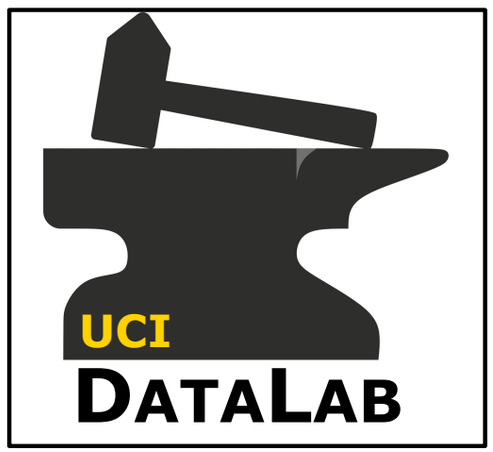
Deep Learning: A Synthesis from Probabilistic Foundations

Eric Nalisnick and **Padhraic Smyth**

University of California, Irvine



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You: "*Umm……*"

Motivation for This Talk

- Deep learning/neural networks are attracting a lot of attention

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- [ ] Nonetheless, deep learning has statistical ideas at the core

  This talk: bridge the gap between statistics and deep learning

- [ ] **Caveat:** Deep learning is a huge field….and this is a 50 minute talk
  (not speaking about convolutional neural networks, for instance)

Audience

- **Applied statisticians:** Be aware of…
  - (a) what deep learning is.
  - (b) what it can do well.
  - (c) what its limits are.

- **Research statisticians**: Opportunities to…
  - (a) use deep learning ideas in statistical modeling.
  - (b) bring more statistical thinking to deep learning.

Notation: A Simple Prediction Problem

- Data Set : $\{(\mathbf{x}_i, y_i)\}, \quad i = 1, \ldots, N$

  Would like to build a model to predict *y* given ***x***

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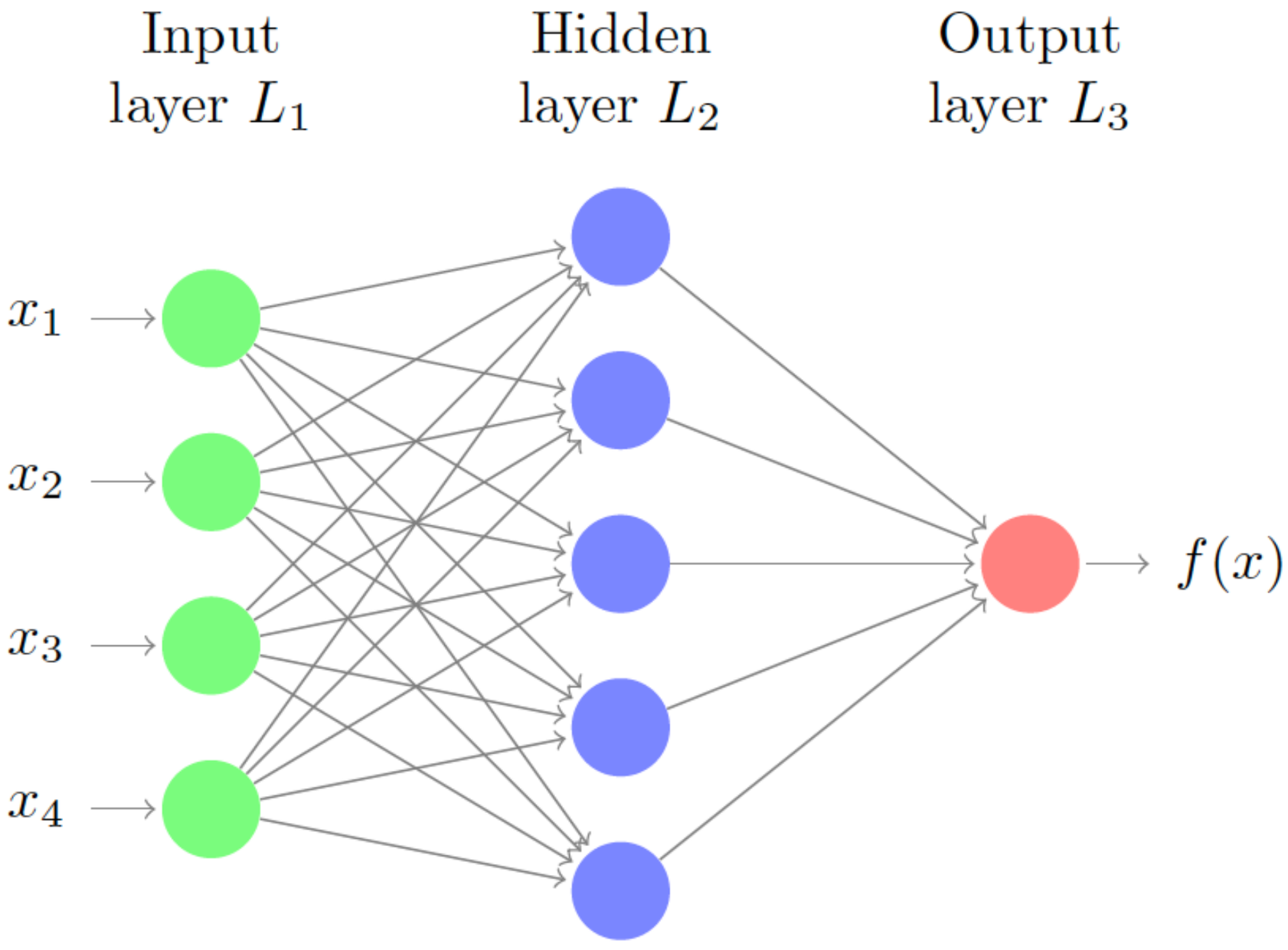
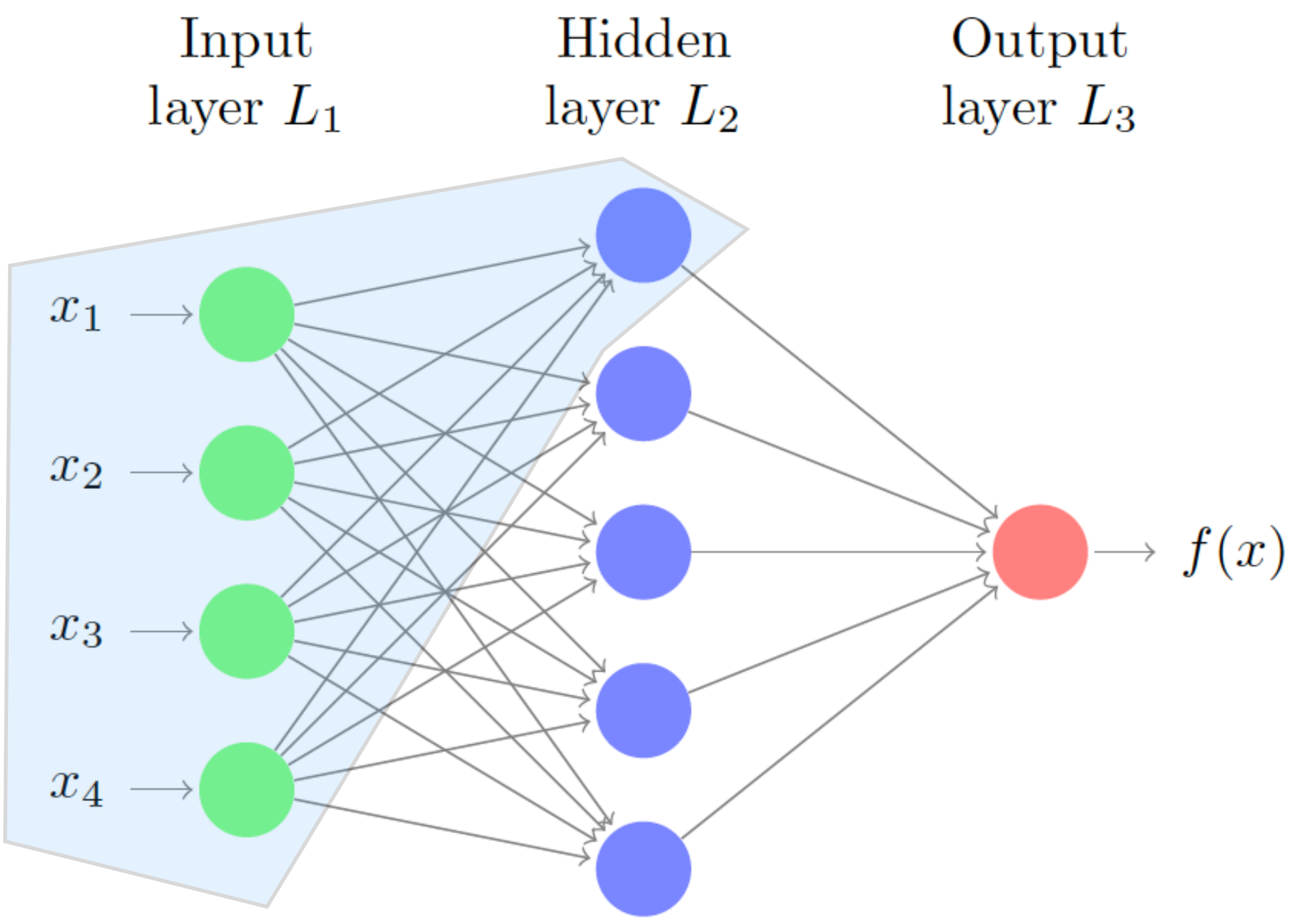
- **Example:**
  x = high-dimensional data (e.g., pixels)
  y = categorical label

