Introduction to Deep Neural Networks (2)

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Introduction to Machine Learning (CS771A)

October 25, 2018

Plan for today

- Quick recap of feedforward networks
- Backprop via a small example
- Variations/improvements to basic feedforward networks
  - Convolutional Neural Networks (CNN)
  - Neural Networks for sequential data (RNN and LSTM)
- Neural networks for unsupervised learning (deep autoencoders)
- Some other recent advances (GAN and VAE)

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- Note: The attempt (this as well as previous lecture) is to convey basic principles of deep neural networks. For a more in-depth treatment, you are advised to take a dedicated deep learning course

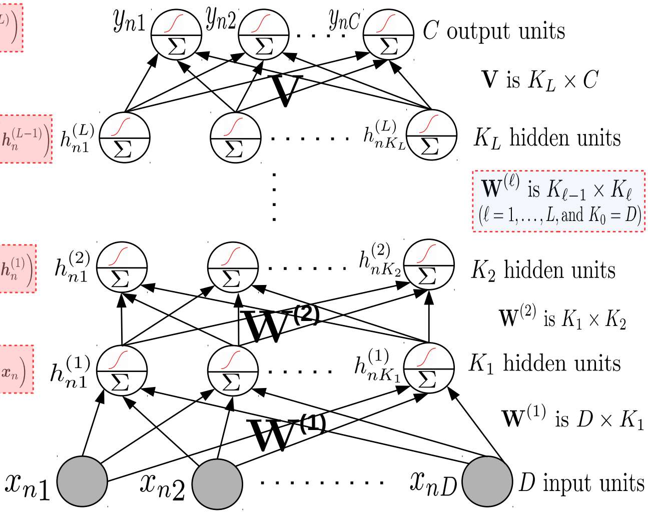
Recap: Feedforward Neural Networks (MLP)

$y_n = o\left(\mathbf{V}^\top h_n^{(L)}\right)$

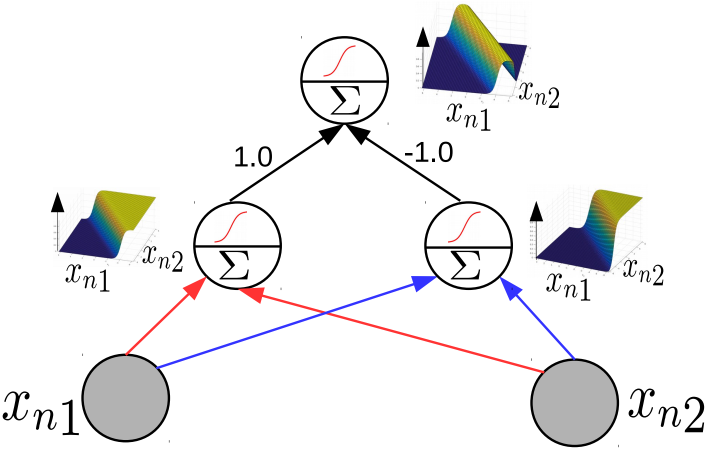
$h_n^{(L)} = g\left({\mathbf{W}^{(L)}}^\top h_n^{(L-1)}\right)$

$h_n^{(2)} = g\left({\mathbf{W}^{(2)}}^\top h_n^{(1)}\right)$

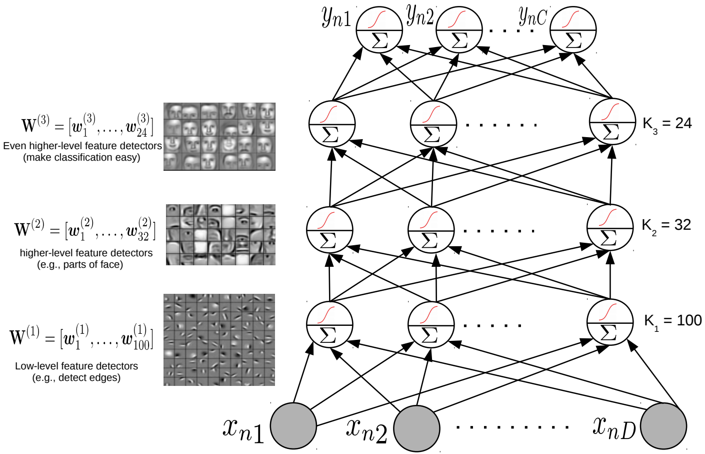
$h_n^{(1)} = g\left({\mathbf{W}^{(1)}}^\top x_n\right)$



Recap: MLP as Composition of Functions



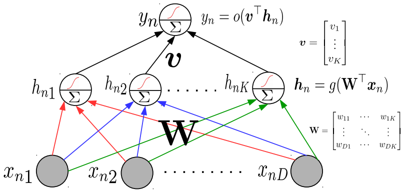
Recap: MLP as Multi-layer Feature Detector



Note: If no. of hidden units $< D$, then it can also be seen as doing (supervised) dim-red

Learning MLP via Backpropagation: A Simple Example

- Consider a single hidden layer MLP



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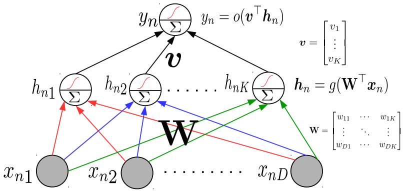

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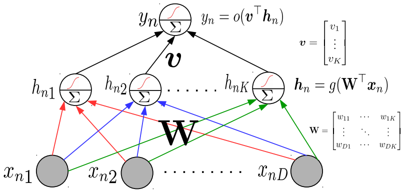

