Large-Scale Machine Learning

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Machine Learning

Outline

1. **When ML Meets Big Data**

2. **Advantages of Deep Learning**
   - Representation Learning
   - Exponential Gain of Expressiveness
   - Memory and GPU Friendliness
   - Online & Transfer Learning

3. **Learning Theory Revisited**
   - Generalizability and Over-Parametrization
   - Wide-and-Deep NN is a Gaussian Process before Training*
   - Gradient Descent is an Affine Transformation
   - Wide-and-Deep NN is a Gaussian Process after Training

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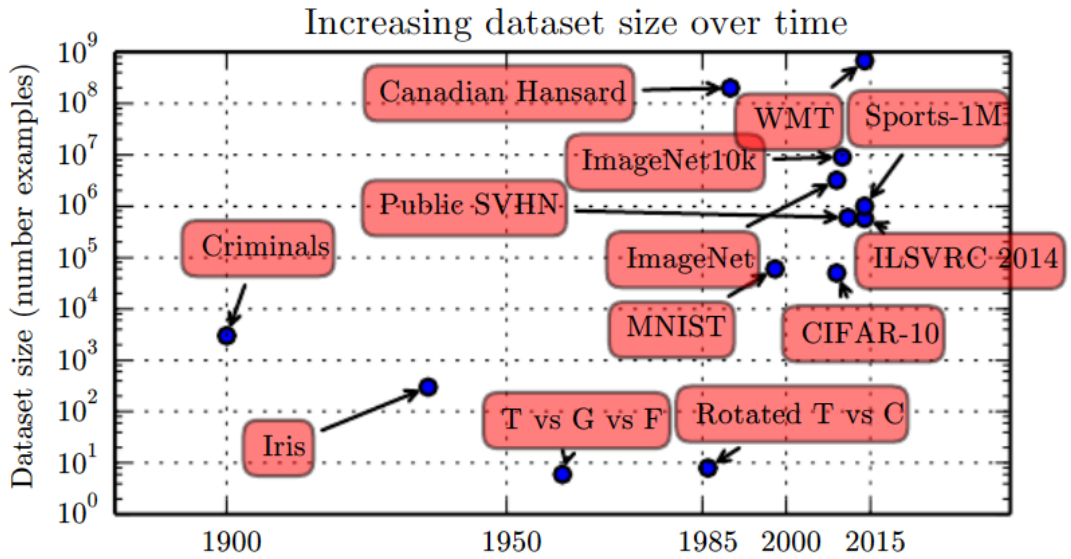
The Big Data Era



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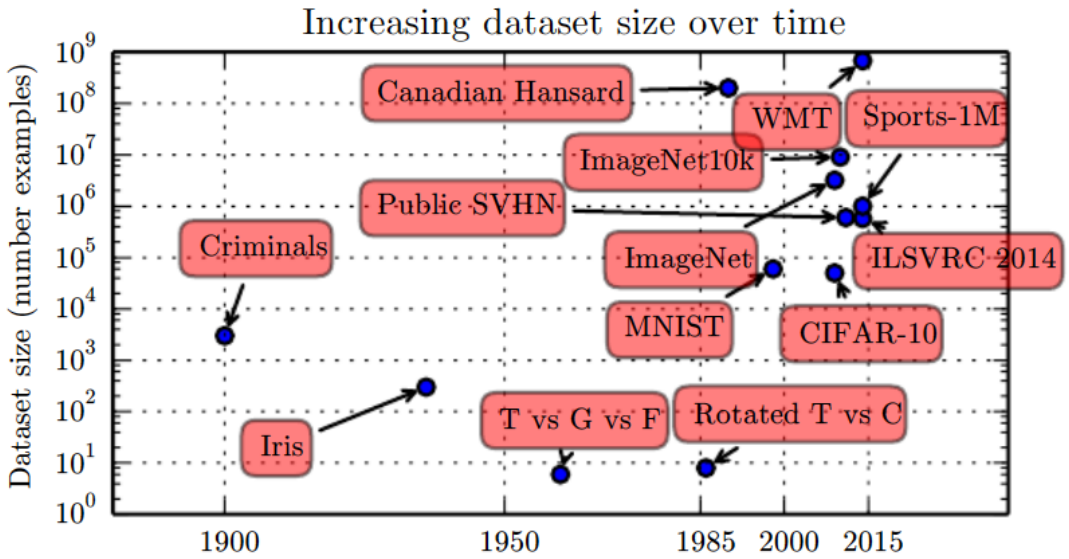

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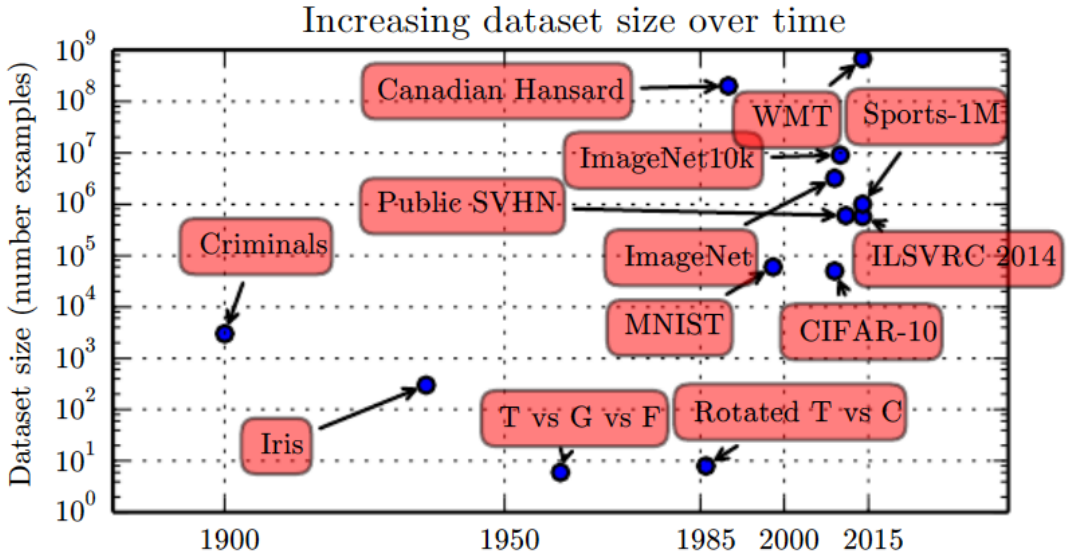
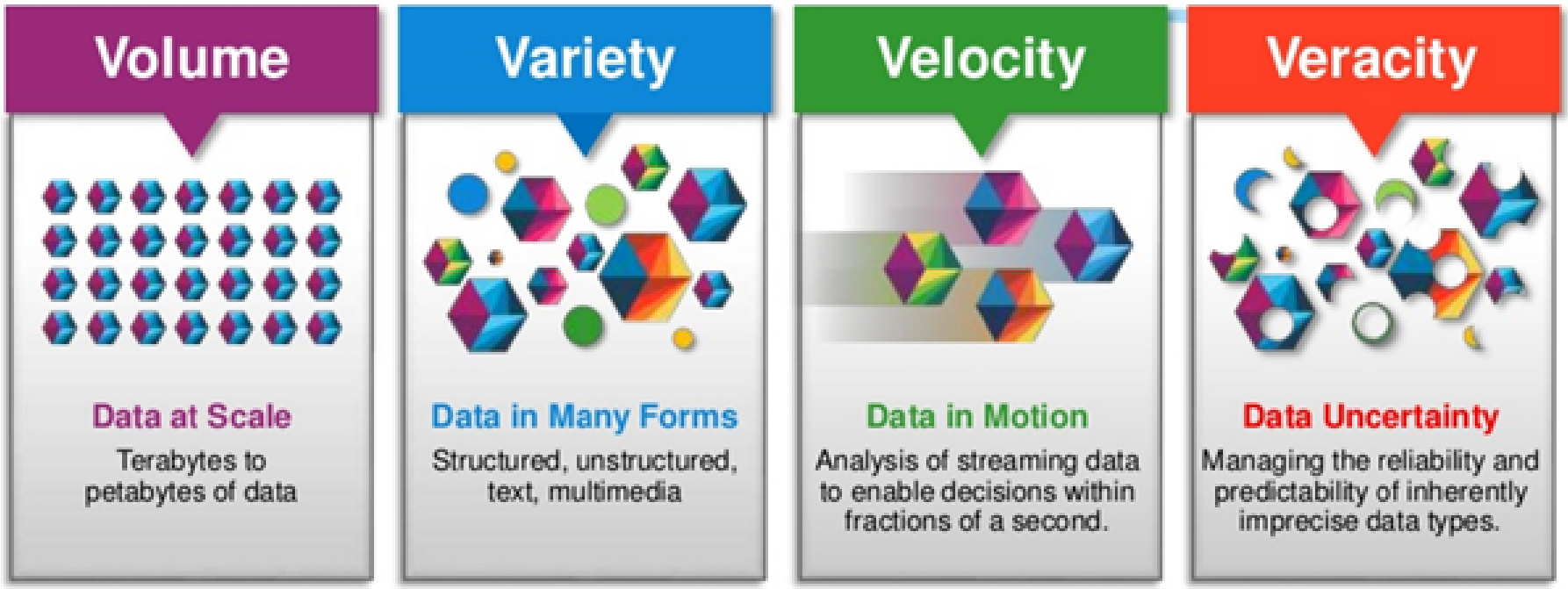


- Today, more and more of our activities are recorded by ubiquitous computing devices
- Networked computers make it easy to centralize these records and curate them into a ***big*** dataset
- ***Large-scale machine learning*** techniques solve problems by leveraging the posteriori knowledge learned from the big data

Characteristics of Big Data



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A group of young people playing a game of Frisbee

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- Velocity
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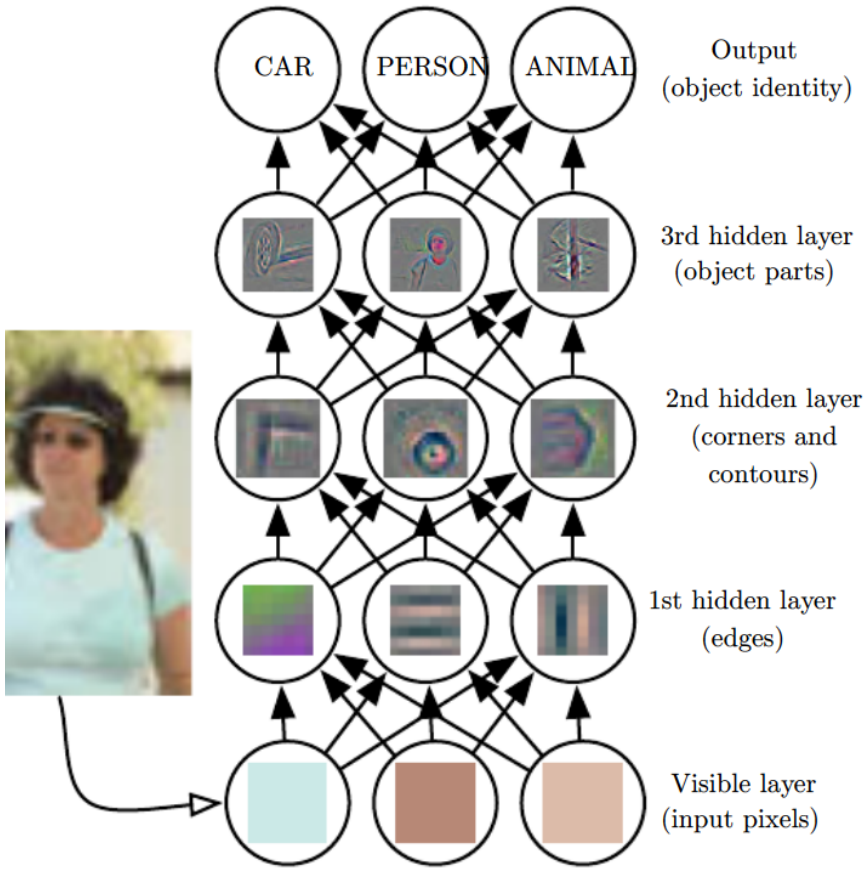
Advantages of Deep Learning



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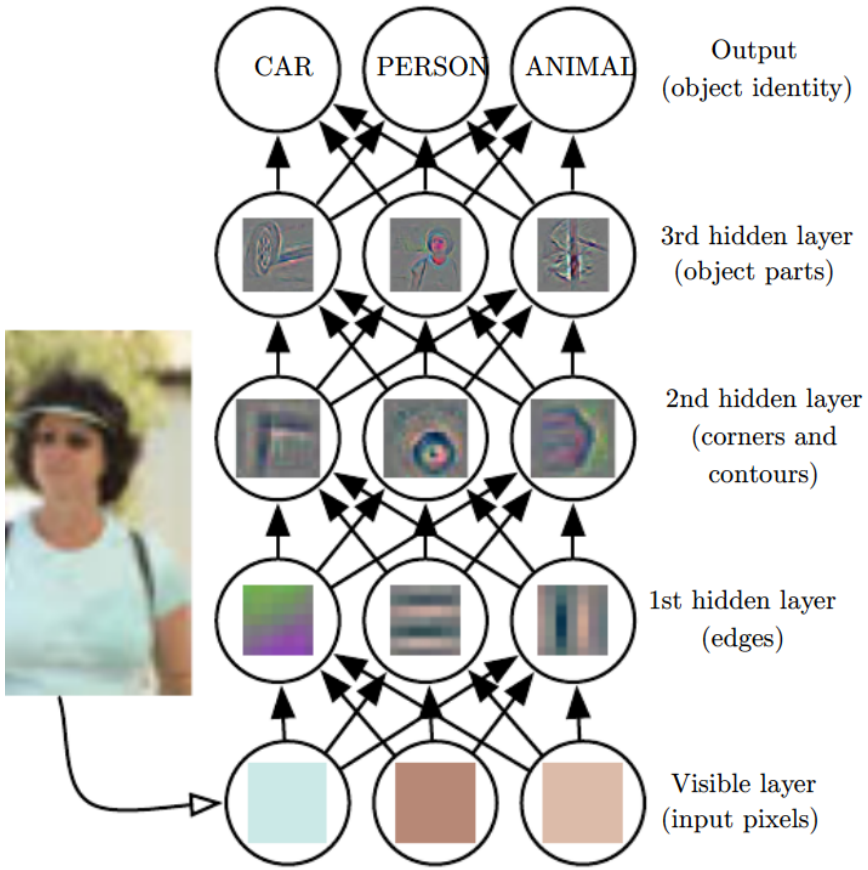