  Could use a logistic (linear) model…
  ….. but would like to explore more complex models



State-of-the-art Neural Network in early 1990's

From Efron and Hastie, Computer Age Statistical Inference, 2016



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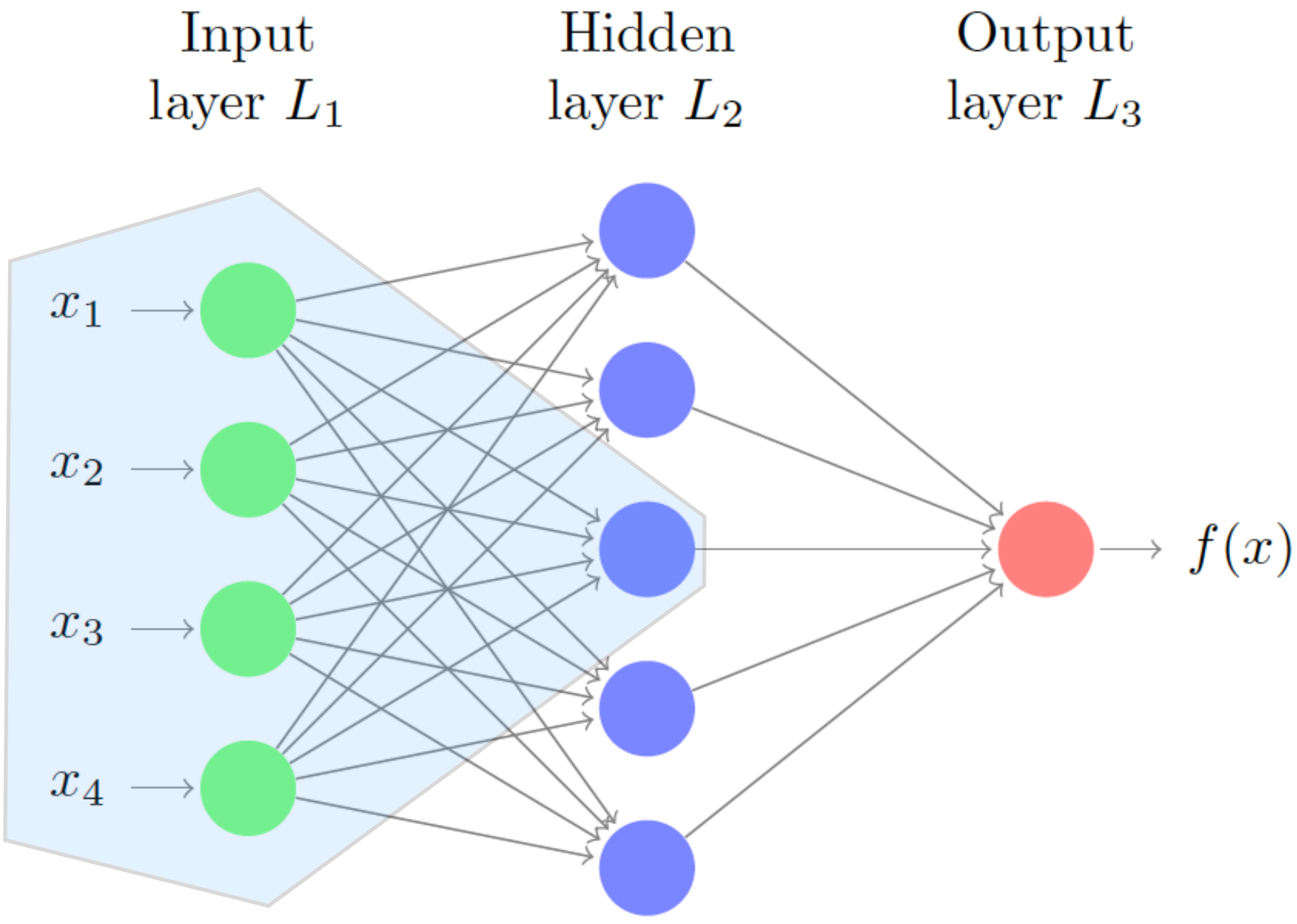

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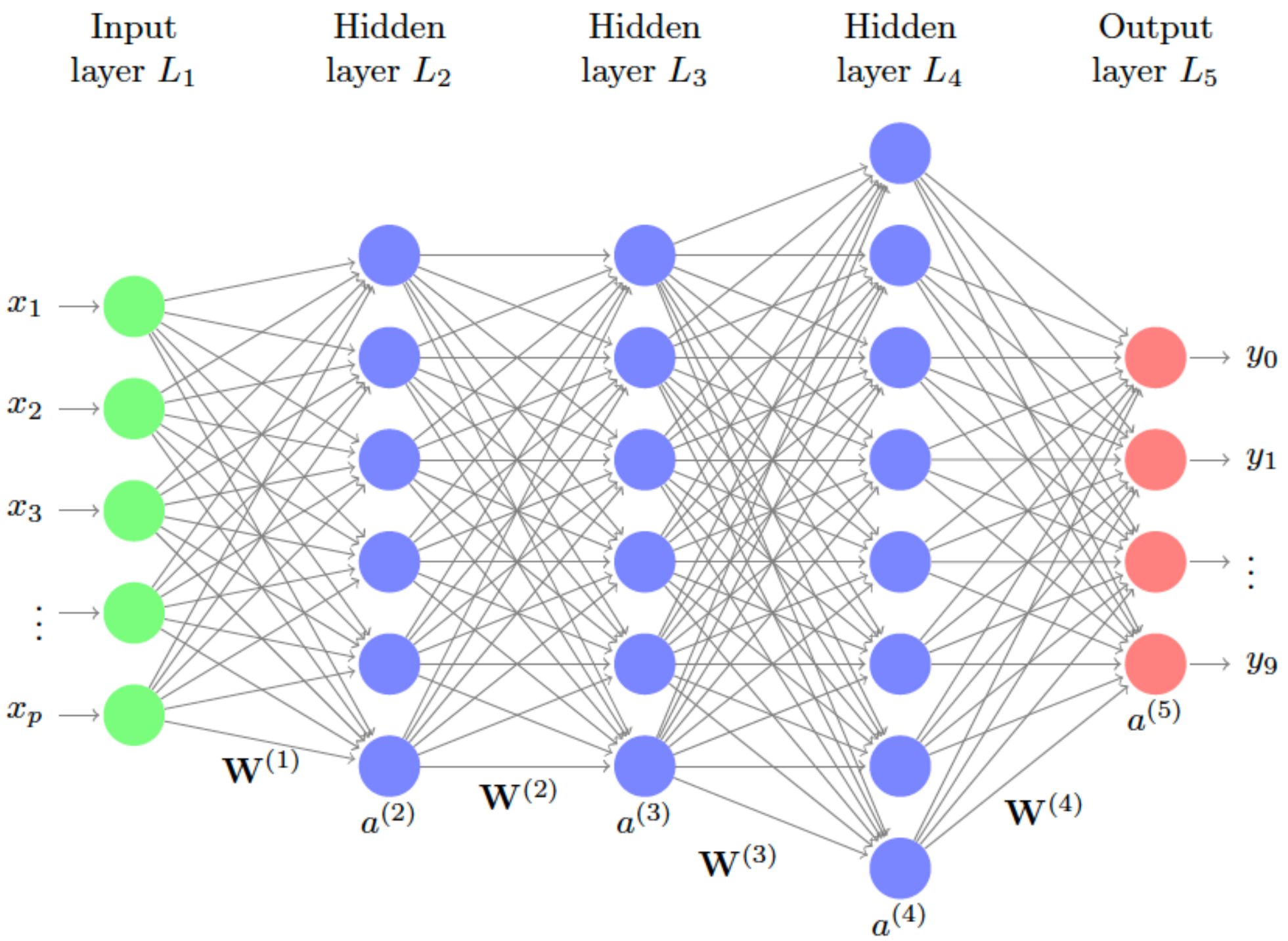