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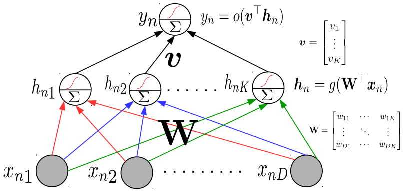

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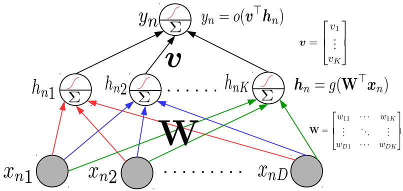

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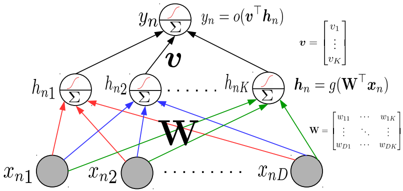

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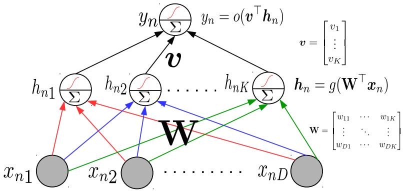

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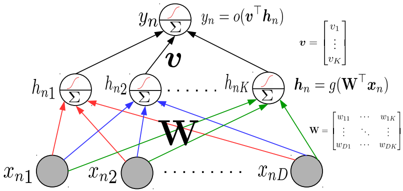

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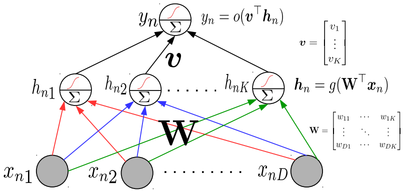

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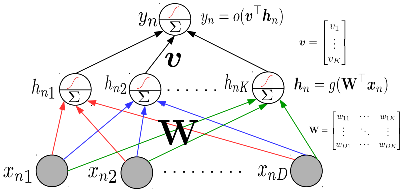

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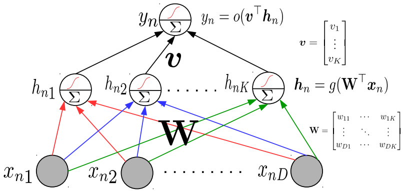

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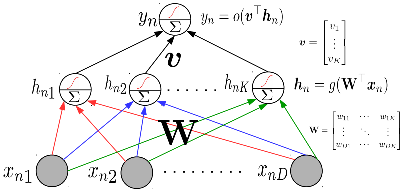

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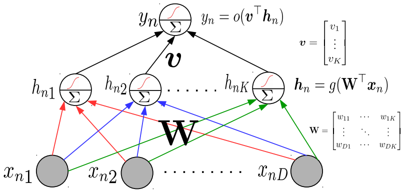

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- Backprop caches many of the calculations for reuse

Some Considerations w.r.t. Optimization in Deep NN

- Gradient based first-order methods are among the most popular ones
- Typically mini-batch SGD based method are used
- However, due to non-convexity, care needs to be exercised
  - Adaptive learning rates (Adam, Adagrad, RMSProp)
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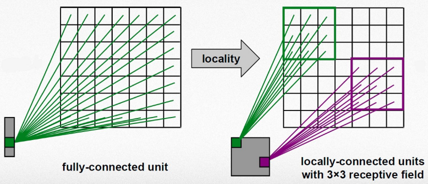
  - Momentum based or "look ahead" gradient methods
- Initialization is also very important
  - Layer-wise pre-training was one of the first successful schemes
  - Many other heuristics exist now

Some Limitations of Feedforward Networks

- Require a huge number of parameters (note that the consecutive layers are fully connected)
- Not ideal for data that exhibit locality structure, e.g., (e.g., images, sentences)
  - Kind of works but would be better to exploit locality in the data more explicitly



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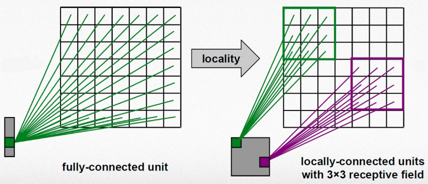
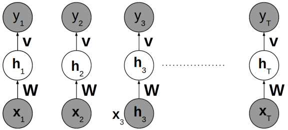
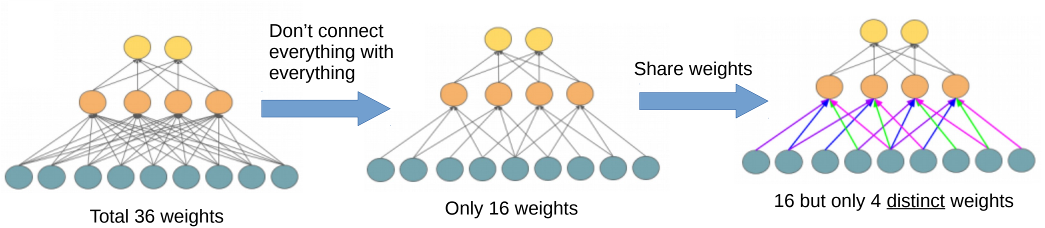


- Doesn't have a "memory", so not ideal when modeling sequence of observations



Convolutional Neural Network (CNN)

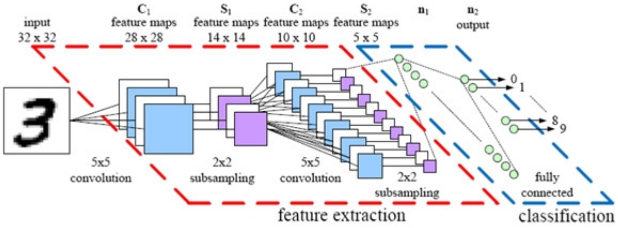
- A feedforward neural network with a special structure