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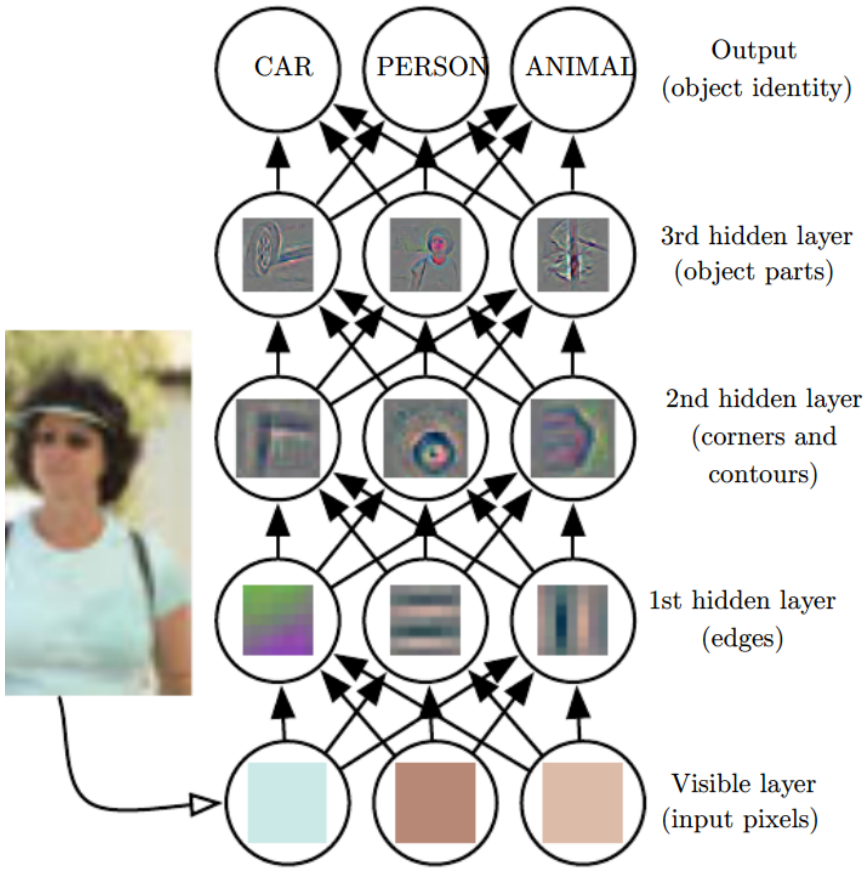

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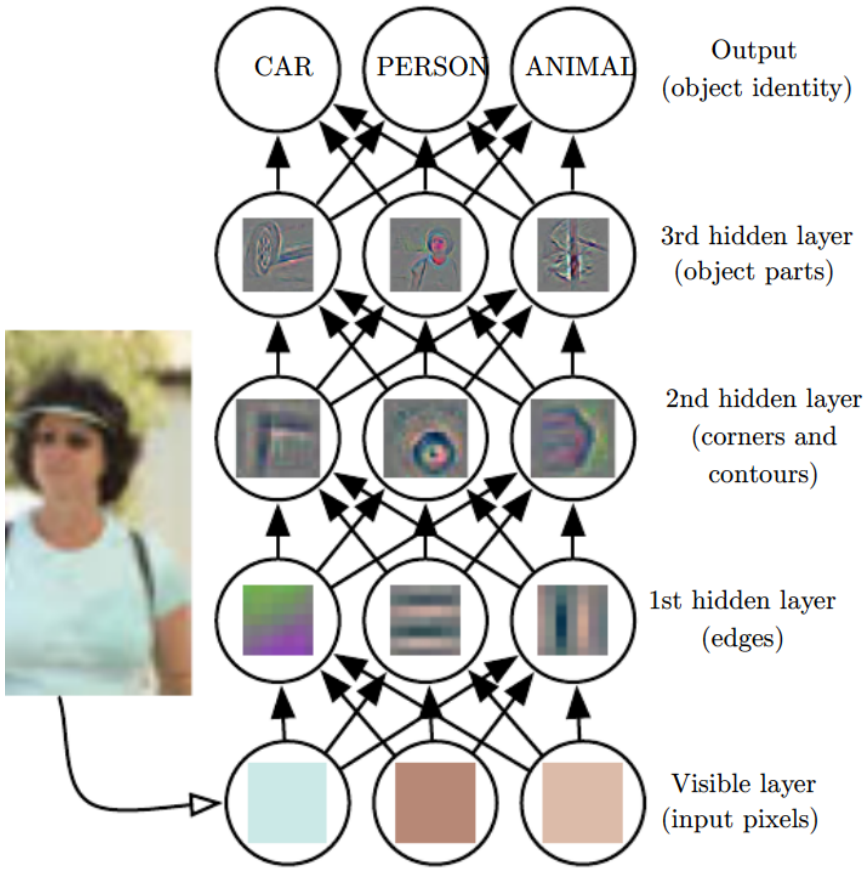

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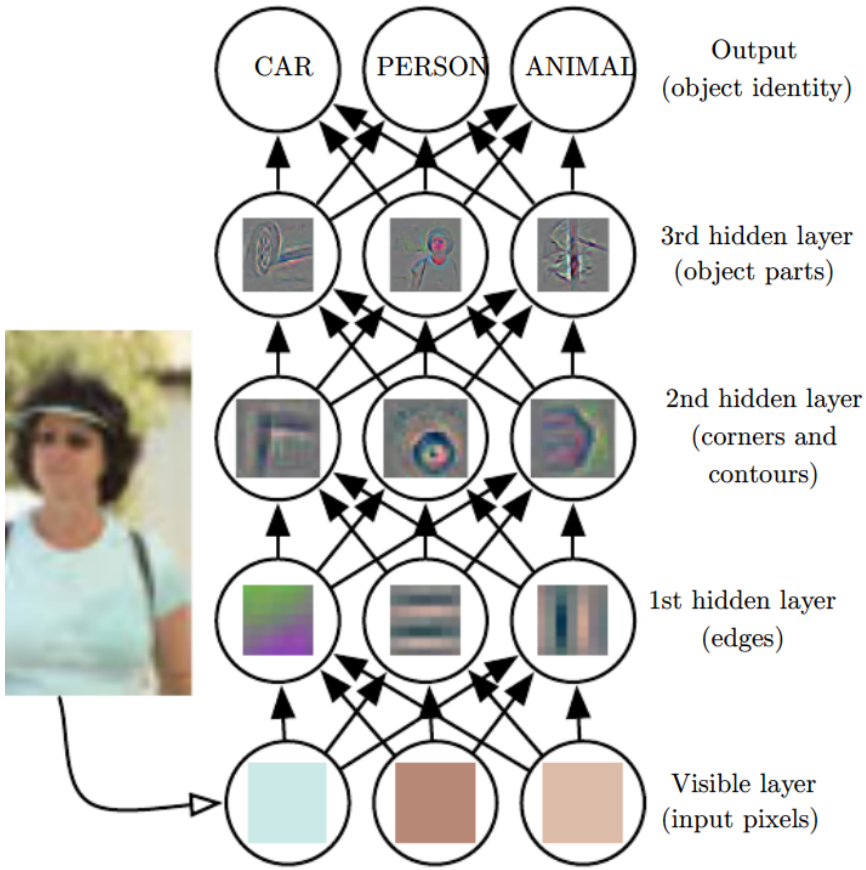

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- Supporting online & transfer learning

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- For simple (linear) f, there are specialized large-scale ML techniques (e.g., LIBLINEAR [6]) that are much more efficient

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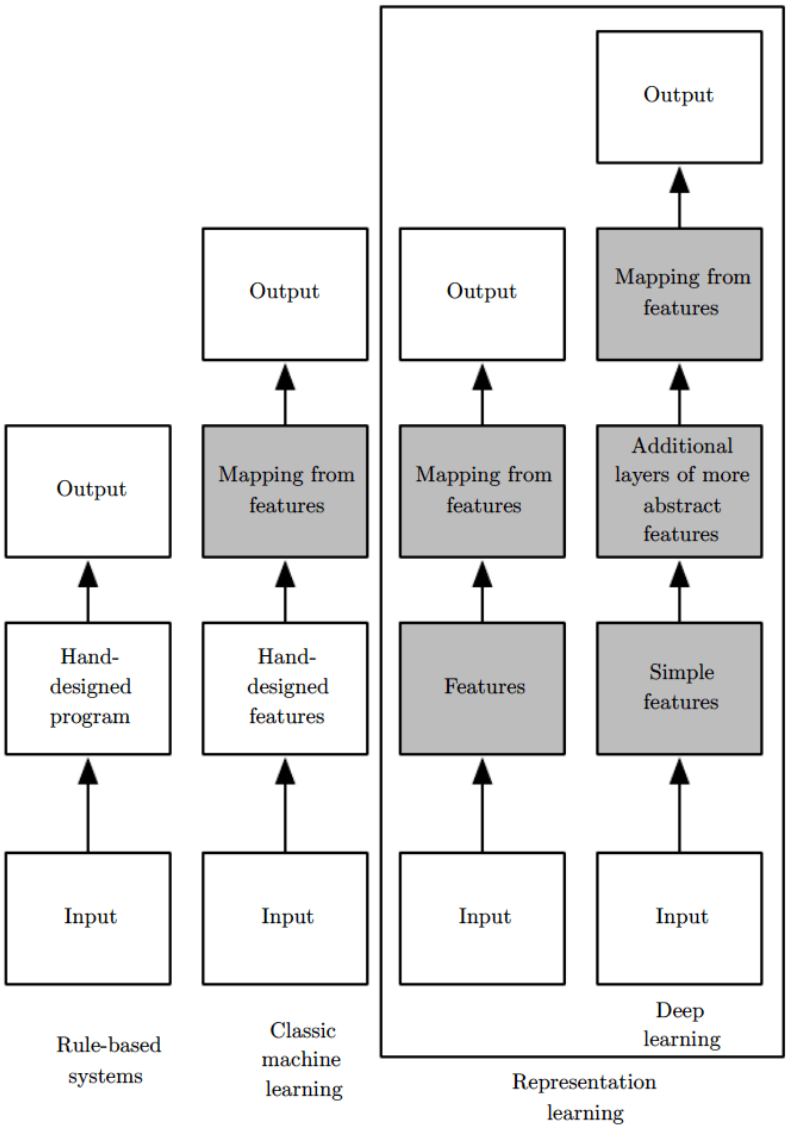

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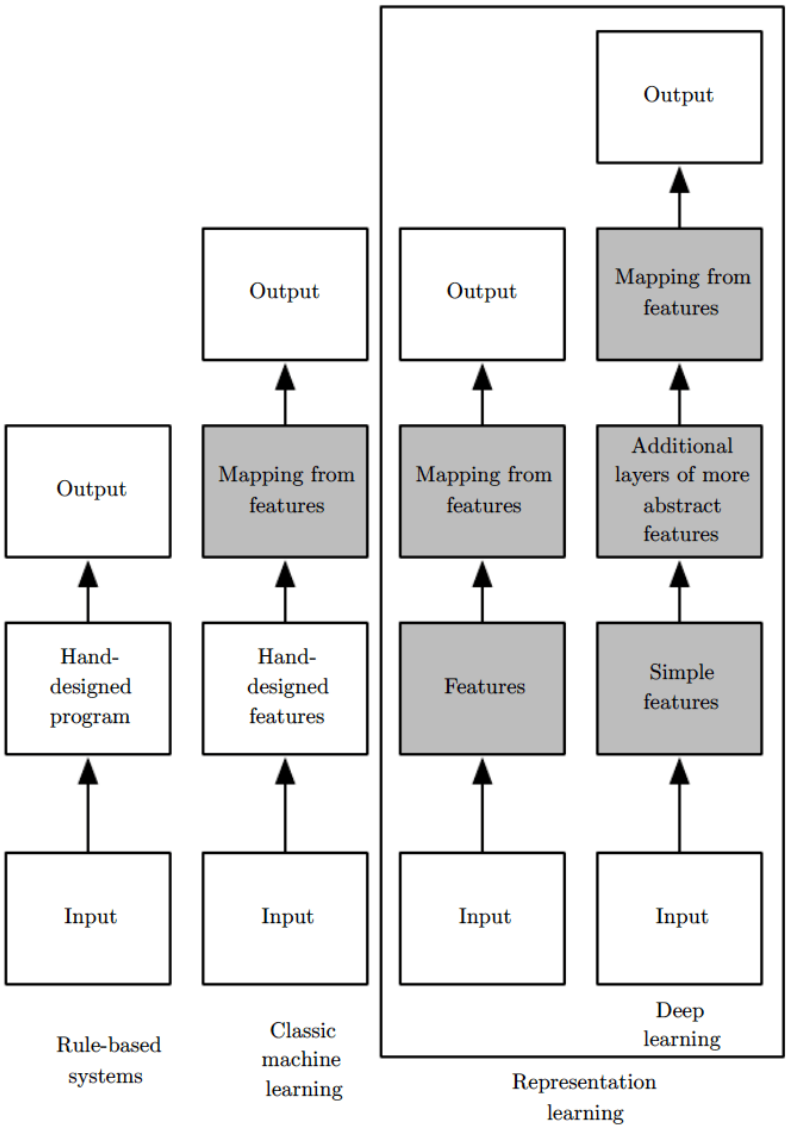

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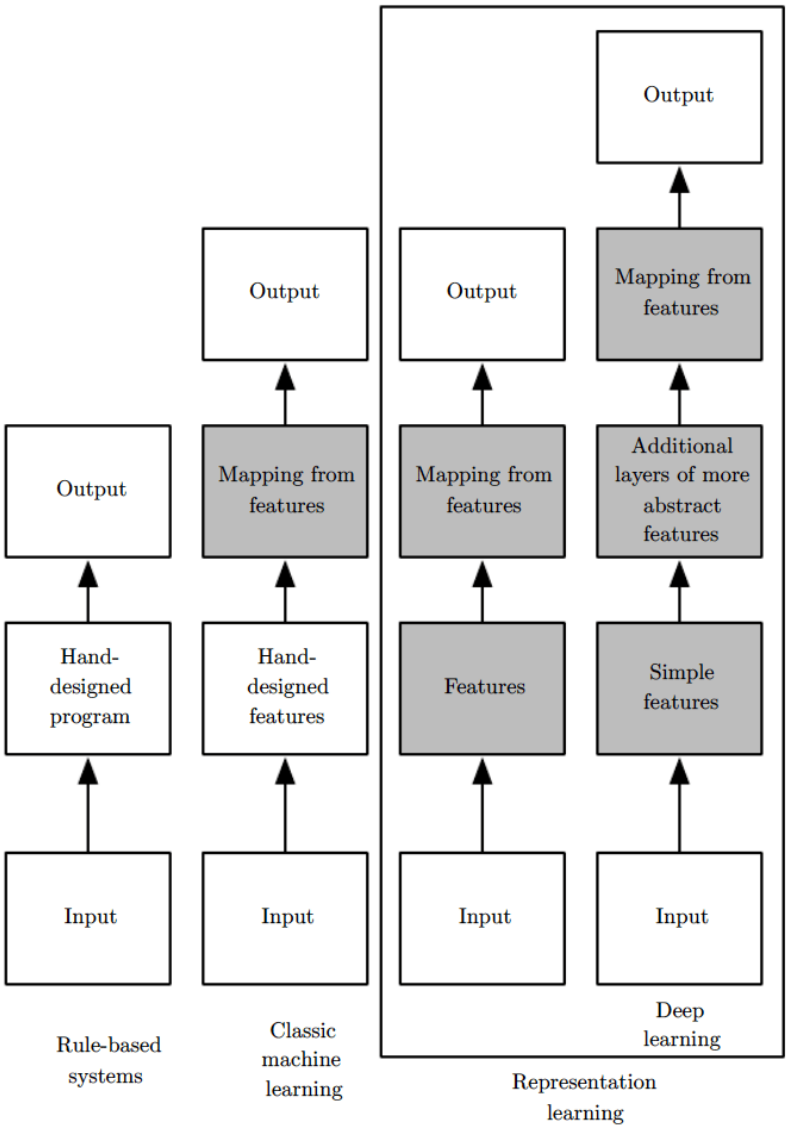