Deep Neural Network in 2018

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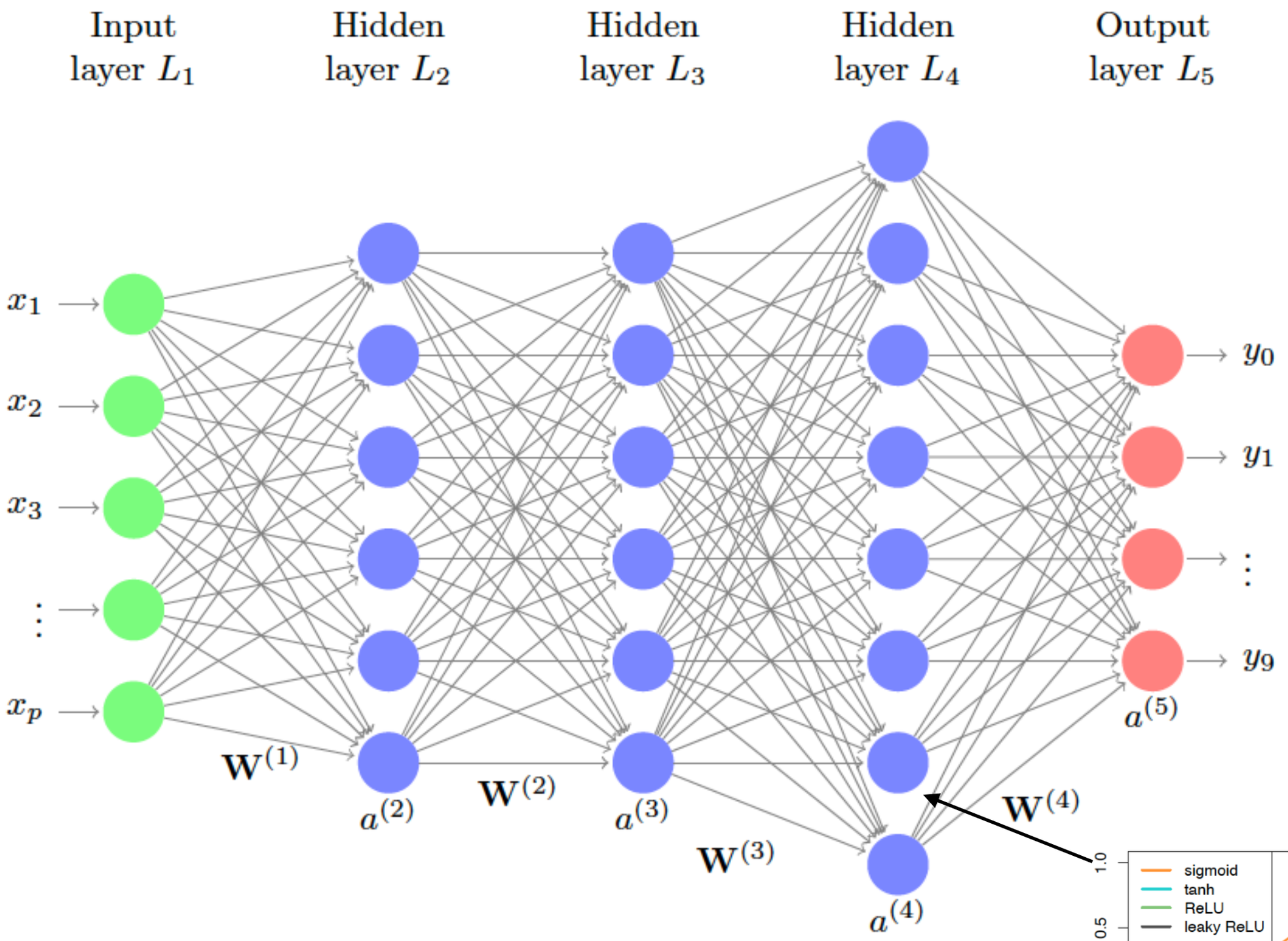

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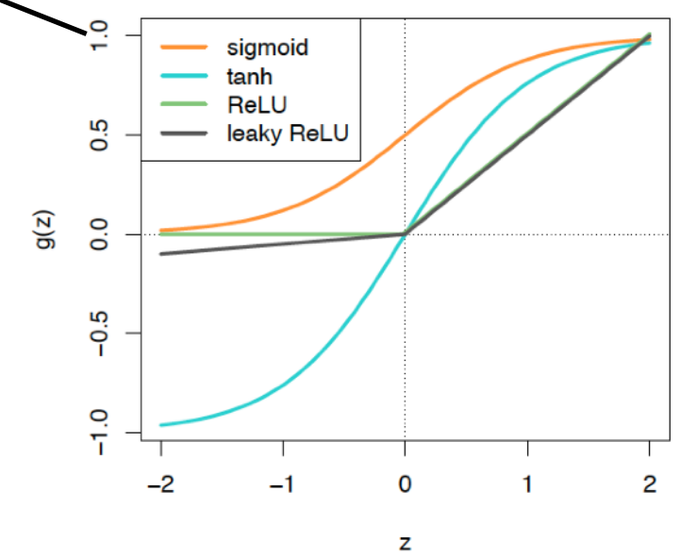

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Example of a Network for Image Recognition