- Not all pairs of nodes are connected
- Weights are also "tied" (many connections have the same weights; color-coded above)
- The set of distinct weights defines a "filter" or "local" feature detector

Convolutional Neural Network (CNN)

- Applies 2 operations, convolution and pooling (subsampling), repeatedly on the input data



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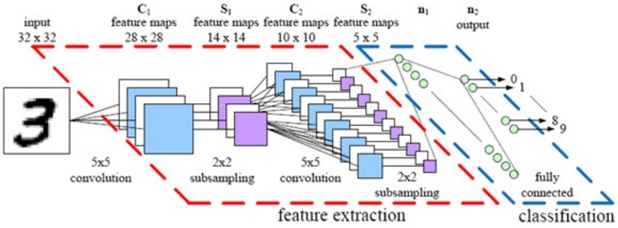

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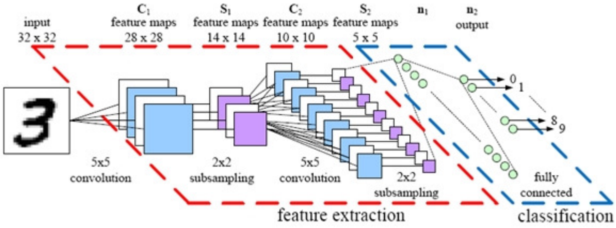

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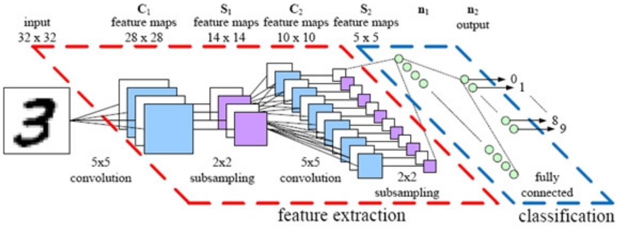

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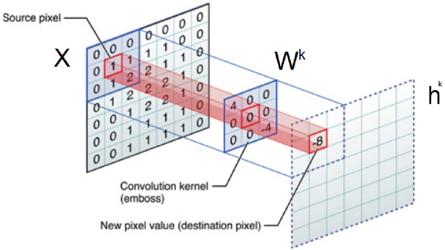
- Note: A nonlinearity is also introduced after the convolution layer

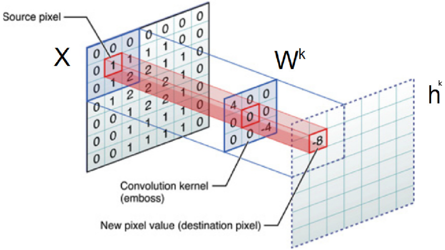
Convolution

- An operation that captures local (e.g., spatial) properties of a signal



Convolution

- An operation that captures local (e.g., spatial) properties of a signal



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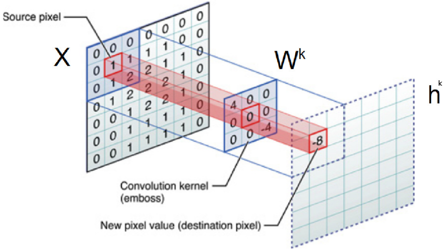

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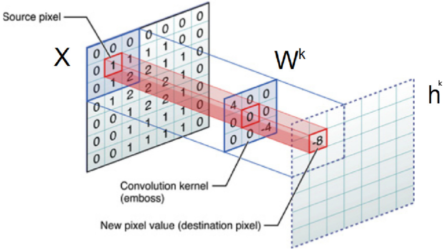

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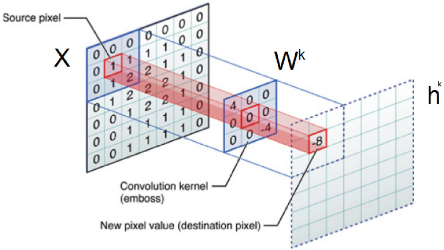

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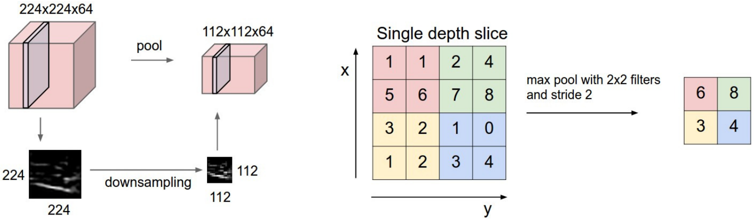

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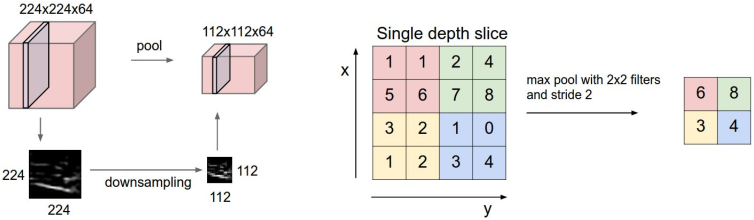

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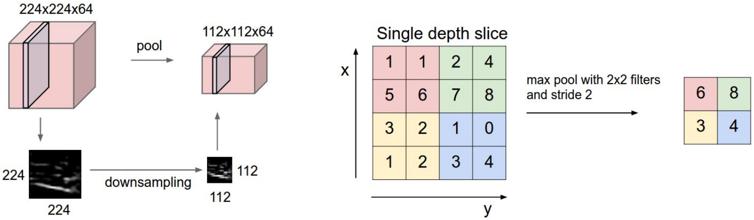