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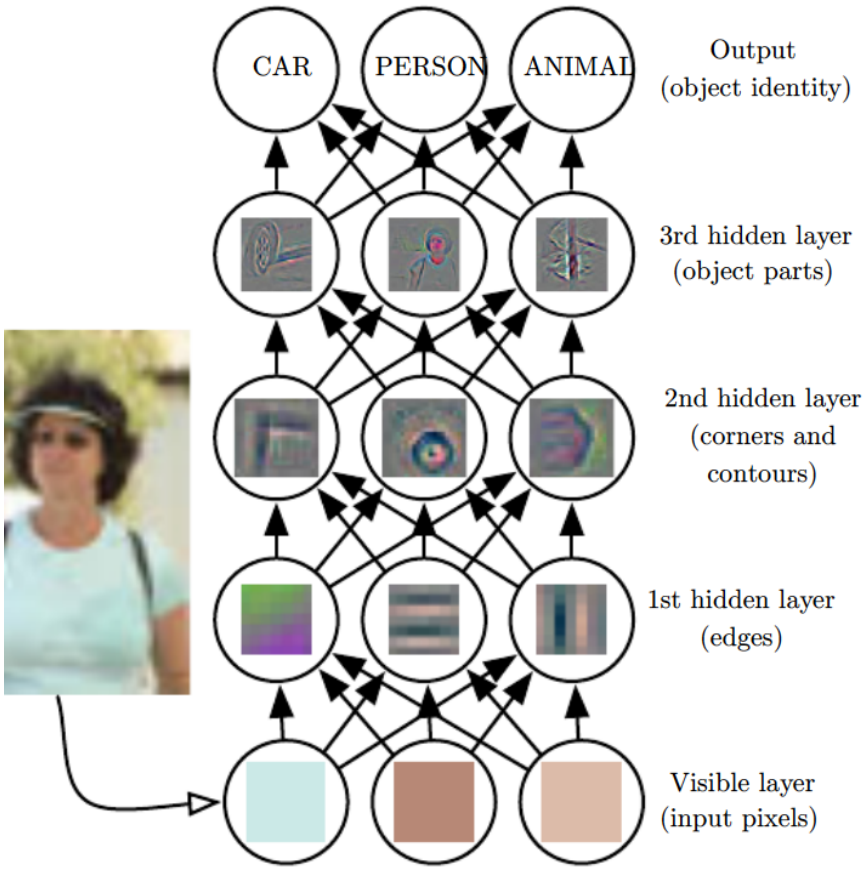
- In deep learning, features/presentations are ***distributed***

Distributed Representations of Data



- In deep learning, we assume that $\boldsymbol{x}$'s were generated by ***compositions of factors***, potentially ***at multiple levels*** in a hierarchy
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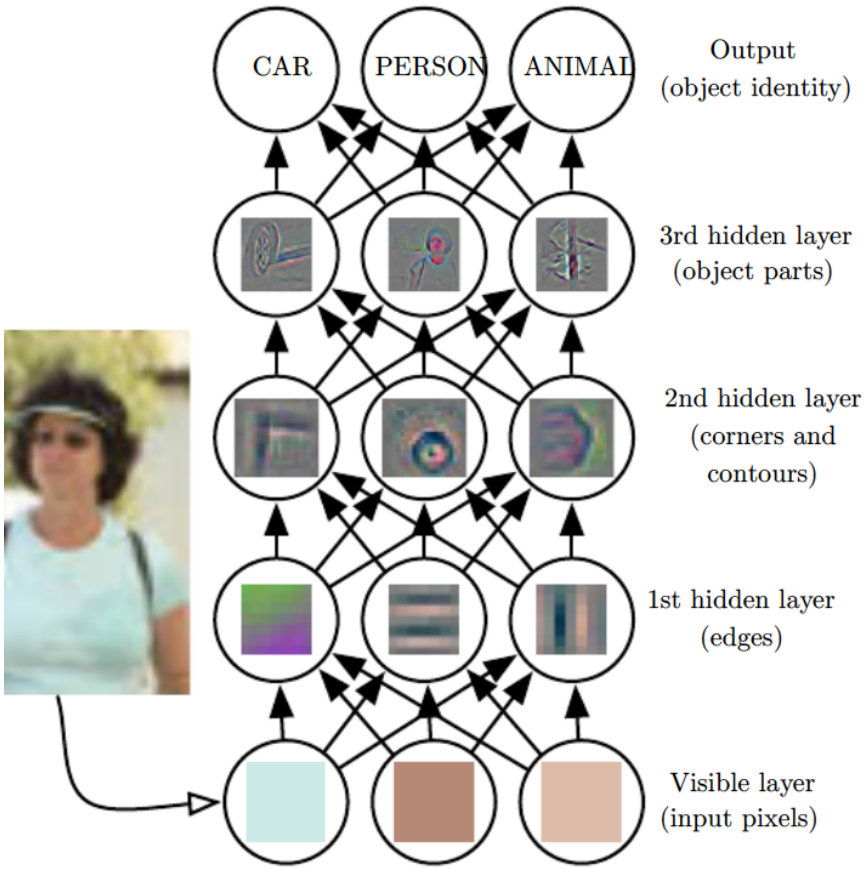

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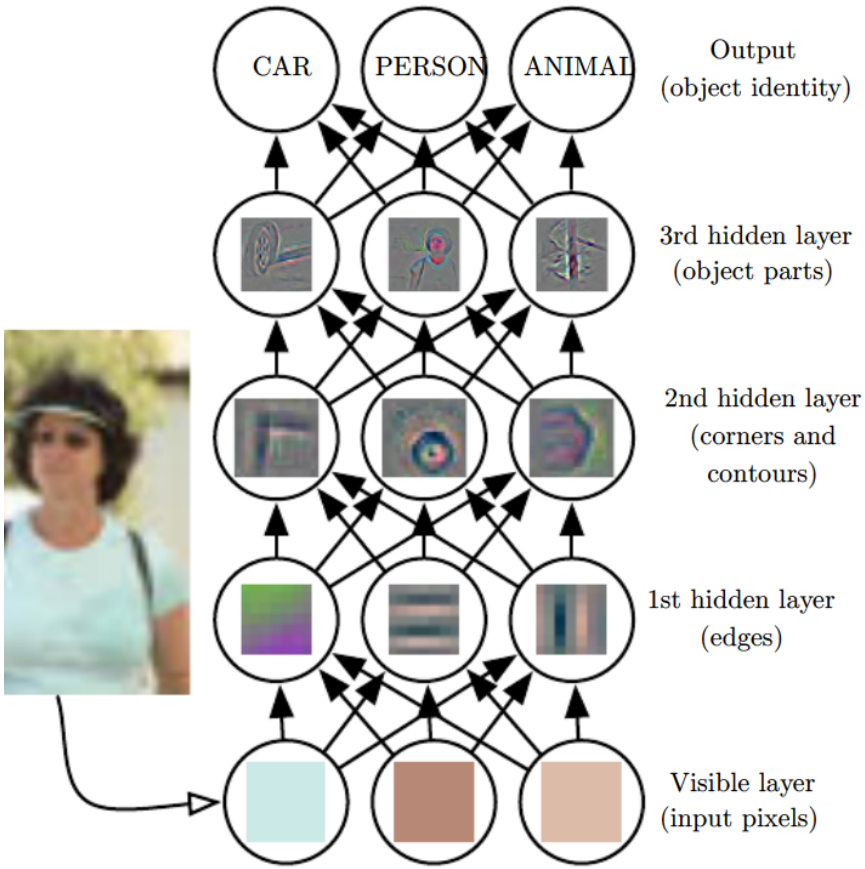

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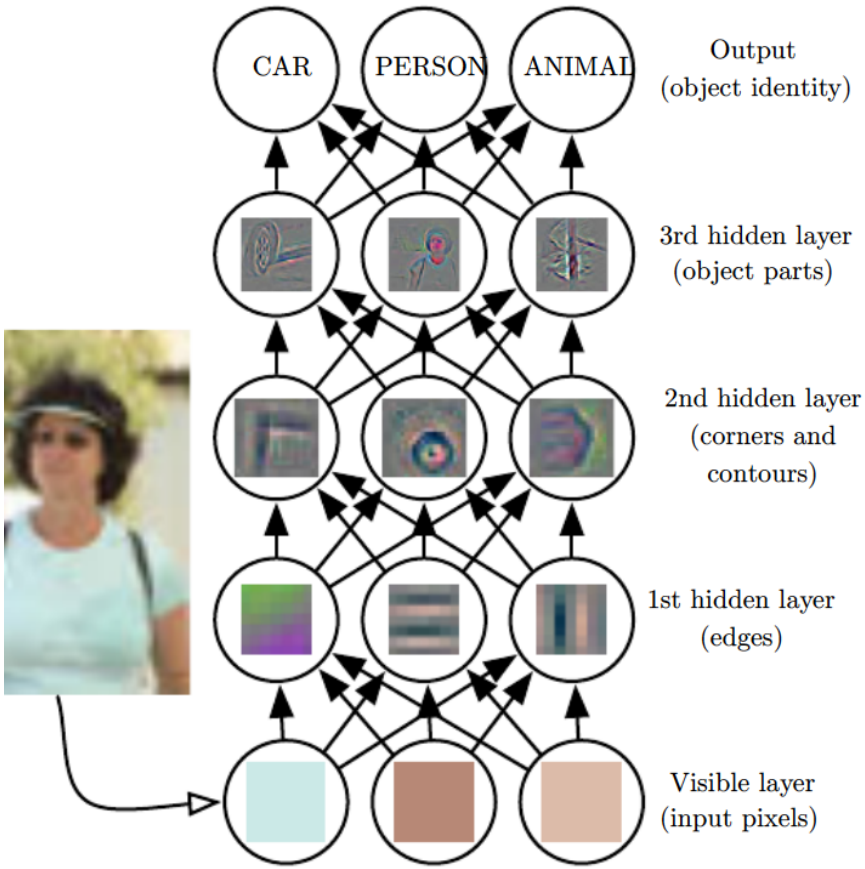

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- To be fed into the factors in the next (deeper) level
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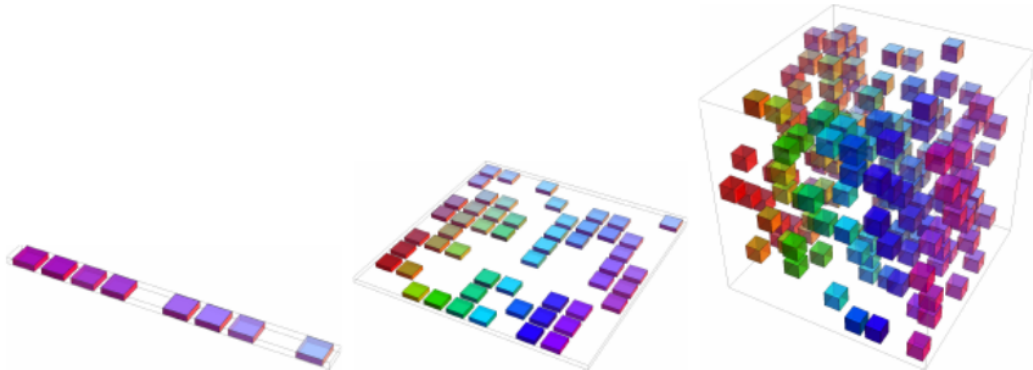

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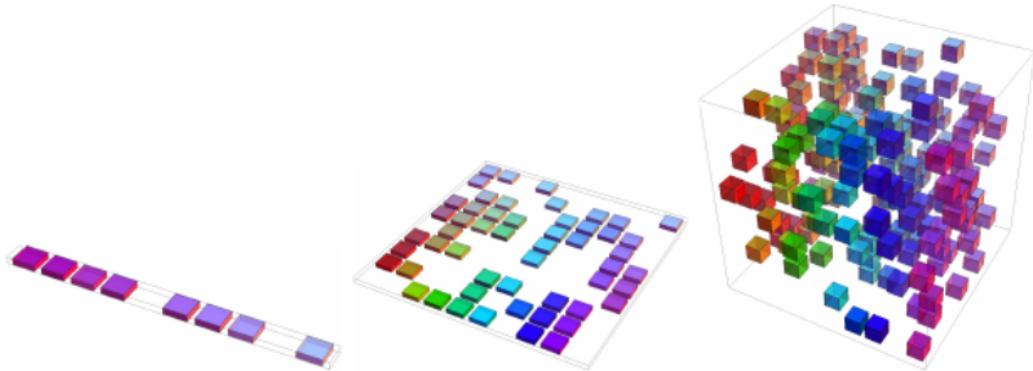

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$$\hat{y} = \sum_i \alpha_i y^{(i)} k(\boldsymbol{x}^{(i)}, \boldsymbol{x}) + b, \text{ where } k(\boldsymbol{x}^{(i)}, \boldsymbol{x}) = \exp(-\gamma \|\boldsymbol{x}^{(i)} - \boldsymbol{x}\|^2)$$

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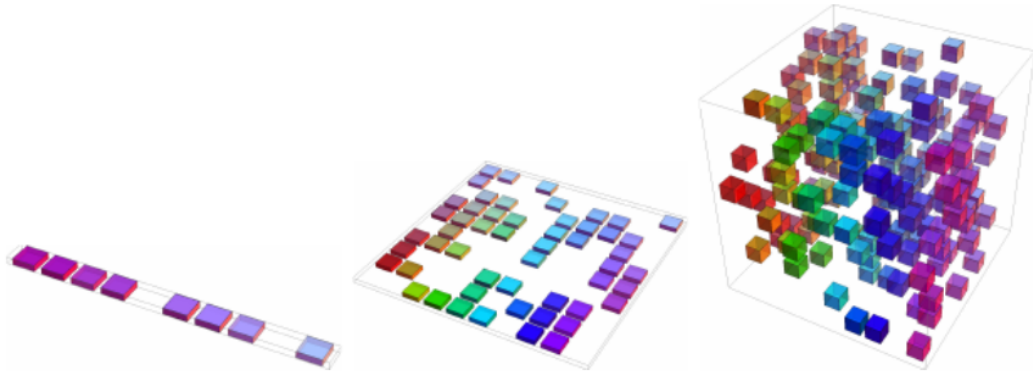

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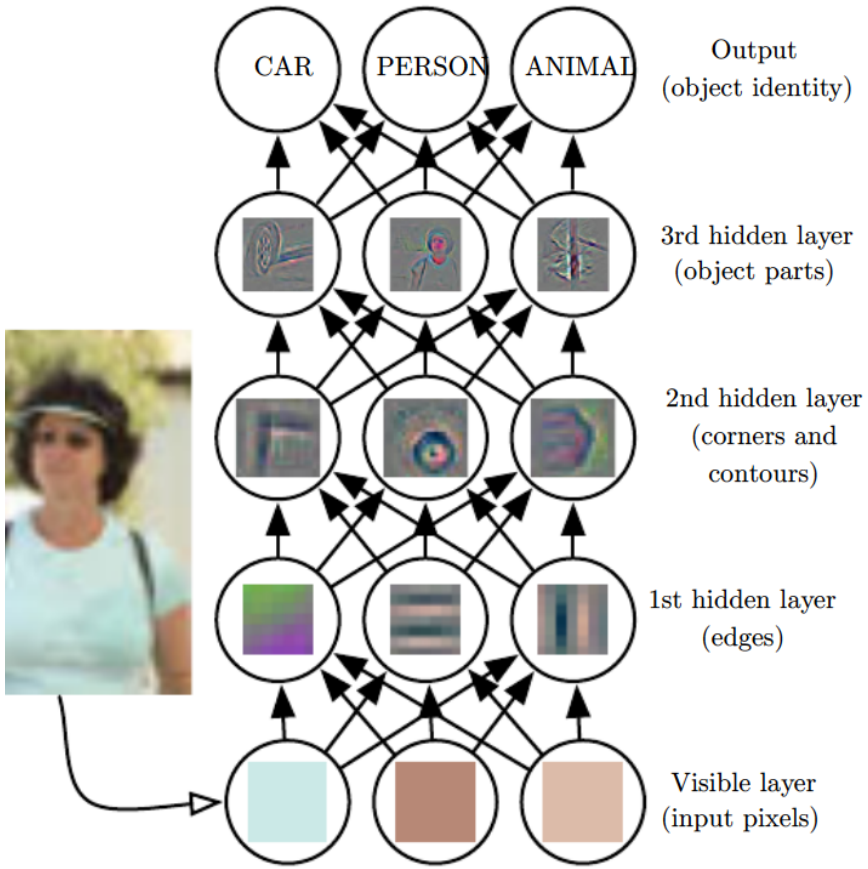
- Suppose f is smooth within a bin, we need ***exponentially more examples*** to get a good interpolation as D increases