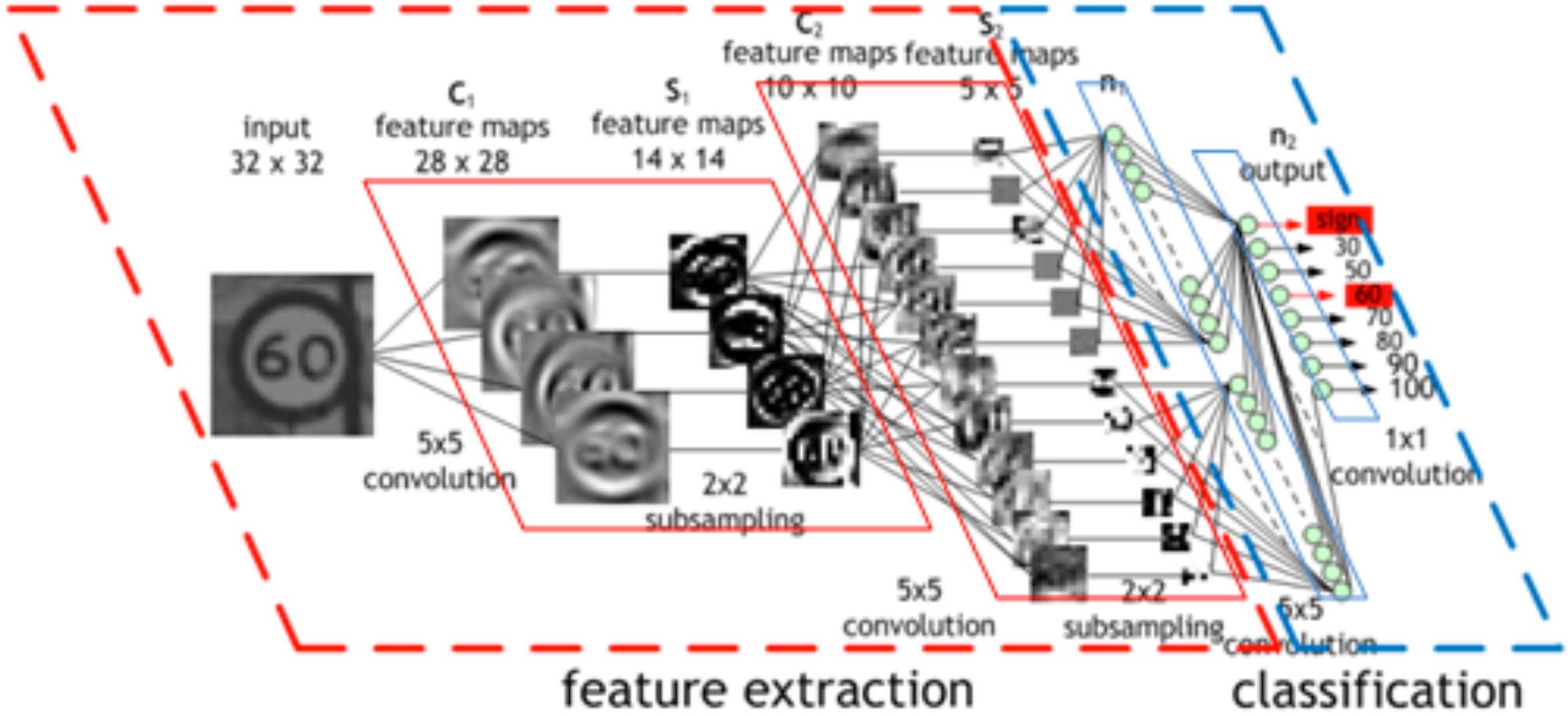
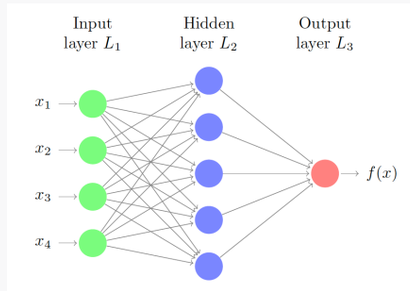


Figure from https://developer.nvidia.com/discover/convolutionalneuralnetwork

How are the Weights Estimated?

Simple Network Model

$$f(\mathbf{x}; \mathbf{W}) = \text{logistic}\left(\sum_{k=1}^{H} w_k^o \; h_k(\mathbf{w}_k^T \mathbf{x}) \right)$$



Model output

Weights/Parameters

Output of kth hidden unit

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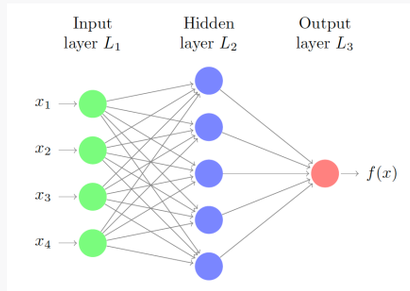

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Optimization Problem

$$\text{minimize}\left\{ -\sum_{i=1}^{N} \log f(\mathbf{x}_i;\mathbf{W}) + \lambda J(\mathbf{W}) \right\}$$

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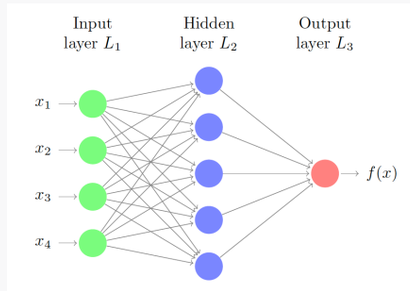

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Negative Conditional Log-likelihood

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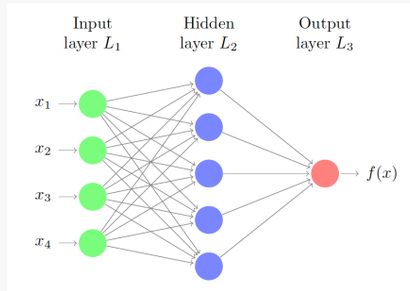