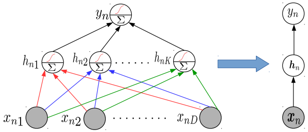
- Also ensures robustness against minor rotations, shifts, corruptions in the image
- Popular approaches: Max-pooling, averaging pooling, etc

Strides

- Stride defines the number of nodes a filter moves between two consecutive convolution operations
- Likewise, we have a stride to define the same when applying pooling

Modeling Sequential Data

- FFNN for a single observation looks like this (denoting all hidden units as $\boldsymbol{h}_n$)



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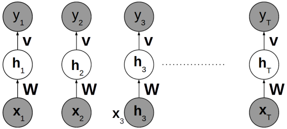

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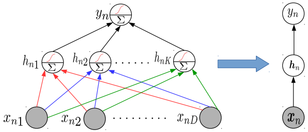

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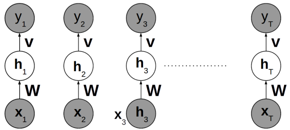

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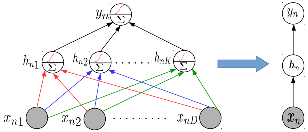

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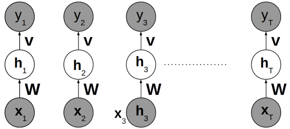

- For such sequential data, we want dependencies between $\boldsymbol{h}_t$'s of different observations
- Desirable when modeling sentence/paragraph/document, video (sequence of frames), etc.

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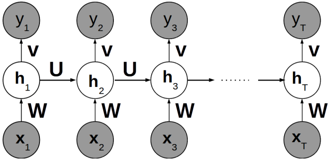

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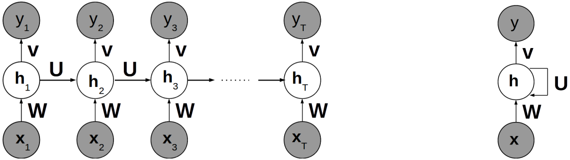

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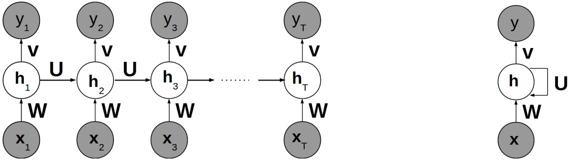

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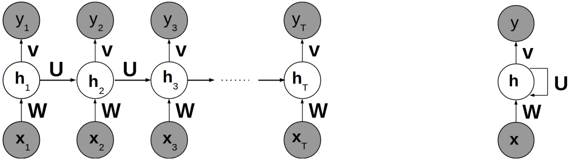

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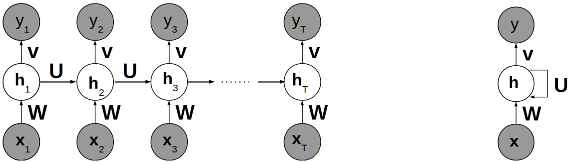

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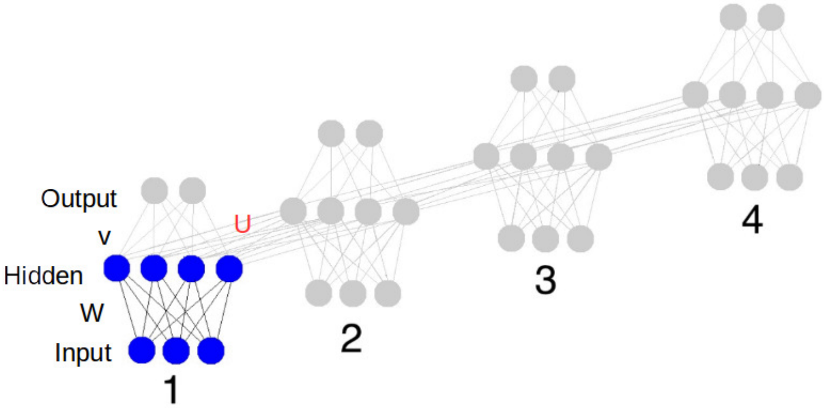
- RNNs can also be extended to have more than one hidden layer

Recurrent Neural Nets (RNN)

- A more "micro" view of RNN (the transition matrix **U** connects the hidden states across observations, propagating information along the sequence)



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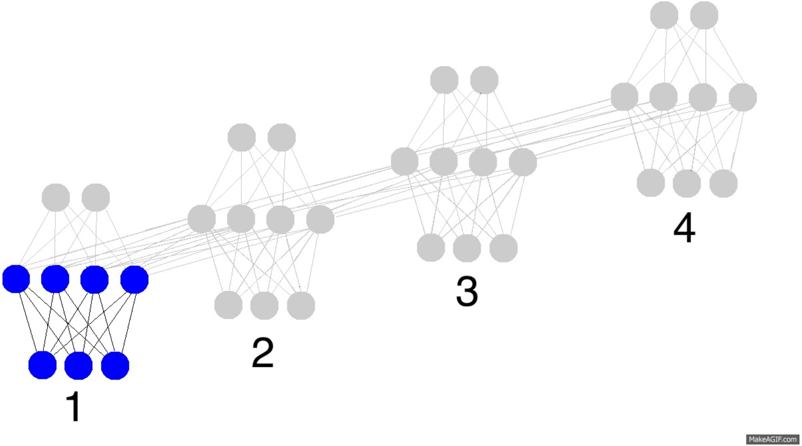