Exponential Gains from Depth I



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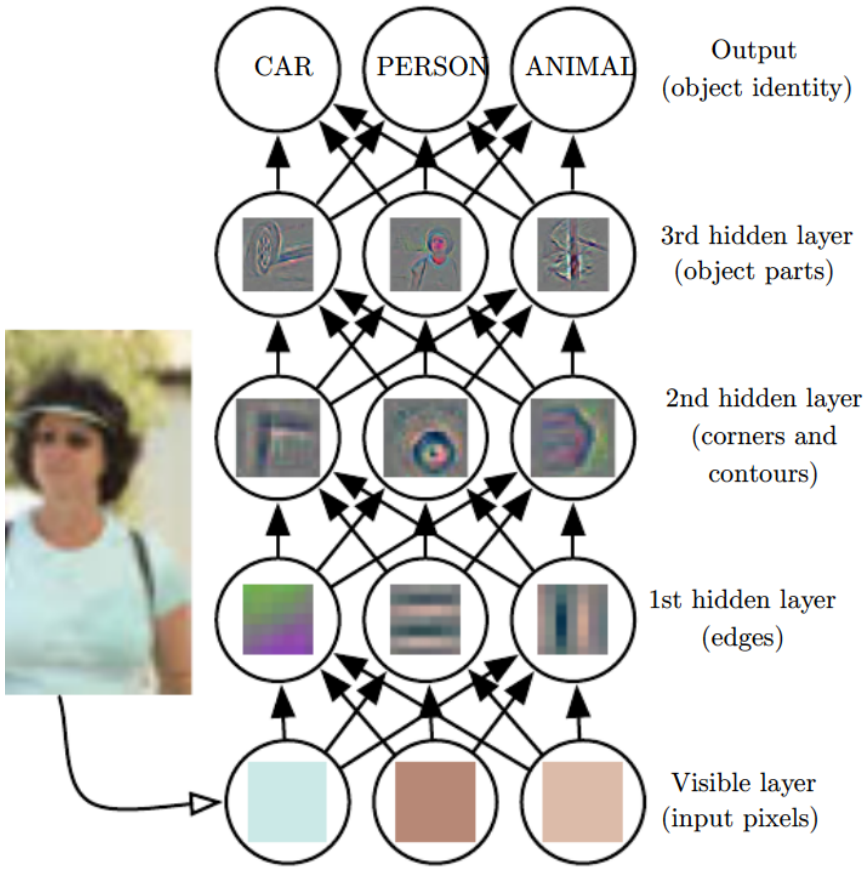

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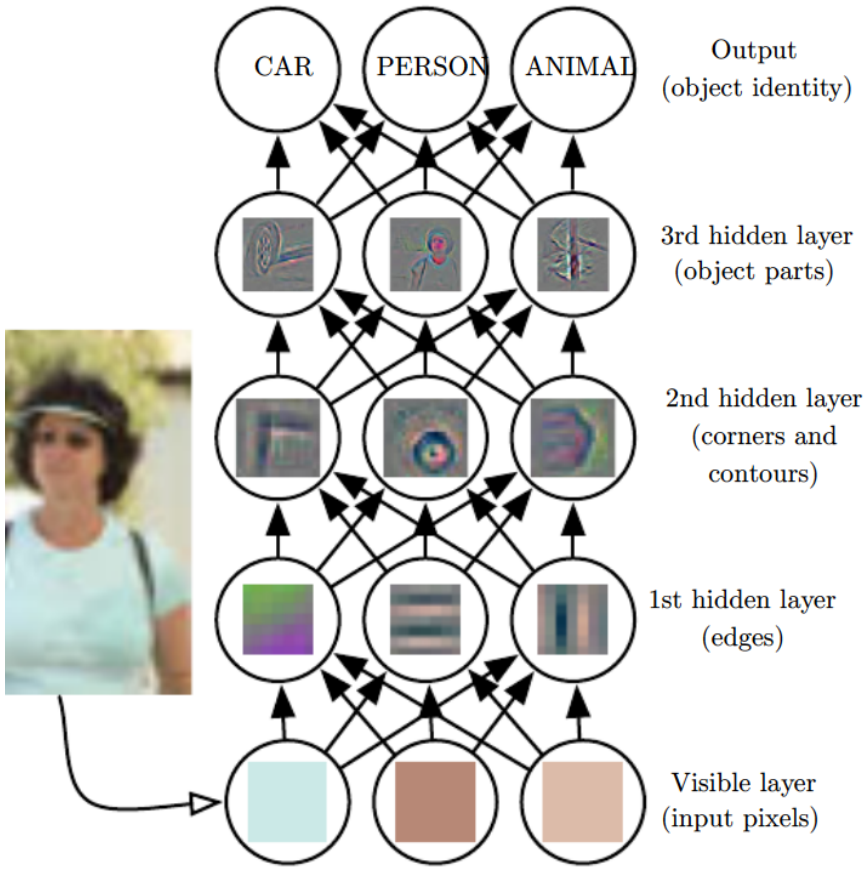

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- With a shallow structure, a deep factor needs to be replaced by ***exponentially many*** factors
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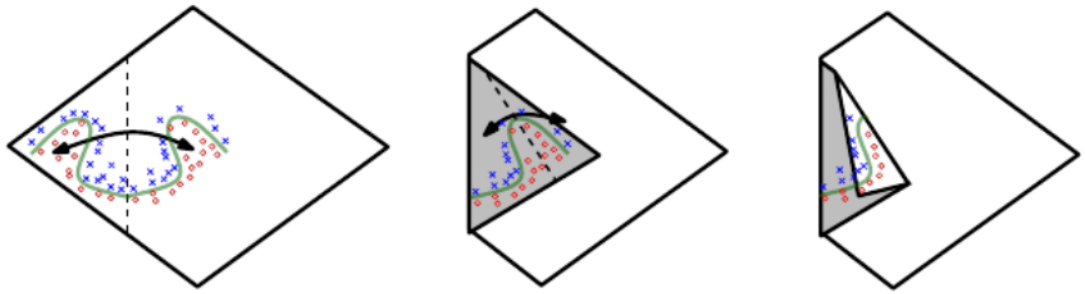
Exponential Gains from Depth II

- Another example: an NN with absolute value rectification units



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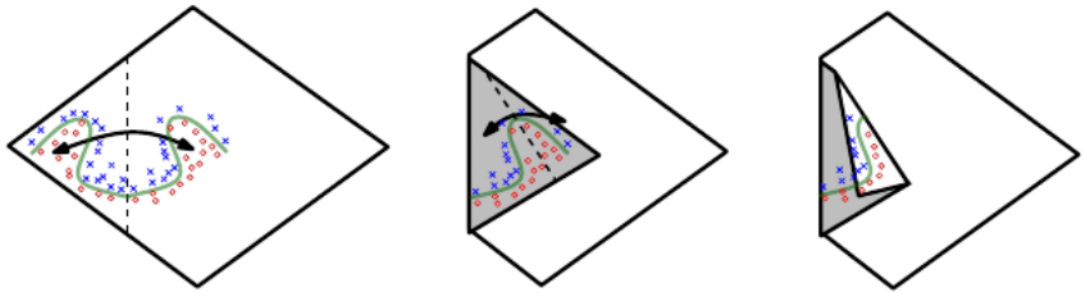

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- This exponential gain counters the exponential challenges posed by the curse of dimensionality

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Stochastic Gradient Descent

Gradient Descent (GD)

$\boldsymbol{w}^{(0)} \leftarrow$ a randon vector;
Repeat until convergence $\{$
$\quad \boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \eta \nabla_{\boldsymbol{w}} C_N(\boldsymbol{w}^{(t)}; \mathbb{X})$;
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- **No I/O** if the next mini-batch can be prefetched

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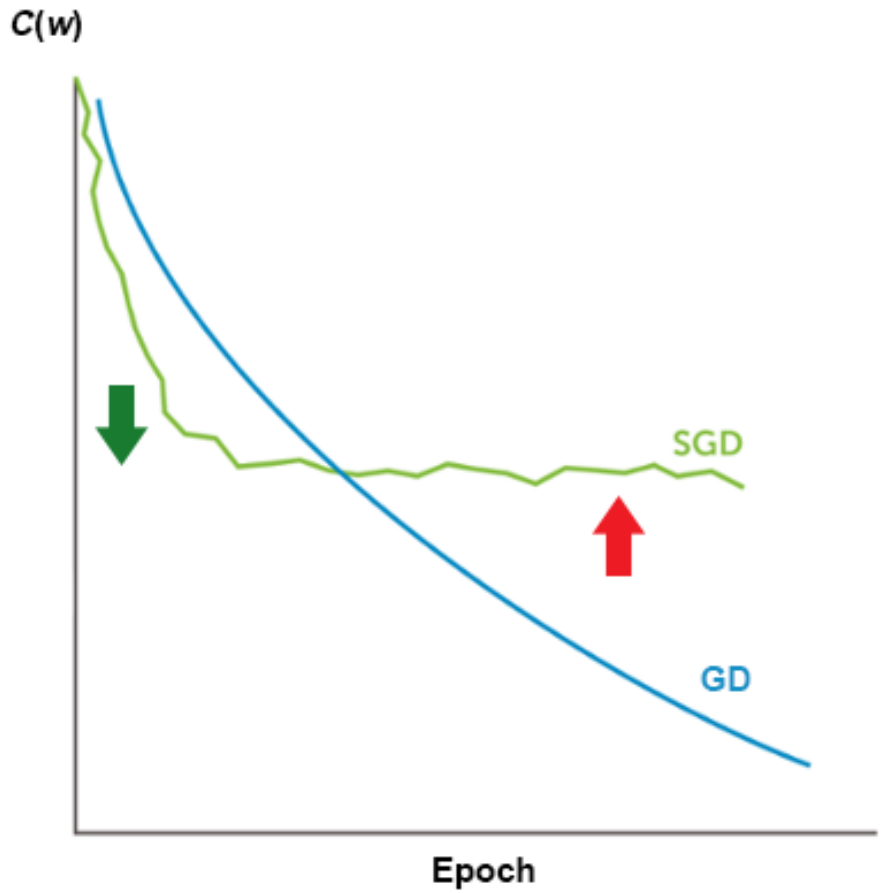

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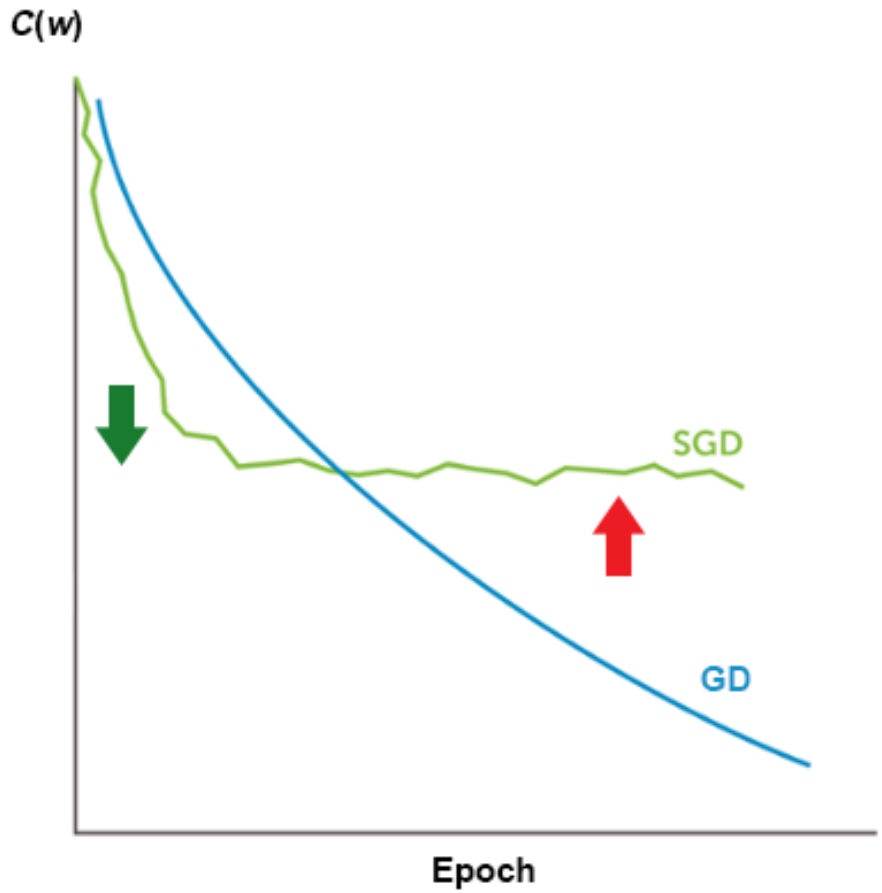


- Is SGD really a better algorithm?