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Regularization -> Log Prior

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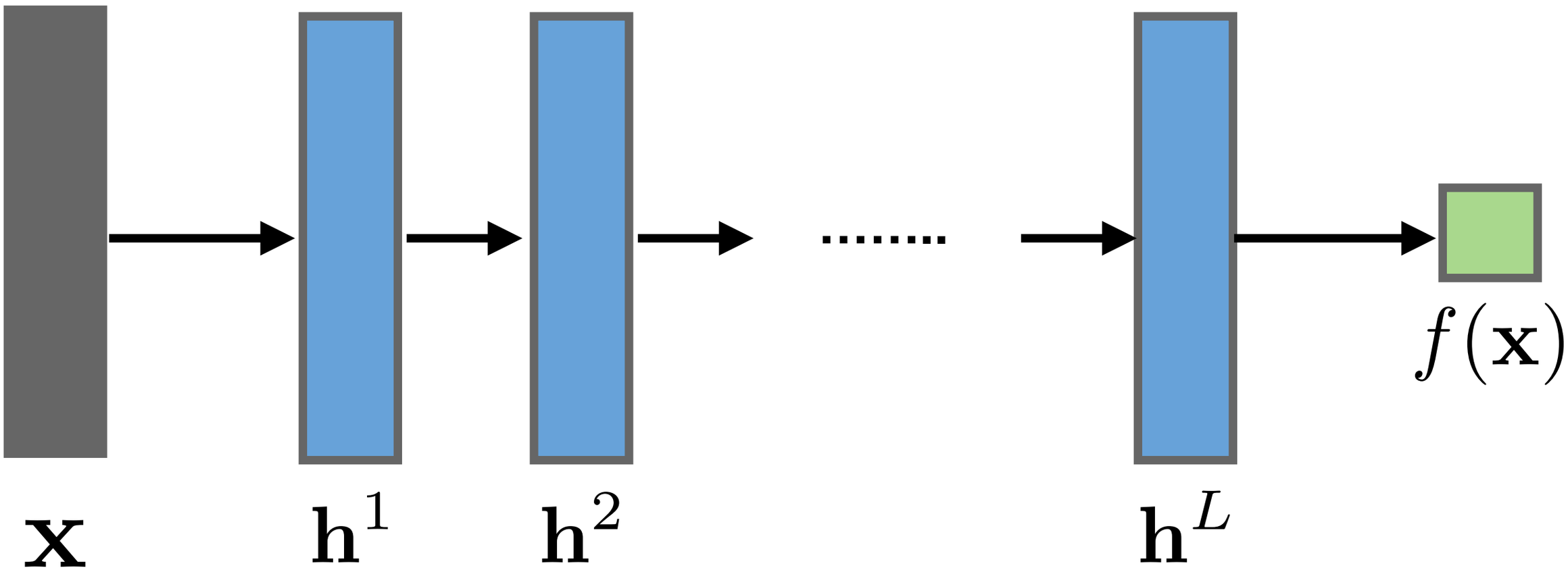
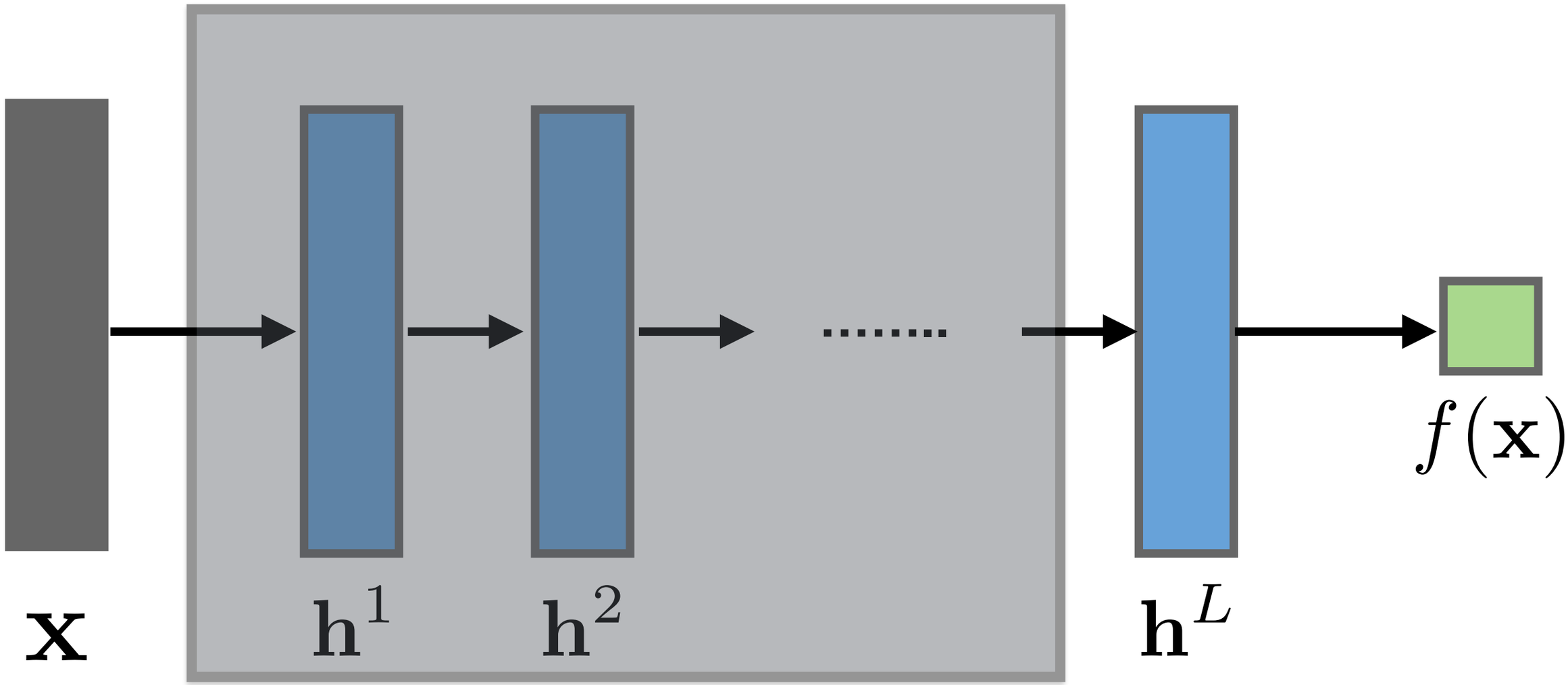
Negative Conditional Log-likelihood

Deep Neural Networks



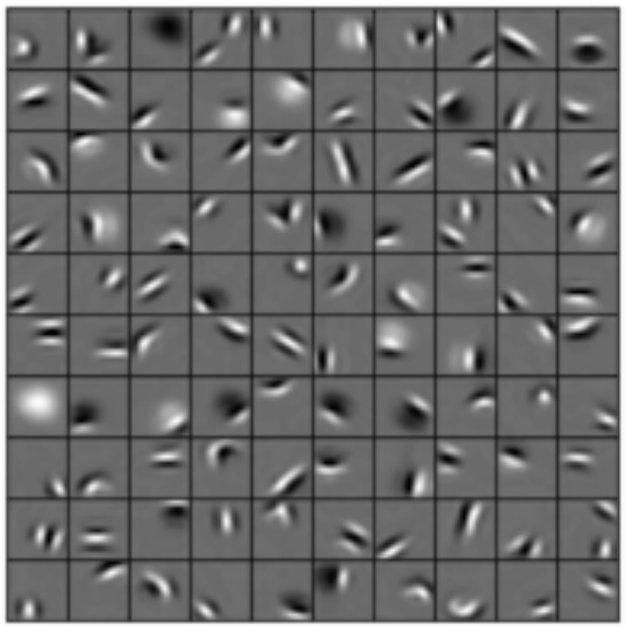
Parameters = matrices of weights between layers

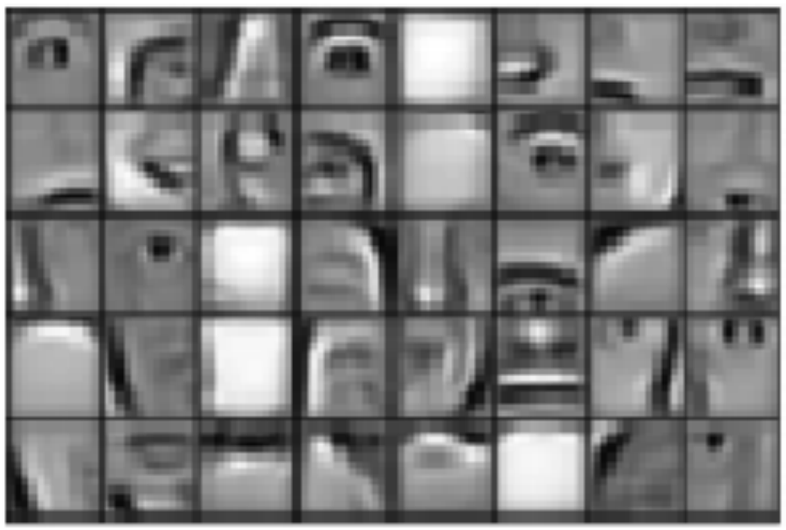
Deep Neural Networks



Feature Extractor **Statistical Model**

What Representations do Networks Learn?