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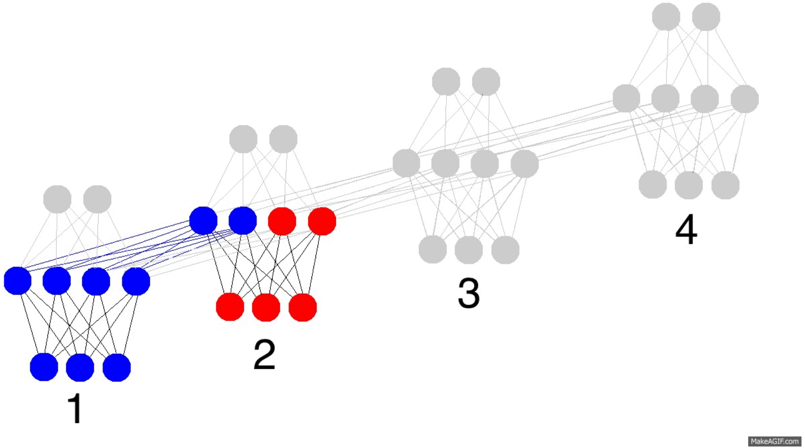

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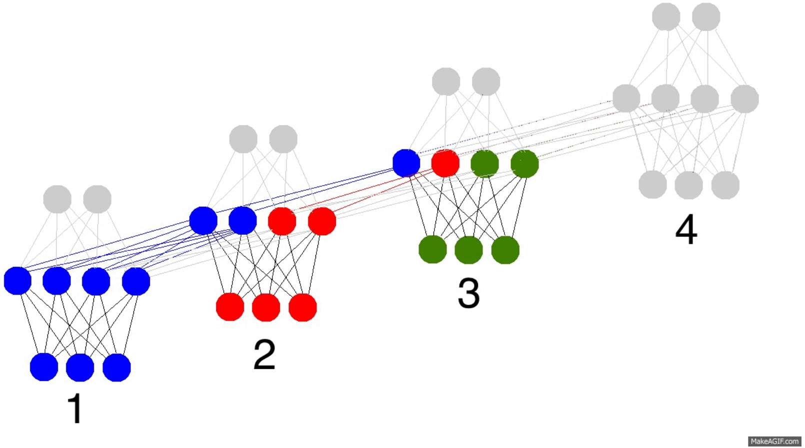

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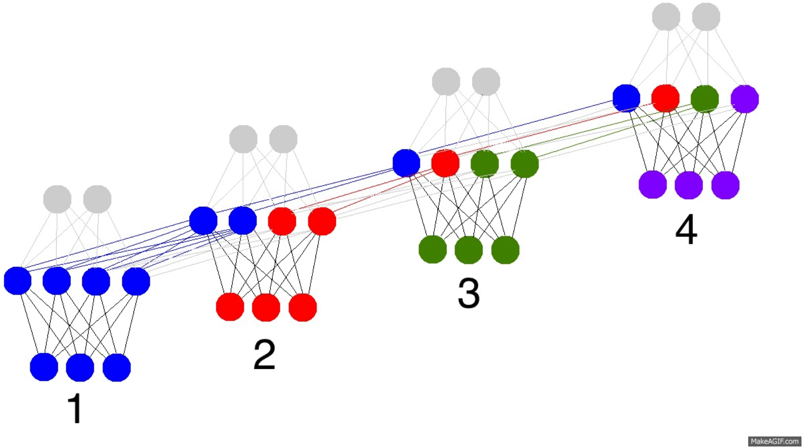
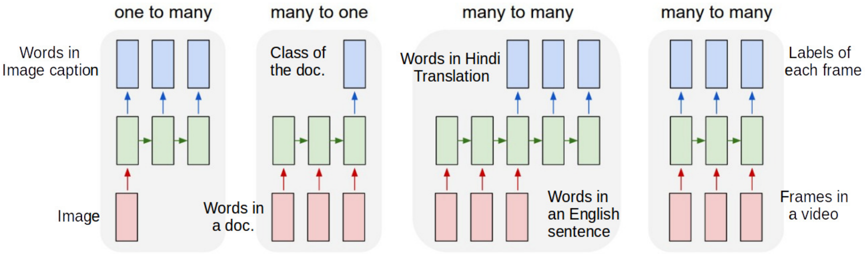


RNN: Applications



- RNNs are widely applicable and are also very flexible.

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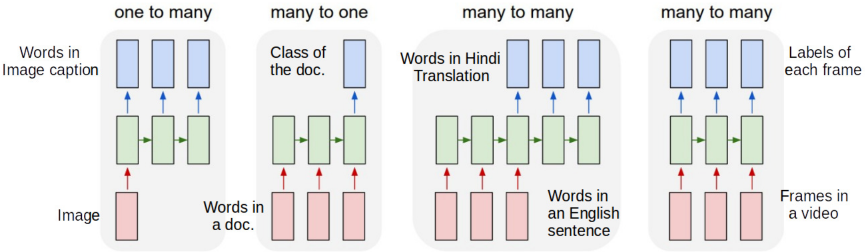

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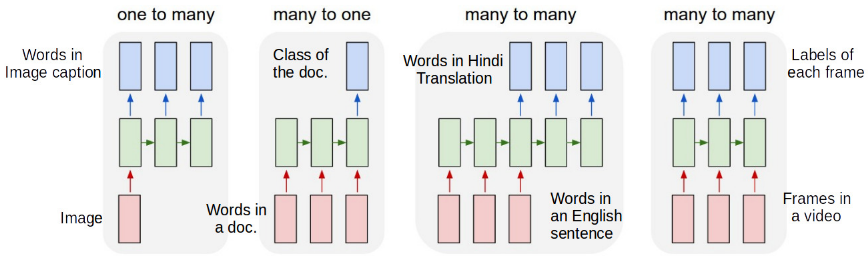