Yes, If You Have Big Data

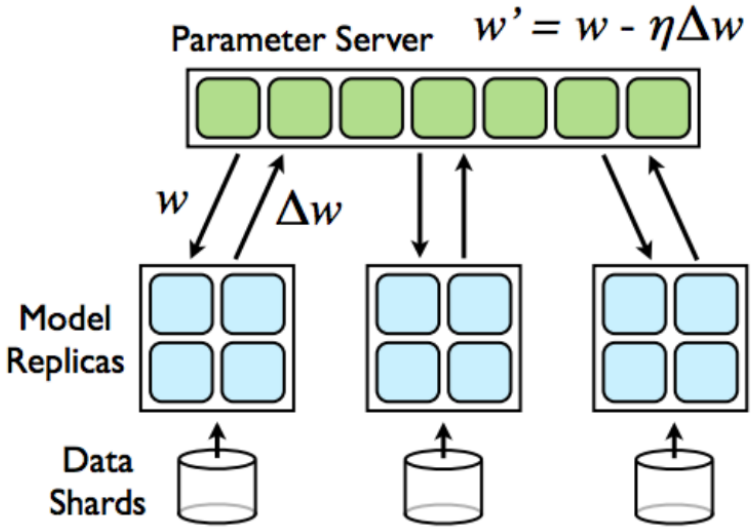
- Performance is limited by ***training time***

Asymptotic Analysis [3]

	GD	SGD
Time per iteration	N	1
#Iterations to opt. error ρ	$\log \frac{1}{\rho}$	$\frac{1}{\rho}$
Time to opt. error ρ	$N \log \frac{1}{\rho}$	$\frac{1}{\rho}$
Time to excess error ε	$\frac{1}{\varepsilon^{1/\alpha}} \log \frac{1}{\varepsilon}$, where $\alpha \in [\frac{1}{2}, 1]$	$\frac{1}{\varepsilon}$

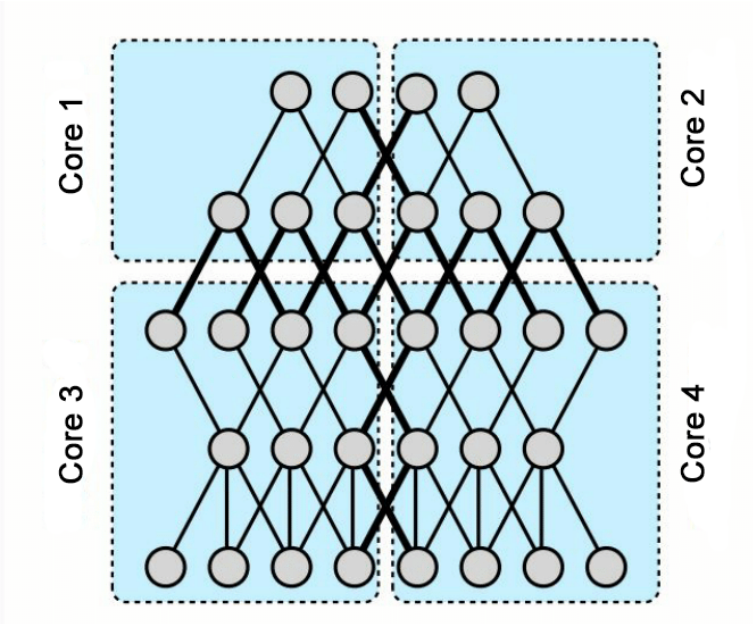
Parallelizing SGD

Data Parallelism



Every core/GPU trains the full model given partitioned data.

Model Parallelism



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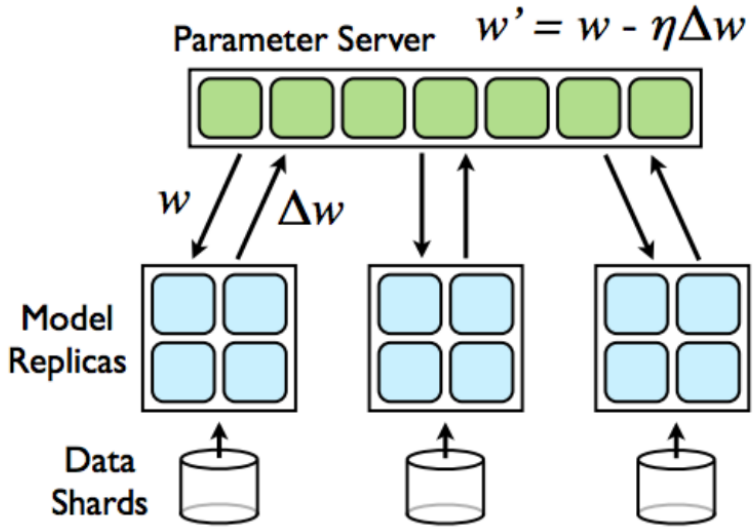

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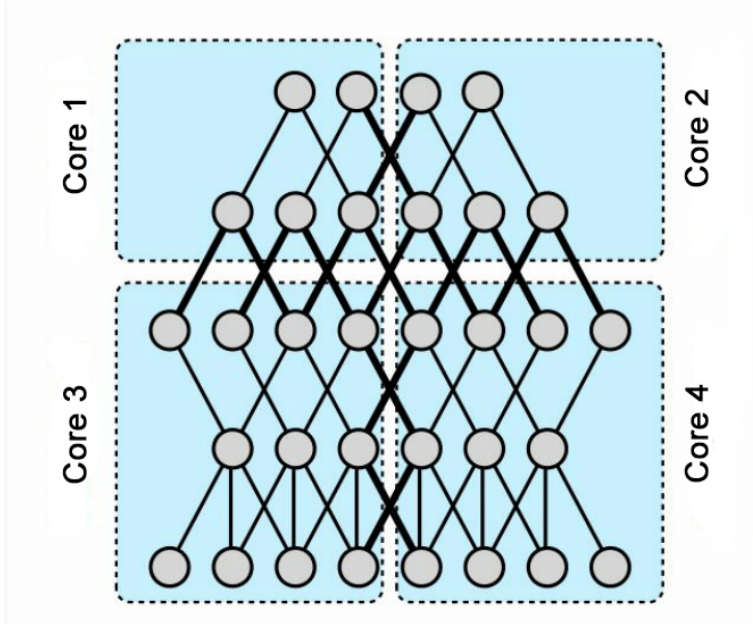

Every core/GPU train a partitioned model given full data.

- The effectiveness depends on applications and available hardware
  - E.g., CPU/GPU speed, communication latency, bandwidth, etc.

Outline

1. When ML Meets Big Data
2. **Advantages of Deep Learning**
   - Representation Learning
   - Exponential Gain of Expressiveness
   - Memory and GPU Friendliness
   - Online & Transfer Learning
3. Learning Theory Revisited
   - Generalizability and Over-Parametrization
   - Wide-and-Deep NN is a Gaussian Process before Training*
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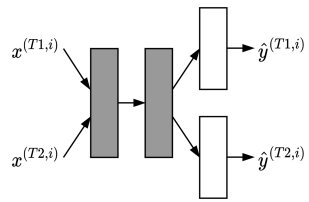

Muti-Task and Transfer Learning

- ***Multi-task learning***: to learning a single model for multiple tasks
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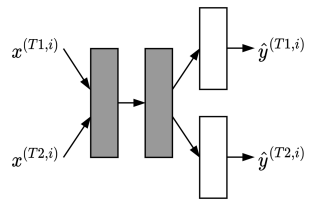
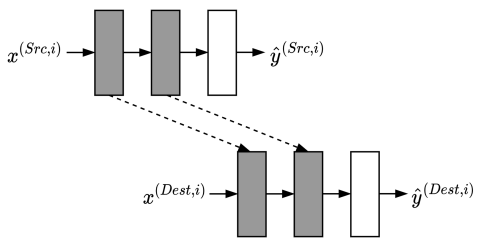
  - Via pretrained layers (whose weights may be further updated when a smaller learning rate)





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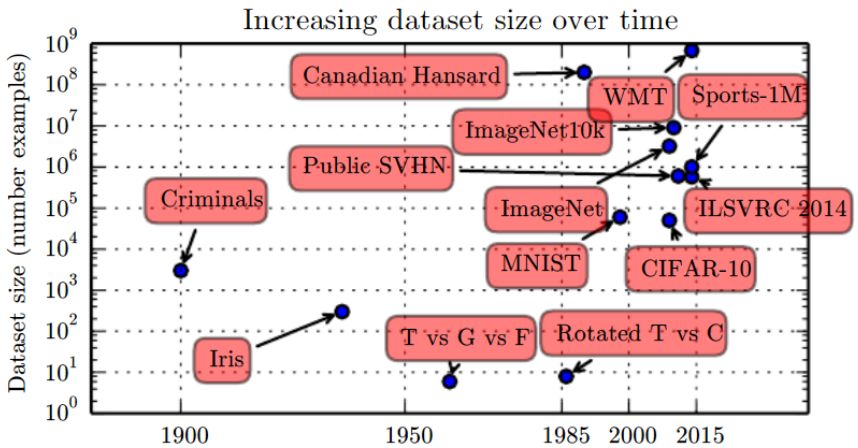
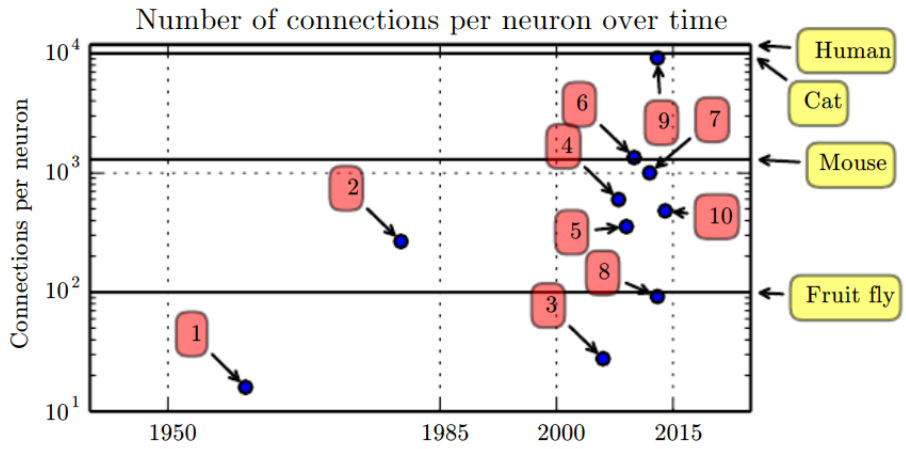
Big Data + Big Models





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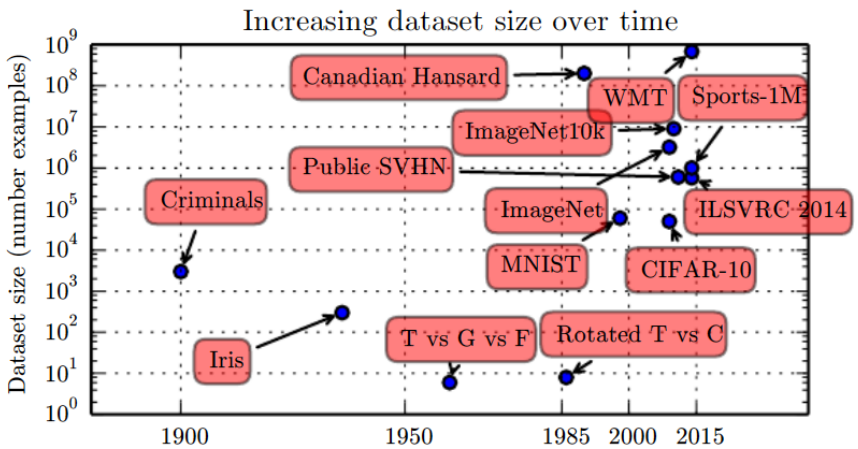

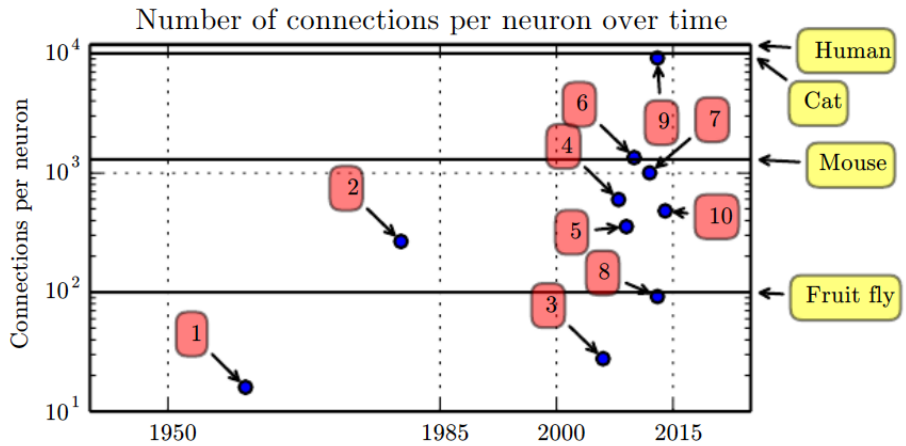

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- With domain-specific architecture such as ***convolutional NNs*** (CNNs) and ***recurrent NNs*** (RNNs)

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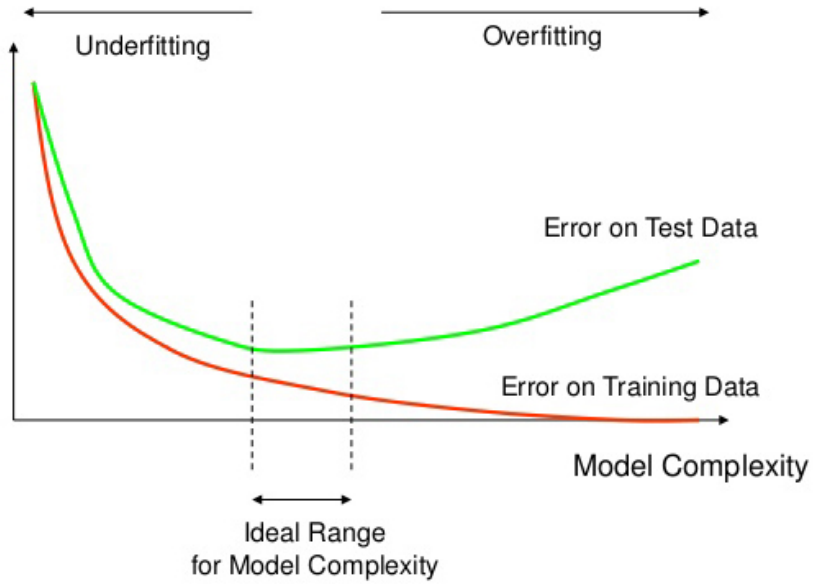
Over-Parametrized NNs

- Let $D^{(l)}$ be the output dimension ("width") of a layer $f^{(l)}(\cdot;\theta^{(l)})$ of an NN
  - Examples $(\boldsymbol{x},\boldsymbol{y}) \in \mathbb{R}^{D^{(0)}} \times \mathbb{R}^{D^{(L)}}$
  - $D = D^{(1)} + \cdots + D^{(L)}$ the total number of neurons
- From the statistical learning theory point of view, the larger the D, the worse the generalizability



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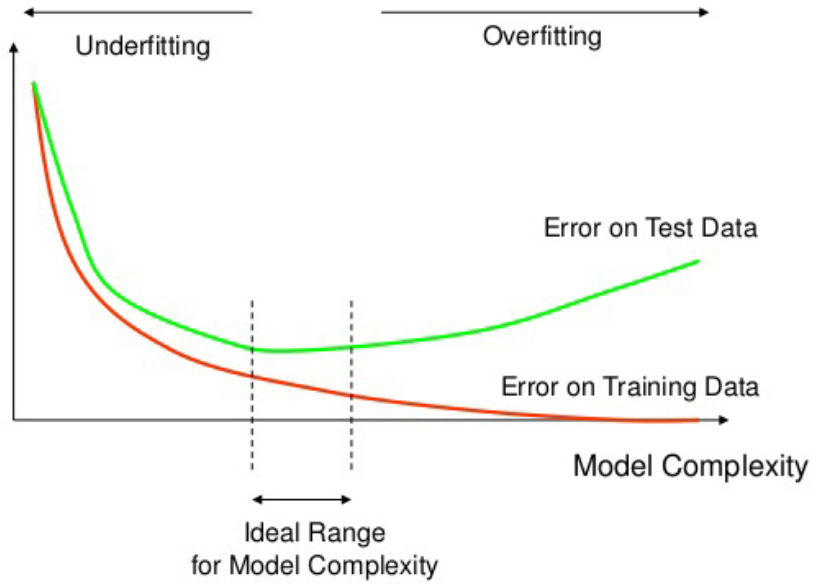

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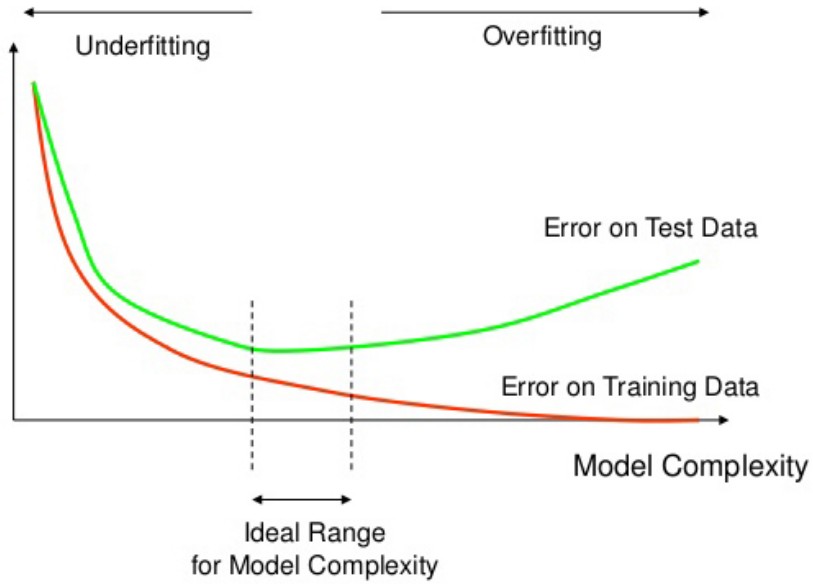

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- Why such a paradox?