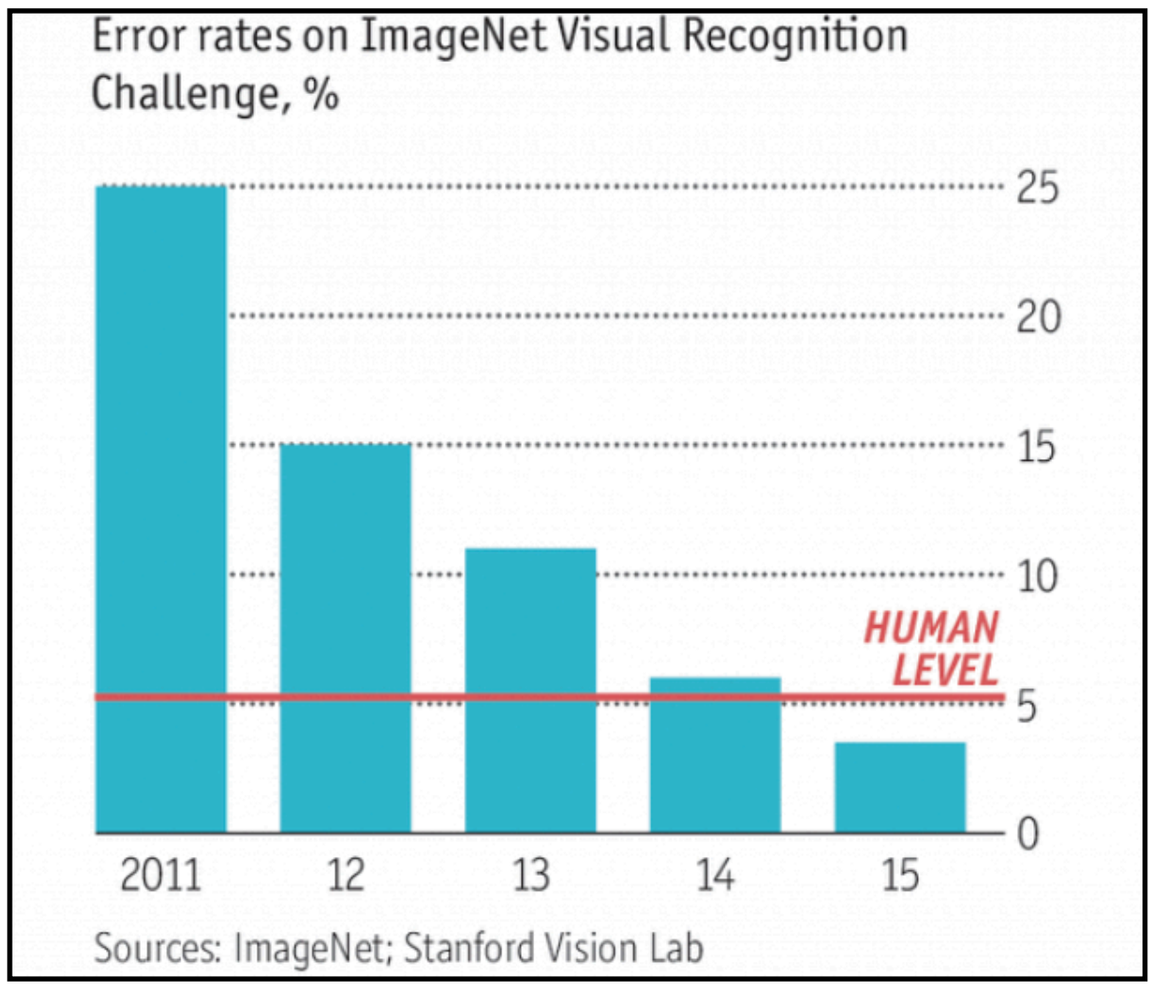


Weight Matrices (or Filters) Learned at Different Layers for Face Detection

Figures from Lee et al, ICML 2009

Deep Learning Results

- **Computer Vision**: Results on ImageNet object classification dataset.



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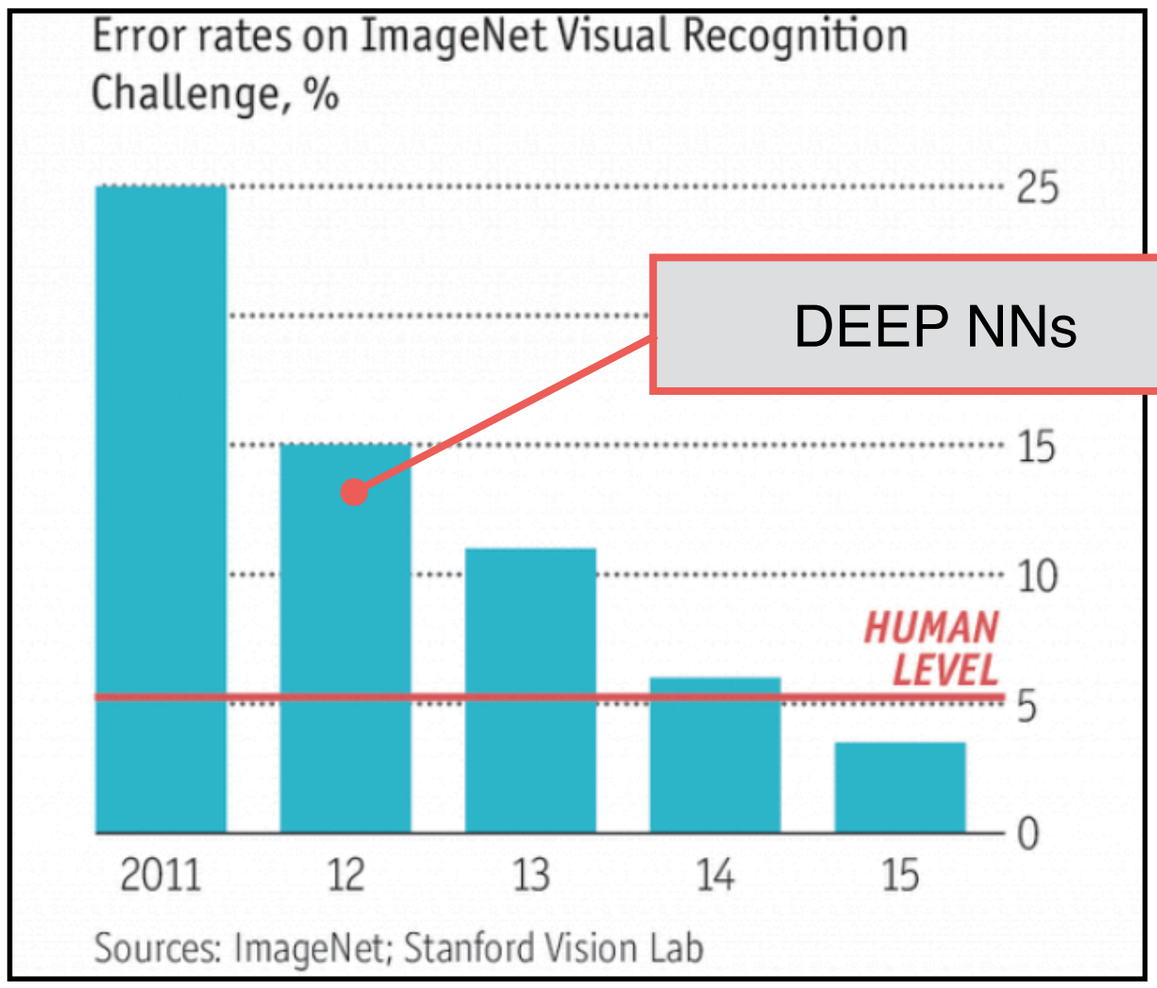

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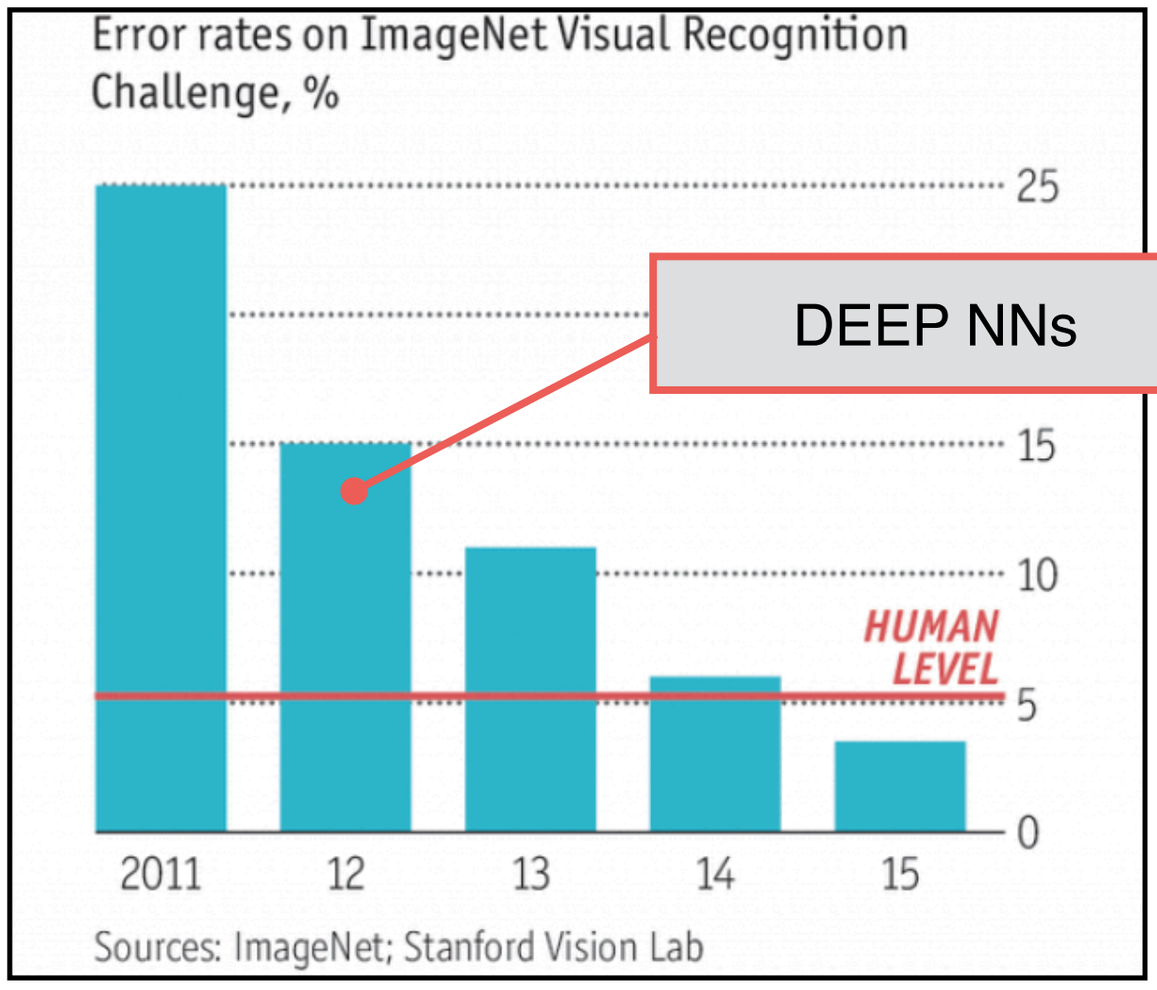