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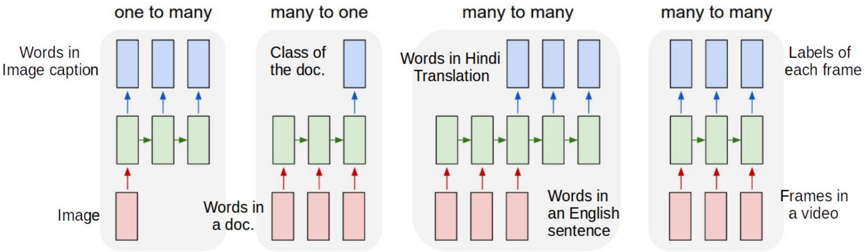

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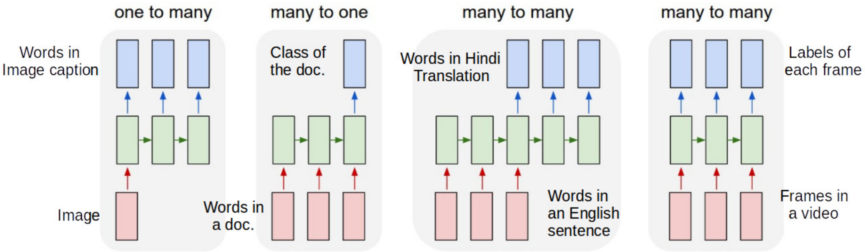

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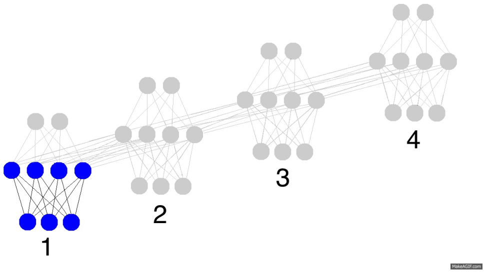
  - Input, output, or both, can be sequences (possibly of different lengths)
  - Different inputs (and different outputs) need not be of the same length
  - Regardless of the length of the input sequence, RNN will learn a fixed size embedding for the input sequence

Training RNN

- Trained using Backpropagation Through Time (forward propagate from step 1 to end, and then backward propagate from end to step 1)
- Think of the time-dimension as another hidden layer and then it is just like standard backpropagation for feedforward neural nets



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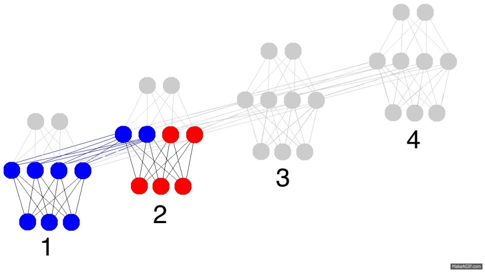

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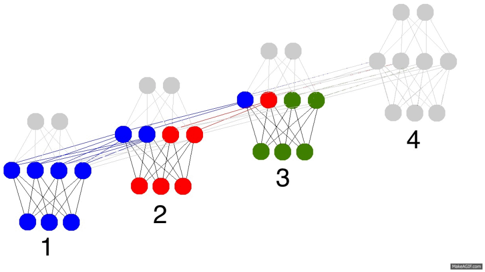

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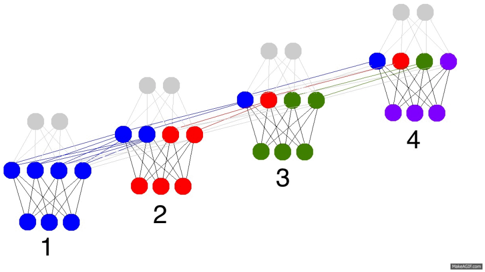

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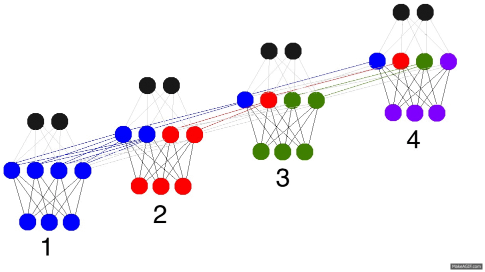

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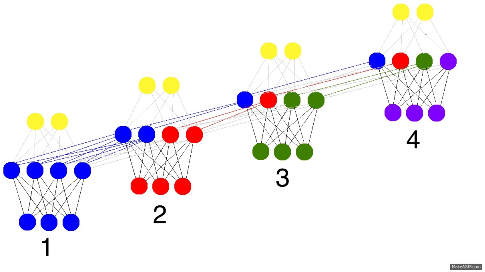

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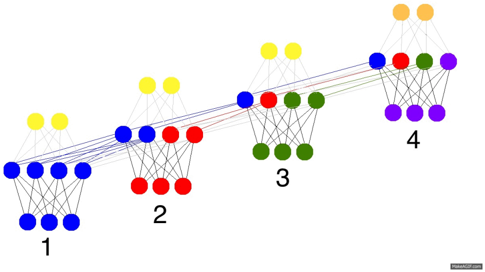