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- Recent studies [9, 8, 10] show that ***a wide NN of any depth can be approximated by a Gaussian process (GP)***
  - Either before, during, or after training
- Recall that a GP is a non-parametric model whose complexity depends only on the size of training set $|\mathbb{X}|$ and the hyperparameters of kernel function $k(\cdot, \cdot)$:

$$\begin{bmatrix} \boldsymbol{y}_N \\ \boldsymbol{y}_M \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \boldsymbol{m}_N \\ \boldsymbol{m}_M \end{bmatrix}, \begin{bmatrix} \boldsymbol{K}_{N,N} & \boldsymbol{K}_{N,M} \\ \boldsymbol{K}_{M,N} & \boldsymbol{K}_{M,M} \end{bmatrix} \right.$$

with Bayesian inference for test points $\mathbb{X}'$:

$$\mathrm{P}(\boldsymbol{y}_M \,|\, \mathbb{X}', \mathbb{X}) = \mathcal{N}(\boldsymbol{K}_{M,N}\boldsymbol{K}_{N,N}^{-1}\boldsymbol{y}_N \,, \boldsymbol{K}_{M,M} - \boldsymbol{K}_{M,N}\boldsymbol{K}_{N,N}^{-1}\boldsymbol{K}_{N,M})$$

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  - Either before, during, or after training
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$$\begin{bmatrix} \boldsymbol{y}_N \\ \boldsymbol{y}_M \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \boldsymbol{m}_N \\ \boldsymbol{m}_M \end{bmatrix}, \begin{bmatrix} \boldsymbol{K}_{N,N} & \boldsymbol{K}_{N,M} \\ \boldsymbol{K}_{M,N} & \boldsymbol{K}_{M,M} \end{bmatrix} \right.$$

  with Bayesian inference for test points $\mathbb{X}'$:

$$\mathrm{P}(\boldsymbol{y}_M \,|\, \mathbb{X}', \mathbb{X}) = \mathcal{N}(\boldsymbol{K}_{M,N}\boldsymbol{K}_{N,N}^{-1}\boldsymbol{y}_N \,, \boldsymbol{K}_{M,M} - \boldsymbol{K}_{M,N}\boldsymbol{K}_{N,N}^{-1}\boldsymbol{K}_{N,M})$$

- Therefore, wide-and-deep NNs do not overfit as one may expect
  - The D, once becoming large, does ***not*** reflect true model complexity

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   - Exponential Gain of Expressiveness
   - Memory and GPU Friendliness
   - Online & Transfer Learning
3. **Learning Theory Revisited**
   - Generalizability and Over-Parametrization
   - Wide-and-Deep NN is a Gaussian Process before Training*
   - Gradient Descent is an Affine Transformation
   - Wide-and-Deep NN is a Gaussian Process after Training

Example: NN for Regression

- For simplicity, we consider an L-layer NN $f(\cdot;\theta)$ for the regression problem:

$$f(\boldsymbol{x};\theta) = \boldsymbol{a}^{(l)} = \boldsymbol{\phi}^{(l)}(\boldsymbol{W}^{(l)\top}\boldsymbol{a}^{(l-1)} + \boldsymbol{b}^{(l)}), \text{ for } l = 1,\dots,L,$$

  where
  - the activation functions $\phi^{(1)}(\cdot) = \cdots = \phi^{(L-1)}(\cdot) \equiv \phi(\cdot)$ and $\phi^{(L-1)}(\cdot)$ is an identify function
  - $\boldsymbol{a}^{(0)} = \boldsymbol{x}$ and $\hat{y} = a^{(L)} = z^{(L)} \in \mathbb{R}$ the mean of a Gaussian
  - $\theta^{(l)} = \text{vec}(\boldsymbol{W}^{(l)}, \boldsymbol{b}^{(l)})$ and $\theta = \text{vec}(\theta^{(1)}, \cdots, \theta^{(L)})$

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  - $\theta^{(l)}=\text{vec}(\boldsymbol{W}^{(l)},\boldsymbol{b}^{(l)})$ and $\theta=\text{vec}(\theta^{(1)},\cdots,\theta^{(L)})$
- Let $\hat{\boldsymbol{y}}=[f(\boldsymbol{x}^{(1)};\theta),\cdots,f(\boldsymbol{x}^{(N)};\theta)]^\top\in\mathbb{R}^N$ be the predictions for the points $\boldsymbol{X}\in\mathbb{R}^{N\times D^{(0)}}$ in training set $\mathbb{X}=\{(\boldsymbol{x}^{(i)},y^{(i)})\}_i=\{\boldsymbol{X},\boldsymbol{y}\}$
- Maximum-likelihood estimation:

$$\arg\max_\theta \mathrm{P}(\mathbb{X}\,|\,\theta)=\arg\min_\theta C(\hat{\boldsymbol{y}},\boldsymbol{y})=\arg\min_\theta \frac{1}{2}\|\hat{\boldsymbol{y}}-\boldsymbol{y}\|^2$$

Weight Initialization and Normalization

$$\boldsymbol{a}^{(l)} = \boldsymbol{\phi}^{(l)}(\boldsymbol{W}^{(l)\top}\boldsymbol{a}^{(l-1)} + \boldsymbol{b}^{(l)})$$

- Common initialization: $W_{i,j}^{(l)} \sim \mathcal{N}(0, \sigma_w^2)$ and $b_i^{(l)} \sim \mathcal{N}(0, \sigma_b^2)$

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- To normalize the forward and backward gradient signals w.r.t. layer width $D^{(l)}$, we can define an equivalent NN:

$$\boldsymbol{a}^{(l)} = \boldsymbol{\phi}^{(l)}(\boldsymbol{W}^{(l)\top}\boldsymbol{a}^{(l-1)} + \boldsymbol{b}^{(l)}),$$

where $W_{i,j}^{(l)} = \frac{\sigma_w}{\sqrt{D^{(l-1)}}}\omega_{i,j}^{(l)}$, $b_i^{(l)} = \sigma_b \beta_i^{(l)}$, and $\omega_{i,j}^{(l)}, \beta_i^{(l)} \sim \mathcal{N}(0,1)$

Distribution of $\hat{y}$

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- Since $\omega_j^{(l)}$'s and $\beta^{(l)}$ are Gaussian random variables with zero means, their sum $\hat{y}$ is also a zero-mean Gaussian
- Now consider the predictions $\hat{\boldsymbol{y}} = [\hat{y}(\boldsymbol{x}^{(1)}), \cdots, \hat{y}(\boldsymbol{x}^{(N)})]^\top \in \mathbb{R}^N$ for N points, we have

$$\begin{bmatrix} \hat{y}(\boldsymbol{x}^{(1)}) \\ \vdots \\ \hat{y}(\boldsymbol{x}^{(N)}) \end{bmatrix} = \frac{\sigma_w}{\sqrt{D^{(l-1)}}}\Sigma_j \omega_{j,i}^{(l)} \begin{bmatrix} \phi(z_j^{(l-1)}(\boldsymbol{x}^{(1)})) \\ \vdots \\ \phi(z_j^{(l-1)}(\boldsymbol{x}^{(N)})) \end{bmatrix} + \sigma_b \beta_i^{(l)} \mathbf{1}_N$$

- As $D^{(L-1)} \to \infty$, by multidimensional Central Limit Theorem, $\hat{\boldsymbol{y}}$ is a multivariate Gaussian with mean $\mathbf{0}_N$ and covariance Σ

Wide-and-Deep NN as a Gaussian Process

- The covariance Σ completely describes the behavior of our NN $\hat{y}(\cdot) = f(\cdot)$ over N points
- Furthermore, we will show that Σ can be describe by a ***deterministic*** kernel function $k^{(L)}(\cdot, \cdot)$ independent of a particular initialization such that

$$\Sigma = \begin{bmatrix} k^{(L)}(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(1)}) & \cdots & k^{(L)}(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(N)}) \\ \vdots & \ddots & \vdots \\ k^{(L)}(\boldsymbol{x}^{(N)}, \boldsymbol{x}^{(1)}) & \cdots & k^{(L)}(\boldsymbol{x}^{(N)}, \boldsymbol{x}^{(N)}) \end{bmatrix} \equiv \boldsymbol{K}^{(L)}_{N,N}$$

- This implies that the NN is in correspondent with a GP called ***NN-GP***:

$$\begin{bmatrix} \hat{\boldsymbol{y}}_N \\ \hat{\boldsymbol{y}}_M \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \boldsymbol{0}_N \\ \boldsymbol{0}_M \end{bmatrix}, \begin{bmatrix} \boldsymbol{K}^{(L)}_{N,N} & \boldsymbol{K}^{(L)}_{N,M} \\ \boldsymbol{K}^{(L)}_{M,N} & \boldsymbol{K}^{(L)}_{M,M} \end{bmatrix} \right)$$

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- What's the $k^{(L)}(\cdot, \cdot)$?

Deriving $k^{(1)}(\cdot, \cdot)$

- We use induction to show that $z_i^{(1)}(\cdot), z_i^{(2)}(\cdot), \cdots, z^{(L)}(\cdot) = \hat{y}(\cdot)$ are GPs, which are govern by kernels $k^{(1)}(\cdot, \cdot), \cdots, k^{(L)}(\cdot, \cdot)$ independent with i, respectively

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- Consider $z_i^{(1)}(\boldsymbol{x}) = \frac{\sigma_w}{\sqrt{D^{(0)}}} \Sigma_j \omega_{j,i}^{(l)} \boldsymbol{x} + \sigma_b \beta_i^{(l)}$ a zero-mean Gaussian
- As $D^{(0)} \to \infty$, we have $[z_i^{(1)}(\boldsymbol{x}^{(1)}), \cdots, z_i^{(1)}(\boldsymbol{x}^{(N)})]^\top \sim N(\boldsymbol{0}_N, \boldsymbol{K}_{N,N}^{(1)})$ by multidimensional Central Limit Theorem, where

$$
\begin{aligned}
k^{(1)}(\boldsymbol{x},\boldsymbol{x}') &= \mathrm{Cov}[z_i^{(1)}(\boldsymbol{x}), z_i^{(1)}(\boldsymbol{x}')] = \mathrm{E}_{\omega_{:,i}^{(l)}, \beta_i^{(l)}}[z_i^{(1)}(\boldsymbol{x}) z_i^{(1)}(\boldsymbol{x}')] \\
&= \frac{\sigma_w^2}{D^{(0)}} \mathrm{E}\left[\Sigma_{j,k} \omega_{j,i}^{(l)} \omega_{k,i}^{(l)} x_j x_k'\right] + \frac{\sigma_w \sigma_b}{\sqrt{D^{(0)}}} \mathrm{E}\left[\beta_i^{(l)} \Sigma_j \omega_{j,i}^{(l)} x_j\right] \\
&\quad + \frac{\sigma_w \sigma_b}{\sqrt{D^{(0)}}} \mathrm{E}\left[\beta_i^{(l)} \Sigma_j \omega_{j,i}^{(l)} x_j'\right] + \sigma_b^2 \mathrm{E}\left[\beta_i^{(l)} \beta_i^{(l)}\right] \\
&= \frac{\sigma_w^2}{D^{(0)}} \Sigma_j \mathrm{E}\left[\omega_{j,i}^{(l)} \omega_{j,i}^{(l)}\right] x_j x_j' + \sigma_b^2 \mathrm{E}\left[\beta_i^{(l)} \beta_i^{(l)}\right] \\
&= \frac{\sigma_w^2}{D^{(0)}} \boldsymbol{x}^\top \boldsymbol{x}' + \sigma_b^2,
\end{aligned}
$$

  is independent with i
- Note that $z_i^{(1)}(\cdot)$ and $z_j^{(1)}(\cdot)$ are independent with each other, $\forall i \neq j$

Deriving $k^{(l)}(\cdot,\cdot)$

- Given that $D^{(0)} \to \infty, \cdots, D^{(l-2)} \to \infty$ and
  - $[z_i^{(l-1)}(\boldsymbol{x}^{(1)}), \cdots, z_i^{(l-1)}(\boldsymbol{x}^{(N)})]^\top \sim N(\mathbf{0}_N, \boldsymbol{K}_{N,N}^{(l-1)})$
  - $z_i^{(l-1)}(\cdot)$ and $z_j^{(l-1)}(\cdot)$ are independent with each other, $\forall i \neq j$

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  - $z_i^{(l-1)}(\cdot)$ and $z_j^{(l-1)}(\cdot)$ are independent with each other, $\forall i \neq j$
- Consider $z_i^{(l)}(\boldsymbol{x}) = \frac{\sigma_w}{\sqrt{D^{(l-1)}}} \Sigma_j \omega_{j,i}^{(l)} \phi(z_j^{(l-1)}(\boldsymbol{x})) + \sigma_b \beta_i^{(l)}$ a zero-mean Gaussian
- As $D^{(l-1)} \to \infty$, we have $[z_i^{(l)}(\boldsymbol{x}^{(1)}), \cdots, z_i^{(l)}(\boldsymbol{x}^{(N)})]^\top \sim N(\boldsymbol{0}_N, \boldsymbol{K}_{N,N}^{(l)})$ by multidimensional Central Limit Theorem, where

$$
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k^{(l)}(\boldsymbol{x},\boldsymbol{x}') &= \mathrm{Cov}[z_i^{(l)}(\boldsymbol{x}), z_i^{(l)}(\boldsymbol{x}')] = \mathrm{E}_{\omega_{:,i}^{(l)}, \beta_i^{(l)}, \boldsymbol{z}^{(l-1)}(\boldsymbol{x})}[z_i^{(l)}(\boldsymbol{x}) z_i^{(l)}(\boldsymbol{x}')] \\
&= \frac{\sigma_w^2}{D^{(l-1)}} \mathrm{E}\left[\Sigma_{j,k} \omega_{j,i}^{(l)} \omega_{k,i}^{(l)} \phi(z_j^{(l-1)}(\boldsymbol{x})) \phi(z_j^{(l-1)}(\boldsymbol{x}'))\right] + \sigma_b^2 \mathrm{E}\left[\beta_i^{(l)} \beta_i^{(l)}\right] \\
&\quad + \frac{\sigma_w \sigma_b}{\sqrt{D^{(l-1)}}} \left(\mathrm{E}\left[\beta_i^{(l)} \Sigma_j \omega_{j,i}^{(l)} \phi(z_j^{(l-1)}(\boldsymbol{x}))\right] + \mathrm{E}\left[\beta_i^{(l)} \Sigma_j \omega_{j,i}^{(l)} \phi(z_j^{(l-1)}(\boldsymbol{x}'))\right]\right) \\
&= \frac{\sigma_w^2}{D^{(l-1)}} \Sigma_j \mathrm{E}\left[\omega_{j,i}^{(l)} \omega_{j,i}^{(l)}\right] \mathrm{E}\left[\phi(z_j^{(l-1)}(\boldsymbol{x})) \phi(z_j^{(l-1)}(\boldsymbol{x}'))\right] + \sigma_b^2 \mathrm{E}\left[\beta_i^{(l)} \beta_i^{(l)}\right] \\
&= \sigma_w^2 \mathrm{E}_{(z_i^{(l-1)}(\boldsymbol{x}), z_i^{(l-1)}(\boldsymbol{x}')) \sim \mathcal{N}(\boldsymbol{0}_2, \boldsymbol{K}_{2,2}^{(l-1)})} \left[\phi(z_i^{(l-1)}(\boldsymbol{x})) \phi(z_i^{(l-1)}(\boldsymbol{x}'))\right] + \sigma_b^2,
\end{aligned}
$$

where

$$
\boldsymbol{K}_{2,2}^{(l-1)} = \begin{bmatrix} k^{(l-1)}(\boldsymbol{x},\boldsymbol{x}) & k^{(l-1)}(\boldsymbol{x},\boldsymbol{x}') \\ k^{(l-1)}(\boldsymbol{x},\boldsymbol{x}') & k^{(l-1)}(\boldsymbol{x}',\boldsymbol{x}') \end{bmatrix}
$$