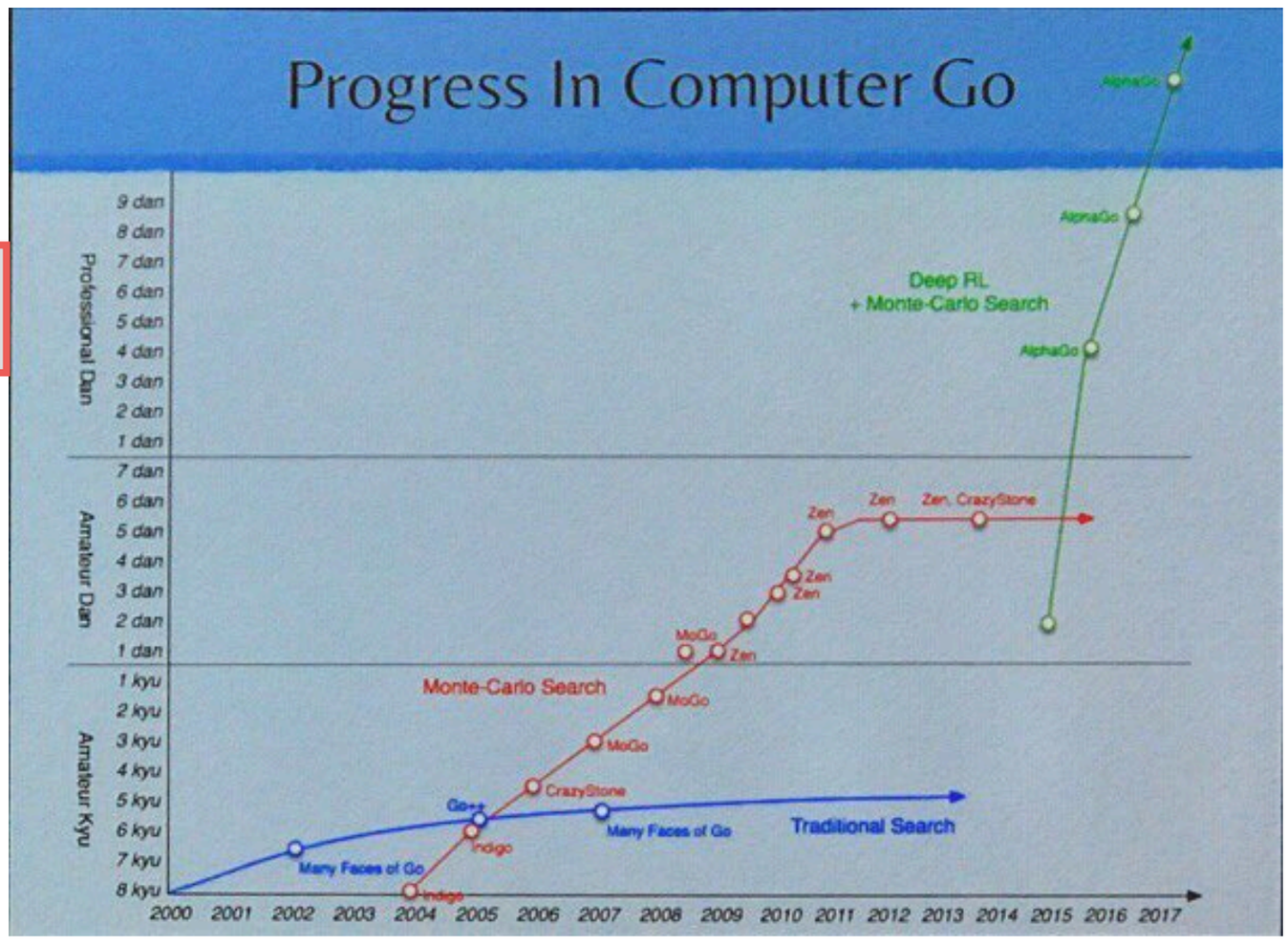

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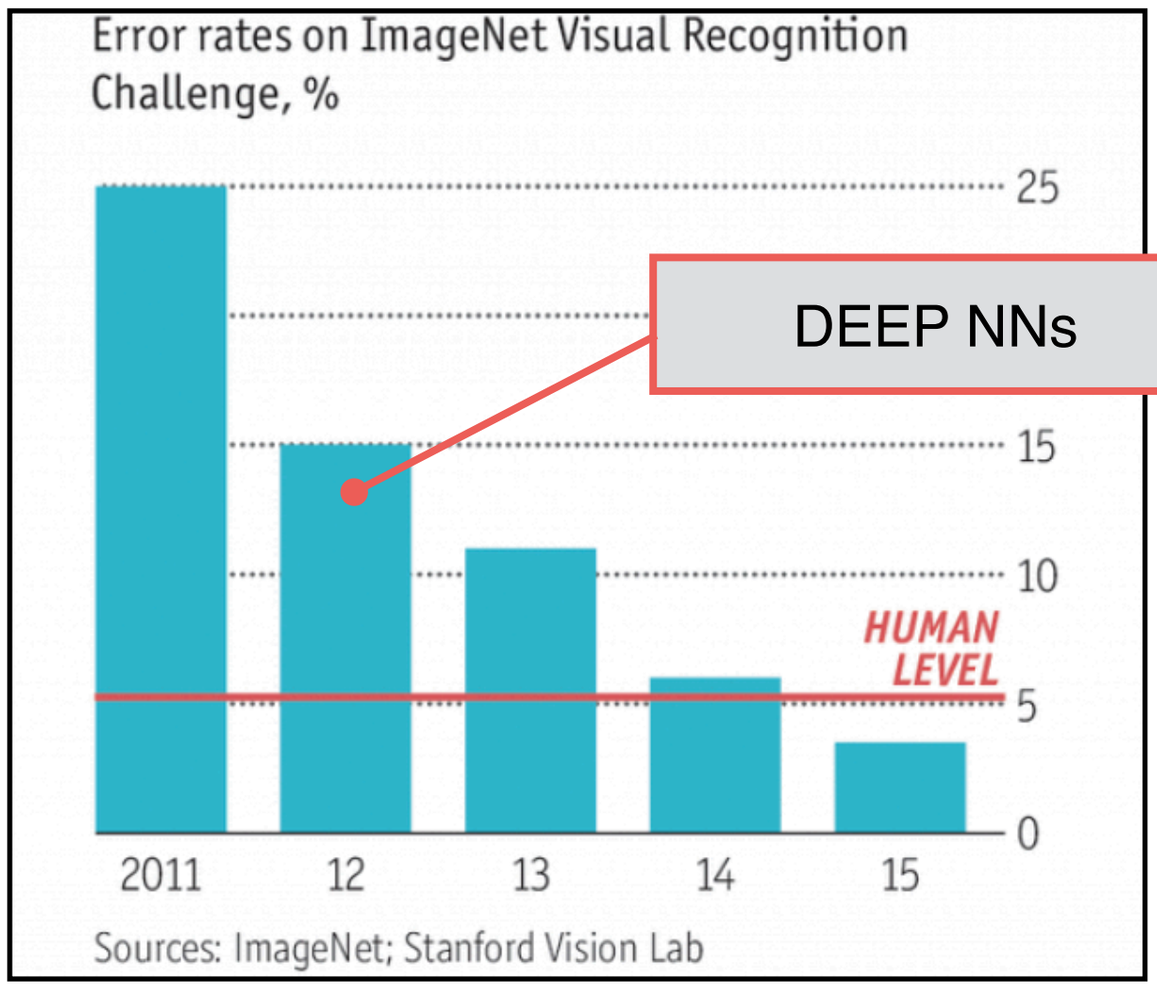