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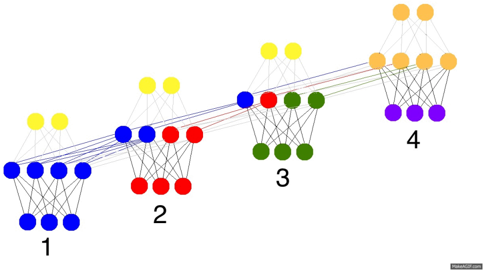

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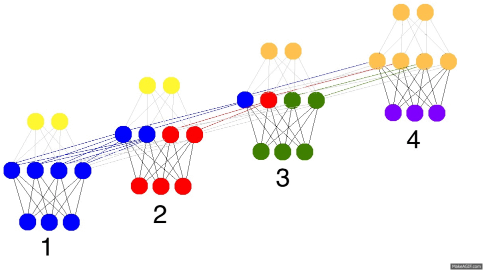

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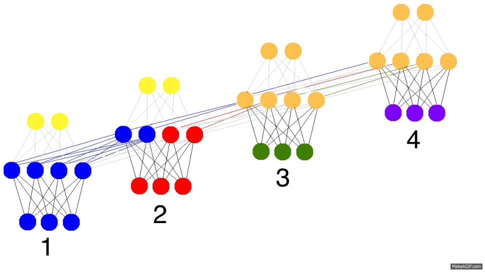

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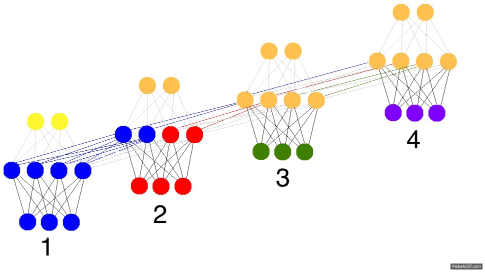

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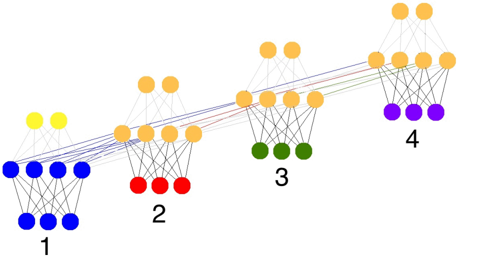

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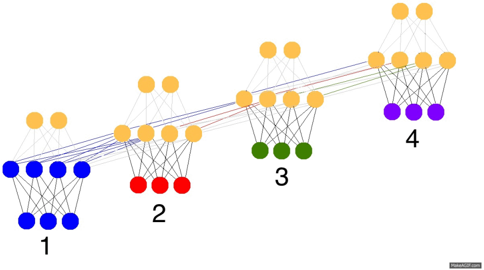

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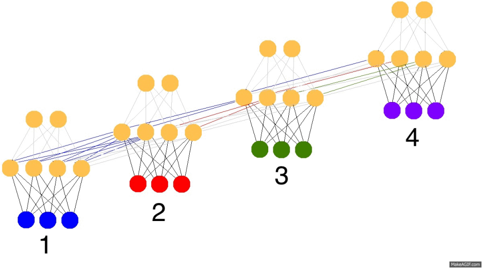

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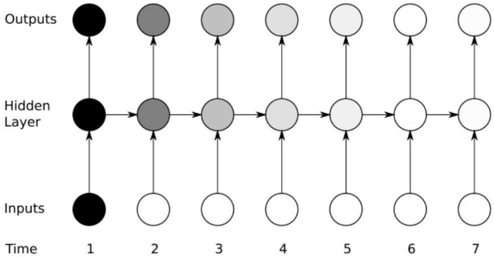
RNN Limitation



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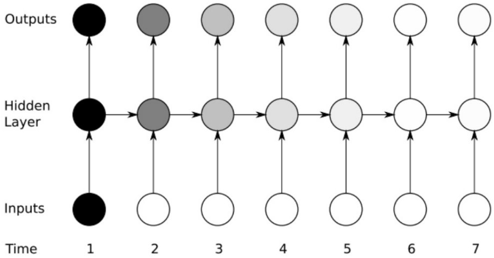

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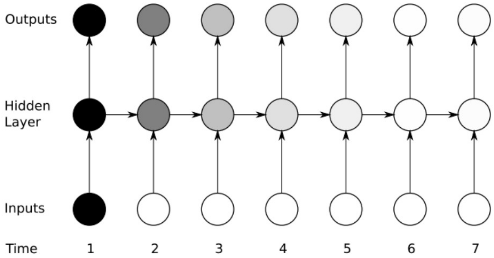

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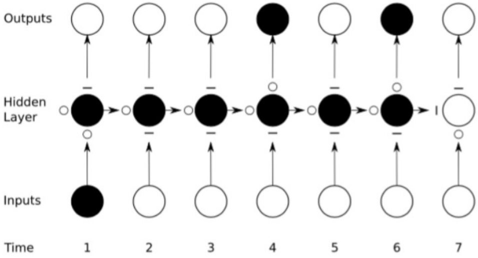
- New inputs "overwrite" the activations of previous hidden states
- Repeated multiplications can cause the gradients to vanish or explode

Capturing Long-Range Dependencies

- Idea: Augment the hidden states with gates (with parameters to be learned)
- These gates can help us remember and forget information "selectively"



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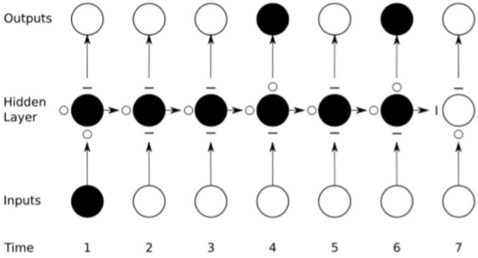