Evaluating $\boldsymbol{K}^{(l)}$

- For certain activation functions $\phi(\cdot)$, such as tanh and ReLU, $k^{(l)}(\boldsymbol{x},\boldsymbol{x}')$ has a closed form [9]
- For other $\phi(\cdot)$'s, Markov Chain Monte Carlo (MCMC) sampling is required to devaluate $k^{(l)}(\boldsymbol{x},\boldsymbol{x}')$

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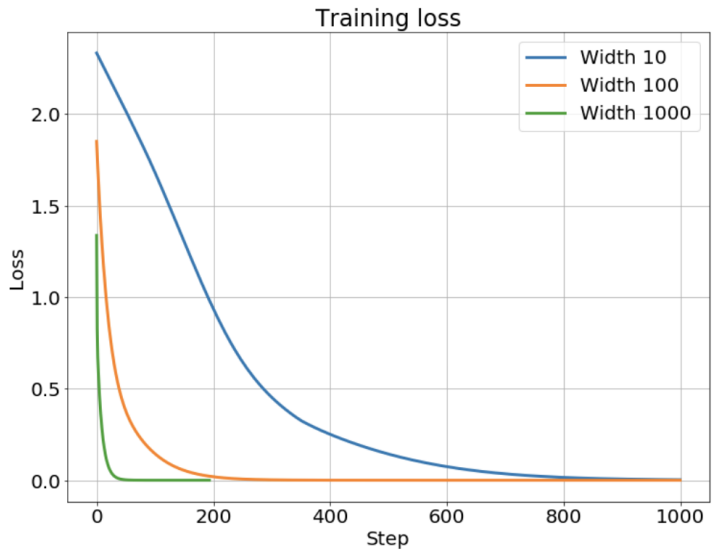
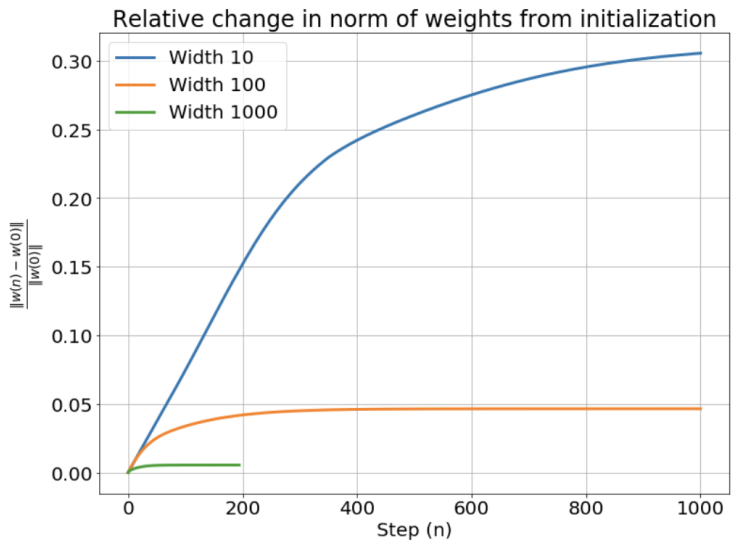
Weight Dynamics

- Observation: the weights of a wide NN do not change much during gradient descent





- Why?

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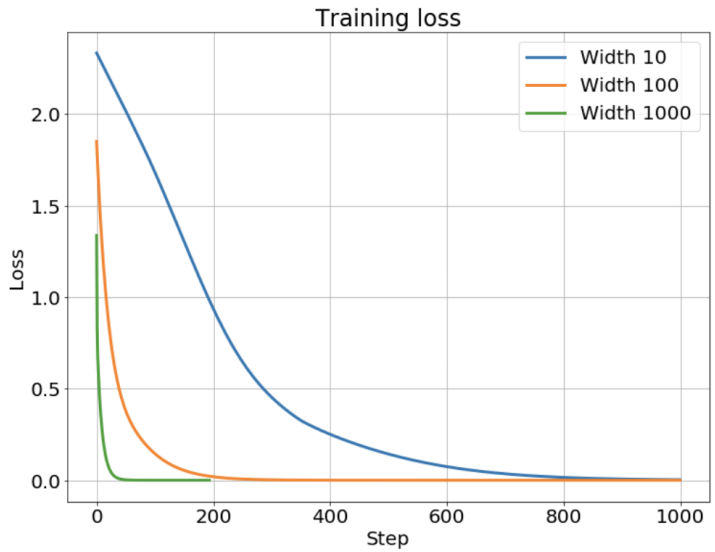

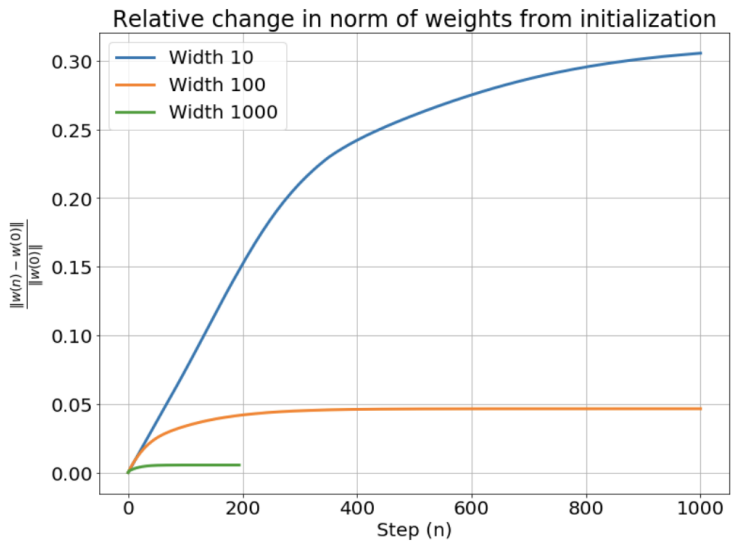

- Why? A small change in a large number of neurons is enough to significantly change the output
- This allows us to approximate an NN $f(\cdot;\theta)$ ***w.r.t. weights*** using the first-order Taylor expansion

Linearization of $f(\cdot;\theta)$

- Let $\theta^{(t)}$ be the parameters of the NN at the t-th step of gradient descent
  - $\hat{\boldsymbol{y}}^{(t)} = [f(\boldsymbol{x}^{(1)};\theta^{(t)}),\cdots,f(\boldsymbol{x}^{(N)};\theta^{(t)})]^\top$ be the predictions over training points
- Since $\theta^{(t)}$ is close to $\theta^{(0)}$ at any time t, we can approximate $f(\cdot;\theta^{(t)})$ using the first-order Taylor expansion ***w.r.t.*** $\theta^{(t)}$ around $\theta^{(0)}$:

$$f(\boldsymbol{x},\theta^{(t)}) \approx \bar{f}(\boldsymbol{x},\theta^{(t)}) = f(\boldsymbol{x},\theta^{(0)}) + \nabla_\theta f(\boldsymbol{x},\theta^{(0)})^\top(\theta^{(t)}-\theta^{(0)})$$

  - $\bar{f}$ is still ***non-linear in terms of x***
  - Let $\bar{\boldsymbol{y}}^{(t)} = [\bar{f}(\boldsymbol{x}^{(1)};\theta^{(t)}),\cdots,\bar{f}(\boldsymbol{x}^{(N)};\theta^{(t)})]^\top$ be the predictions of $\bar{f}$ at time t

Weight and Prediction Dynamics

$$f(\boldsymbol{x}, \boldsymbol{\theta}^{(t)}) \approx \bar{f}(\boldsymbol{x}, \boldsymbol{\theta}^{(t)}) = f(\boldsymbol{x}, \boldsymbol{\theta}^{(0)}) + \nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}, \boldsymbol{\theta}^{(0)})^\top (\boldsymbol{\theta}^{(t)} - \boldsymbol{\theta}^{(0)})$$

- Gradient descent with learning rate η makes the following changes:

$$\begin{aligned} \boldsymbol{\theta}^{(t+1)} - \boldsymbol{\theta}^{(t)} &\approx -\eta \nabla_{\boldsymbol{\theta}} C(\bar{\boldsymbol{y}}^{(t)}, \boldsymbol{y}) \\ &= -\eta \nabla_{\boldsymbol{\theta}} \bar{\boldsymbol{y}}^{(t)} \nabla_{\bar{\boldsymbol{y}}^{(t)}} C(\bar{\boldsymbol{y}}^{(t)}, \boldsymbol{y}) \\ &= -\eta \nabla_{\boldsymbol{\theta}} \hat{\boldsymbol{y}}^{(0)} \nabla_{\bar{\boldsymbol{y}}^{(t)}} C(\bar{\boldsymbol{y}}^{(t)}, \boldsymbol{y}) \end{aligned}$$

and

$$\begin{aligned} \bar{\boldsymbol{y}}^{(t+1)} - \bar{\boldsymbol{y}}^{(t)} &= \nabla_{\boldsymbol{\theta}} \hat{\boldsymbol{y}}^{(0)\top} (\boldsymbol{\theta}^{(t+1)} - \boldsymbol{\theta}^{(t)}) \\ &\approx -\eta \underbrace{\nabla_{\boldsymbol{\theta}} \hat{\boldsymbol{y}}^{(0)\top}}_{N \times D} \underbrace{\nabla_{\boldsymbol{\theta}} \hat{\boldsymbol{y}}^{(0)}}_{D \times N} \nabla_{\bar{\boldsymbol{y}}^{(t)}} C(\bar{\boldsymbol{y}}^{(t)}, \boldsymbol{y}), \end{aligned}$$

where $\boldsymbol{T}_{N,N}^{(0)} \equiv \nabla_{\boldsymbol{\theta}} \hat{\boldsymbol{y}}^{(0)\top} \nabla_{\boldsymbol{\theta}} \hat{\boldsymbol{y}}^{(0)} \in \mathbb{R}^{N \times N}$ is called the ***Neural Tangent Kernel (NTK)*** matrix

Prediction Dynamics in Regression

- In regression where $C(\bar{\boldsymbol{y}}^{(0)}, \boldsymbol{y}) = \frac{1}{2}\|\bar{\boldsymbol{y}}^{(0)} - \boldsymbol{y}\|^2$, we have

$$\bar{\boldsymbol{y}}^{(t+1)} - \bar{\boldsymbol{y}}^{(t)} \approx -\eta \boldsymbol{T}^{(0)}_{N,N} \nabla_{\bar{\boldsymbol{y}}^{(t)}} C(\bar{\boldsymbol{y}}^{(t)}, \boldsymbol{y}) = -\eta \boldsymbol{T}^{(0)}_{N,N} (\bar{\boldsymbol{y}}^{(t)} - \boldsymbol{y})$$

- With a sufficiently small learning rate η, we can think t as continuous time and each GD step as Δt, where

$$\lim_{\Delta t \to 0} \frac{\bar{\boldsymbol{y}}^{(t+\Delta t)} - \bar{\boldsymbol{y}}^{(t)}}{\Delta t} = \frac{\partial \bar{\boldsymbol{y}}^{(t)}}{\partial t} \approx -\eta \boldsymbol{T}^{(0)}_{N,N} (\bar{\boldsymbol{y}}^{(t)} - \boldsymbol{y})$$

- Letting $\boldsymbol{u}^{(t)} = \bar{\boldsymbol{y}}^{(t)} - \boldsymbol{y}$, we have an ordinary differential equation:

$$\frac{\partial \bar{\boldsymbol{y}}^{(t)}}{\partial t} \approx -\eta \boldsymbol{T}^{(0)}_{N,N} (\bar{\boldsymbol{y}}^{(t)} - \boldsymbol{y})$$
$$\Rightarrow \frac{\partial \boldsymbol{u}^{(t)}}{\partial t} \approx -\eta \boldsymbol{T}^{(0)}_{N,N} \boldsymbol{u}^{(t)}$$

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- In regression where $C(\bar{\boldsymbol{y}}^{(0)}, \boldsymbol{y}) = \frac{1}{2}\|\bar{\boldsymbol{y}}^{(0)} - \boldsymbol{y}\|^2$, we have

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$$\Rightarrow \frac{\partial \boldsymbol{u}^{(t)}}{\partial t} \approx -\eta \boldsymbol{T}^{(0)}_{N,N} \boldsymbol{u}^{(t)}$$

- Therefore, $\boldsymbol{u}^{(t)} = e^{-\eta \boldsymbol{T}^{(0)}_{N,N} t} \boldsymbol{u}(0)$
  - Recall that $e^{\boldsymbol{A}t} = \frac{1}{0!}\boldsymbol{I} + \frac{t}{1!}\boldsymbol{A} + \frac{t^2}{2!}\boldsymbol{A}^2 + \cdots$ for a symmetric $\boldsymbol{A}$
  - So, $\frac{\partial e^{\boldsymbol{A}t}}{\partial t} = \frac{1}{0!}\boldsymbol{A} + \frac{t}{1!}\boldsymbol{A}^2 + \cdots = (\frac{1}{0!}\boldsymbol{I} + \frac{t}{1!}\boldsymbol{A} + \cdots)\boldsymbol{A} = \boldsymbol{A}e^{\boldsymbol{A}t}$
- This implies that

$$\bar{\boldsymbol{y}}^{(t)} = e^{-\eta \boldsymbol{T}^{(0)}_{N,N} t} \bar{\boldsymbol{y}}(0) + (\boldsymbol{I} - e^{-\eta \boldsymbol{T}^{(0)}_{N,N} t})\boldsymbol{y} = e^{-\eta \boldsymbol{T}^{(0)}_{N,N} t} \hat{\boldsymbol{y}}(0) + (\boldsymbol{I} - e^{-\eta \boldsymbol{T}^{(0)}_{N,N} t})\boldsymbol{y}$$

Weight Dynamics in Regression

- By definition of $\bar{\boldsymbol{y}}^{(t)}$, we also have $\bar{\boldsymbol{y}}^{(t)} = \hat{\boldsymbol{y}}^{(0)} + \nabla_{\boldsymbol{\theta}} \hat{\boldsymbol{y}}^{(0)\top} (\boldsymbol{\theta}^{(t)} - \boldsymbol{\theta}^{(0)})$
- Solving $\boldsymbol{\theta}^{(t)}$ in

$$e^{-\eta \boldsymbol{T}^{(0)}_{N,N} t} \hat{\boldsymbol{y}}^{(0)} + (\boldsymbol{I} - e^{-\eta \boldsymbol{T}^{(0)}_{N,N} t}) \boldsymbol{y} = \hat{\boldsymbol{y}}^{(0)} + \nabla_{\boldsymbol{\theta}} \hat{\boldsymbol{y}}^{(0)\top} (\boldsymbol{\theta}^{(t)} - \boldsymbol{\theta}^{(0)}),$$

  we have

$$\boldsymbol{\theta}^{(t)} = \boldsymbol{\theta}^{(0)} - \nabla_{\boldsymbol{\theta}} \hat{\boldsymbol{y}}^{(0)} \boldsymbol{T}^{(0)-1}_{N,N} (\boldsymbol{I} - e^{-\eta \boldsymbol{T}^{(0)}_{N,N} t}) (\hat{\boldsymbol{y}}^{(0)} - \boldsymbol{y})$$

Predictions of Trained NN

- Substituting $\theta^{(t)}$ in $\bar{\boldsymbol{y}}^{(t)} = \hat{\boldsymbol{y}}^{(0)} + \nabla_{\boldsymbol{\theta}} \hat{\boldsymbol{y}}^{(0)\top} (\boldsymbol{\theta}^{(t)} - \boldsymbol{\theta}^{(0)})$, we have that:
- For an arbitrary (training or test) point $\boldsymbol{x}'$, the prediction of trained NN is

$$f(\boldsymbol{x}', \boldsymbol{\theta}^{(t)}) \approx \bar{f}(\boldsymbol{x}'; \boldsymbol{\theta}^{(t)}) = \boldsymbol{p}^\top \begin{bmatrix} \hat{\boldsymbol{y}}^{(0)} \\ \hat{y}'^{(0)} \end{bmatrix} + q,$$

where

$$\boldsymbol{p} = [-\boldsymbol{T}^{(0)}_{1',N} \boldsymbol{T}^{(0)-1}_{N,N} (\boldsymbol{I} - e^{-\eta \boldsymbol{T}^{(0)}_{N,N} t}), 1]^\top \in \mathbb{R}^{N+1},$$
$$q = \boldsymbol{T}^{(0)}_{1',N} \boldsymbol{T}^{(0)-1}_{N,N} (\boldsymbol{I} - e^{-\eta \boldsymbol{T}^{(0)}_{N,N} t}) \boldsymbol{y}$$

  - $\boldsymbol{T}^{(0)}_{N,N} = \nabla_{\boldsymbol{\theta}} \hat{\boldsymbol{y}}^{(0)\top} \nabla_{\boldsymbol{\theta}} \hat{\boldsymbol{y}}^{(0)} \in \mathbb{R}^{N \times N}$ is the NTK matrix for $\boldsymbol{X}_N$
  - $\boldsymbol{T}^{(0)}_{1',N} = \nabla_{\boldsymbol{\theta}} \hat{y}'^{(0)\top} \nabla_{\boldsymbol{\theta}} \hat{\boldsymbol{y}}^{(0)} \in \mathbb{R}^{1 \times N}$ is the NTK matrix between $\boldsymbol{x}'$ and $\boldsymbol{X}_N$

Predictions of Trained NN

- Substituting $\theta^{(t)}$ in $\bar{\boldsymbol{y}}^{(t)} = \hat{\boldsymbol{y}}^{(0)} + \nabla_{\boldsymbol{\theta}} \hat{\boldsymbol{y}}^{(0)\top} (\boldsymbol{\theta}^{(t)} - \boldsymbol{\theta}^{(0)})$, we have that:
- For an arbitrary (training or test) point $\boldsymbol{x}'$, the prediction of trained NN is

$$f(\boldsymbol{x}', \boldsymbol{\theta}^{(t)}) \approx \bar{f}(\boldsymbol{x}'; \boldsymbol{\theta}^{(t)}) = \boldsymbol{p}^\top \begin{bmatrix} \hat{\boldsymbol{y}}^{(0)} \\ \hat{y}'^{(0)} \end{bmatrix} + q,$$

where

$$\boldsymbol{p} = [-\boldsymbol{T}^{(0)}_{1',N} \boldsymbol{T}^{(0)-1}_{N,N} (\boldsymbol{I} - e^{-\eta \boldsymbol{T}^{(0)}_{N,N} t}), 1]^\top \in \mathbb{R}^{N+1},$$
$$q = \boldsymbol{T}^{(0)}_{1',N} \boldsymbol{T}^{(0)-1}_{N,N} (\boldsymbol{I} - e^{-\eta \boldsymbol{T}^{(0)}_{N,N} t}) \boldsymbol{y}$$

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  - $\boldsymbol{T}^{(0)}_{1',N} = \nabla_{\boldsymbol{\theta}} \hat{y}'^{(0)\top} \nabla_{\boldsymbol{\theta}} \hat{\boldsymbol{y}}^{(0)} \in \mathbb{R}^{1 \times N}$ is the NTK matrix between $\boldsymbol{x}'$ and $\boldsymbol{X}_N$
- ***No actual training*** needed!

Gradient Descent as an Affine Transformation

Theorem (NTK in infinite width)

*As the NN's width goes to infinity, $\boldsymbol{T}^{(0)}_{N,N}$ and $\boldsymbol{T}^{(0)}_{1',N}$ converges to $\boldsymbol{T}_{N,N}$ and $\boldsymbol{T}_{1',N}$, which can be described by a **deterministic** kernel function independent of a particular initialization [8, 10].*

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- $\boldsymbol{T}_{N,N}$ and $\boldsymbol{T}_{1',N}$ have closed forms for certain activation functions $\phi(\cdot)$'s, including erf and ReLU
- $f(\boldsymbol{x}', \boldsymbol{\theta}^{(t)}) \approx \boldsymbol{p}^\top \begin{bmatrix} \hat{\boldsymbol{y}}^{(0)} \\ \hat{y}'^{(0)} \end{bmatrix} + q$ is an ***affine transformation*** of a random vector $\begin{bmatrix} \hat{\boldsymbol{y}}^{(0)} \\ \hat{y}'^{(0)} \end{bmatrix}$

Outline

1. When ML Meets Big Data
2. Advantages of Deep Learning
   - Representation Learning
   - Exponential Gain of Expressiveness
   - Memory and GPU Friendliness
   - Online & Transfer Learning
3. **Learning Theory Revisited**
   - Generalizability and Over-Parametrization
   - Wide-and-Deep NN is a Gaussian Process before Training*
   - Gradient Descent is an Affine Transformation
   - Wide-and-Deep NN is a Gaussian Process after Training

Wide-and-Deep NN as a Gaussian Process I

- As $D \to \infty$, randomly initialized NN has a corresponding NN-GP:

$$\begin{bmatrix} \hat{\boldsymbol{y}}_N \\ \hat{\boldsymbol{y}}_M \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \boldsymbol{0}_N \\ \boldsymbol{0}_M \end{bmatrix}, \begin{bmatrix} \boldsymbol{K}^{(L)}_{N,N} & \boldsymbol{K}^{(L)}_{N,M} \\ \boldsymbol{K}^{(L)}_{M,N} & \boldsymbol{K}^{(L)}_{M,M} \end{bmatrix} \right)$$

- As $D \to \infty$, GD-based training is an affine transformation:

$$f(\boldsymbol{x}', \theta^{(t)}) \approx \bar{f}(\boldsymbol{x}'; \theta^{(t)}) = \boldsymbol{p}^\top \begin{bmatrix} \hat{\boldsymbol{y}}^{(0)} \\ \hat{y}'^{(0)} \end{bmatrix} + q$$

  where
  - $\boldsymbol{p} = [-\boldsymbol{T}_{1',N}\boldsymbol{T}^{-1}_{N,N}(\boldsymbol{I} - e^{-\eta \boldsymbol{T}_{N,N} t}), 1]^\top \in \mathbb{R}^{N+1}$
  - $q = \boldsymbol{T}_{1',N}\boldsymbol{T}^{-1}_{N,N}(\boldsymbol{I} - e^{-\eta \boldsymbol{T}_{N,N} t})\boldsymbol{y}$
  - $\boldsymbol{T}_{N,N}$ and $\boldsymbol{T}_{1',N}$ the NTK matrices

Wide-and-Deep NN as a Gaussian Process II

- Therefore, as $D \to \infty$, the trained NN is still in correspondent with a GP, called ***NTK-GP***, whose predictions for M test points are

$$\begin{bmatrix} \hat{\boldsymbol{y}}_N \\ \hat{\boldsymbol{y}}_M \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \boldsymbol{A}\boldsymbol{y} \\ \boldsymbol{B}\boldsymbol{y} \end{bmatrix}, \boldsymbol{C}^\top \begin{bmatrix} \boldsymbol{K}^{(L)}_{N,N} & \boldsymbol{K}^{(L)}_{N,M} \\ \boldsymbol{K}^{(L)}_{M,N} & \boldsymbol{K}^{(L)}_{M,M} \end{bmatrix} \boldsymbol{C} \right),$$

  where
  - $\boldsymbol{A} = (\boldsymbol{I} - e^{-\eta \boldsymbol{T}_{N,N} t}) \in \mathbb{R}^{N \times N}$
  - $\boldsymbol{B} = \boldsymbol{T}_{M,N} \boldsymbol{T}_{N,N}^{-1} (\boldsymbol{I} - e^{-\eta \boldsymbol{T}_{N,N} t}) \in \mathbb{R}^{M \times N}$
  - $\boldsymbol{C} = \begin{bmatrix} -\boldsymbol{A} & \boldsymbol{1}_{N,M} \\ -\boldsymbol{B} & \boldsymbol{1}_{M,M} \end{bmatrix} \in \mathbb{R}^{(N+M) \times (N+M)}$

Mean Predictions of NTK-GP

- Prior (unconditioned) mean predictions for training set:

$$\hat{\boldsymbol{y}}_N = \boldsymbol{A}\boldsymbol{y} = (\boldsymbol{I} - e^{-\eta \boldsymbol{T}_{N,N} t})\boldsymbol{y}$$

  - As $t \to \infty$, **the $\hat{y}_N$ always approaches true labels y**
  - This explains why the SGD-based training of large NNs seldom encounters significant obstacles such as local minima [7]

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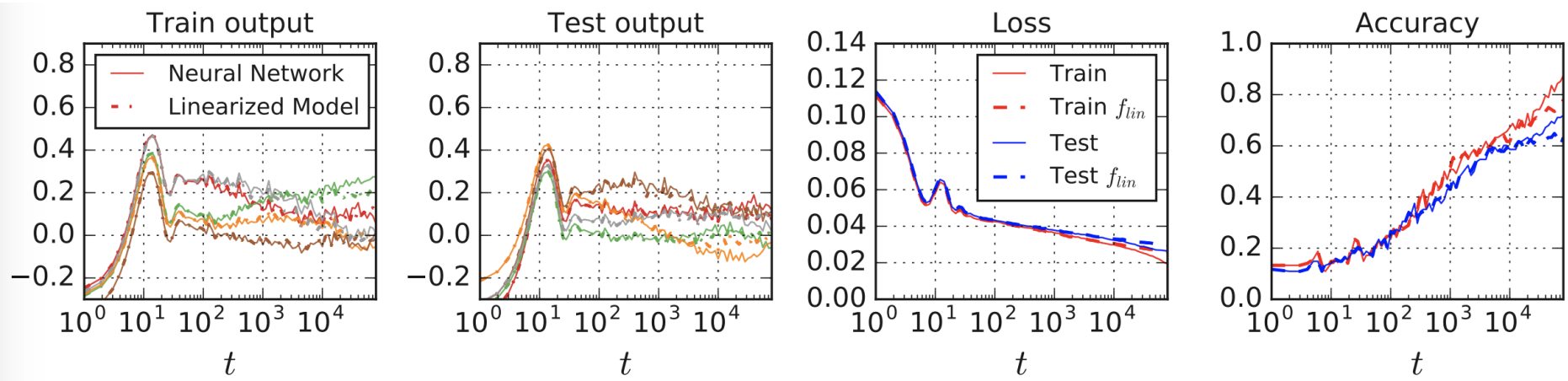
- Prior mean predictions for test set:

$$\hat{\boldsymbol{y}}_M = \boldsymbol{B}\boldsymbol{y} = \boldsymbol{T}_{M,N}\boldsymbol{T}_{N,N}^{-1}(\boldsymbol{I} - e^{-\eta \boldsymbol{T}_{N,N} t})\boldsymbol{y}$$

  - As $t \to \infty$, we have $\hat{\boldsymbol{y}}_M = \boldsymbol{T}_{M,N}\boldsymbol{T}_{N,N}^{-1}\boldsymbol{y}$
  - ***Weight hyperparameters are important*** because they determines $\boldsymbol{T}_{M,N}\boldsymbol{T}_{N,N}^{-1}$

Analytic vs. Real Predictions

- Wide residual network [18] trained by SGD with momentum on MSE loss on CIFAR-10
  - First two panes shows the output dynamics for a randomly selected subset of train and test points



Remarks

- Wide-and-deep NNs can be approximated by a class of GPs
  - Either before, during, or after training
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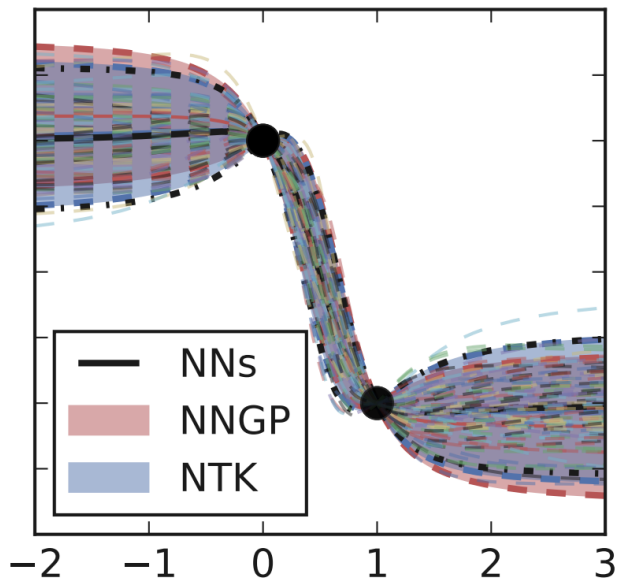
- Wide-and-deep NNs can be approximated by a class of GPs
  - Either before, during, or after training
- Therefore, complexity of wide-and-deep NNs grows with N, not $|\theta|$
- Applicable to other architectures incl. CNN [2, 15], RNN [16, 1], and any architecture [17]

Limitations

- Approximation holds only when the NNs have:
  - Infinite width
  - Small learning rate: $\eta \leq O(1/\lambda_{\max})$ where $\lambda_{\max}$ is the max eigenvalue of $\boldsymbol{T}_{N,N}$
  - Proper initialization (to be discussed next)
- The prior NTK-GP inference is ***inconsistent*** with the Bayesian inference of NN-GP
  - SGP introduces bias



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