- The hidden states have 3 type of gates
  - Input (bottom), Forget (left), Output (top)

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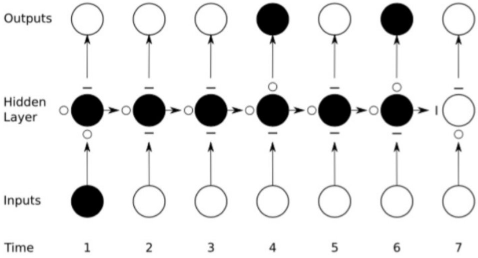

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Capturing Long-Range Dependencies

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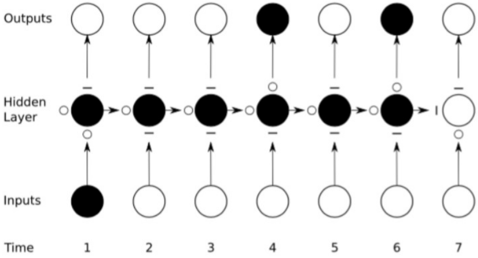

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- LSTM (Hochreiter and Schmidhuber, mid-90s): **Long Short-Term Memory** is one such idea

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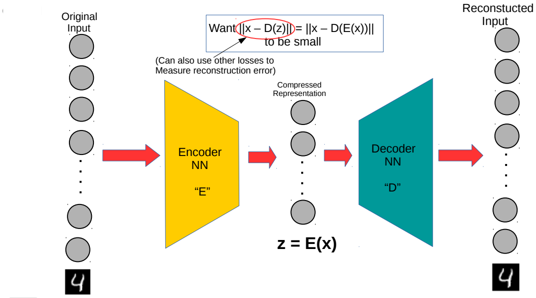
- Many variants of LSTM exists, e.g., using C_{t-1} in local computations, Gated Recurrent Units (GRU), etc. Mostly minor variations of basic LSTM above

Deep Neural Networks for Unsupervised Learning

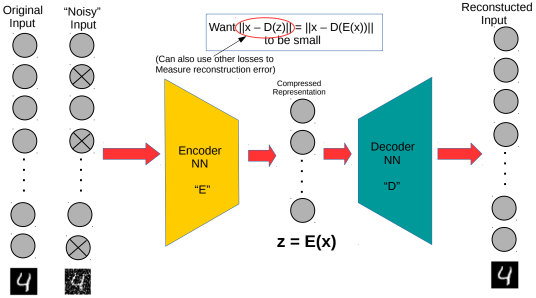
- Auto-encoder (AE) is a popular deep neural network unsupervised feature learning



- If size $\boldsymbol{z}$ is $K < D$, auto-encoders can be used for dimensionality reduction too
- For linear encoder/decodder with $E(\boldsymbol{x}) = \mathbf{W}^\top \boldsymbol{x}$, $D(\boldsymbol{z}) = \mathbf{W}\boldsymbol{z}$ and squared loss, AE is akin to PCA

Deep Neural Networks for Unsupervised Learning

- Denoising auto-encoders: Inject noise in the inputs before passing to to encoder



- Many ways to introduct "noise": Inject zero-mean Gaussian noise, "zero-out" some features, etc
- Especially useful when $K > D$ ($\boldsymbol{z}$ to be a copy of $\boldsymbol{x}$ with $K - D$ zeros) - overcomplete autocoders

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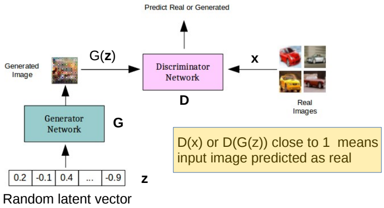
- A game between a Generator and a Discriminator



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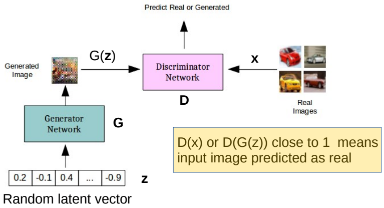

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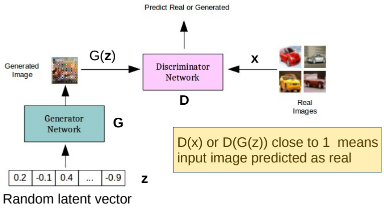

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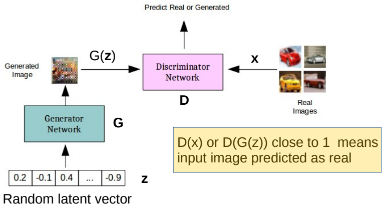

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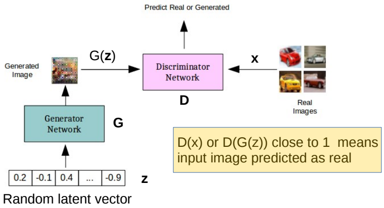

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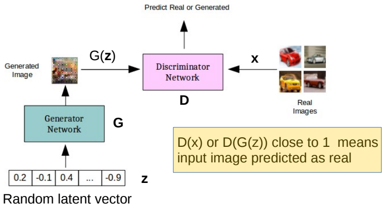

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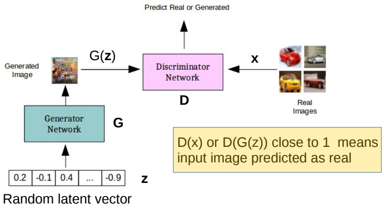

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- Can do MAP estimation of the NN parameters or even infer full posterior (Bayesian Deep Learning)

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