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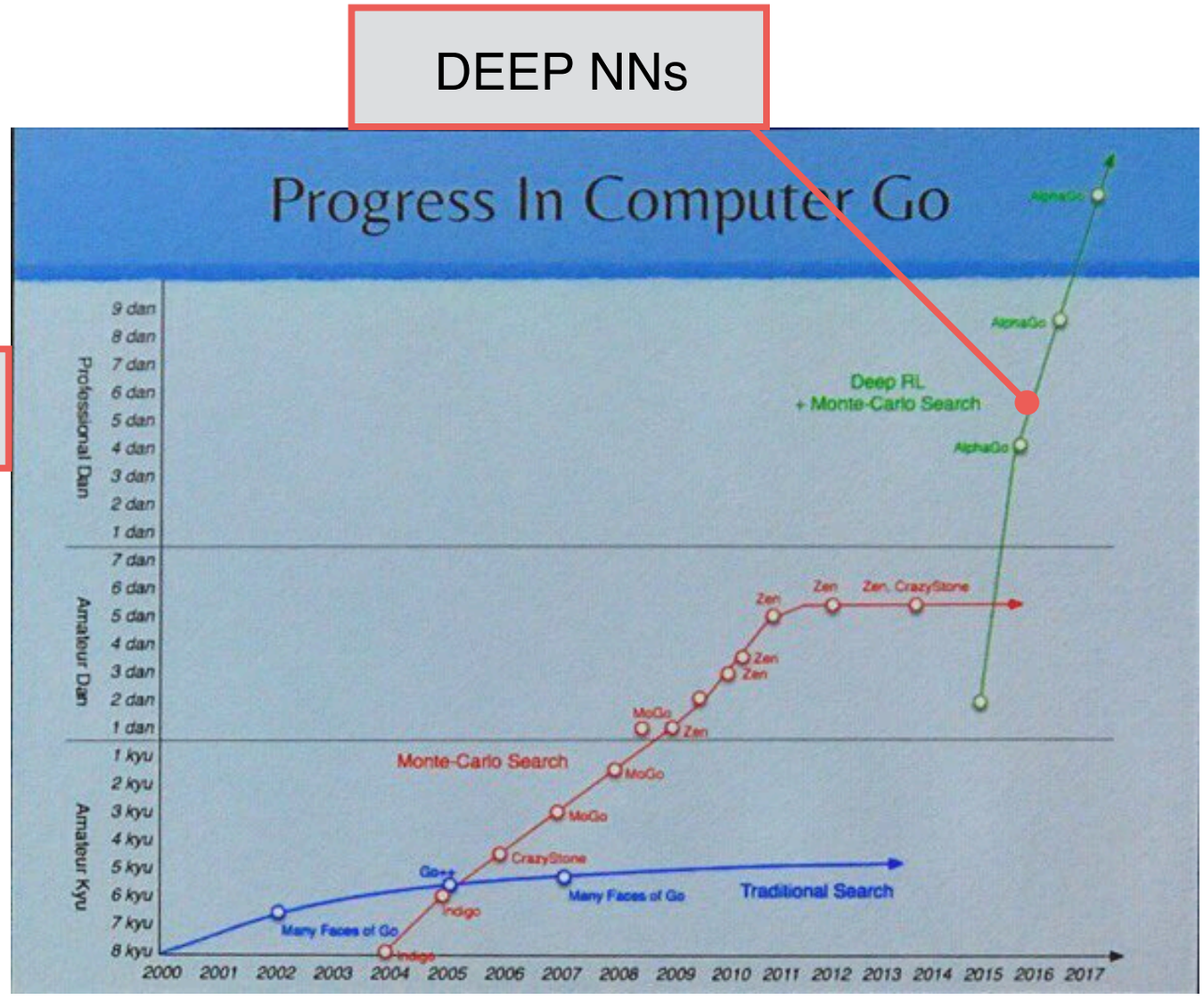

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Some Observations

- **A deep network is a mathematical function with parameters** (in effect a very flexible non-linear regression model)
- **The hidden layers act as latent feature extractors** - but they are deterministic, no distributional semantics (unlike statistical models)

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- [ ] **The hidden layers act as latent feature extractors** - but they are deterministic, no distributional semantics (unlike statistical models)

- [ ] **There can be millions of parameters**: But these are not parameters in a traditional statistical sense. Focus is typically on prediction, not parameter interpretation

- [ ] **The parameters are estimated by minimizing a loss function** - often equivalent to a negative conditional log-likelihood

More Observations

- **Often need very large amounts of labeled training data**
  (N ~ millions)

- **Significant "engineering" to get these models to work:**
  - model structure
  - hyperparameter tuning
  - optimization algorithms

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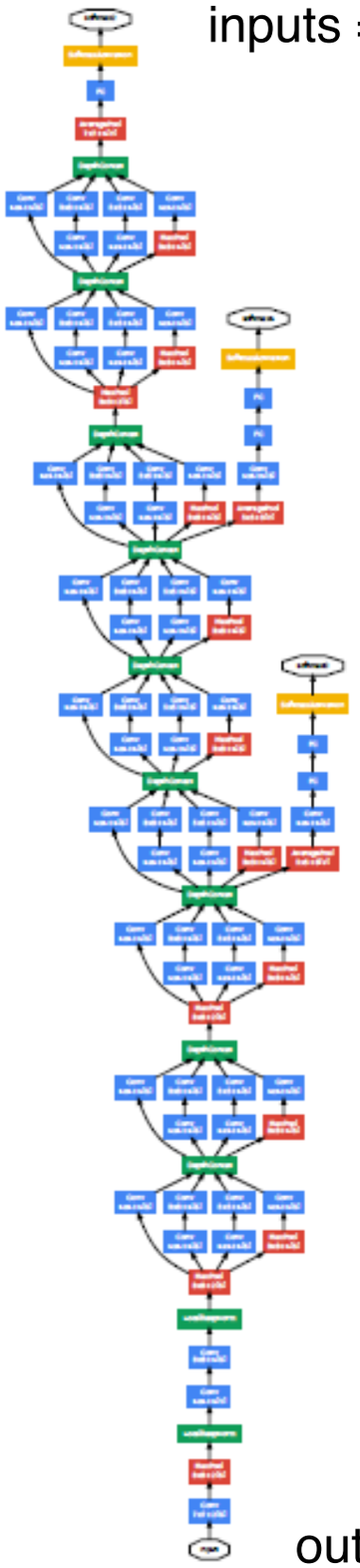
- **Many of the success stories have been in "pattern recognition":**
  - large amounts of labeled data
  - inputs are high-dimensional, need feature extraction (e.g., pixels)
  - model interpretability is not a priority
  - image analysis, speech recognition, text analysis

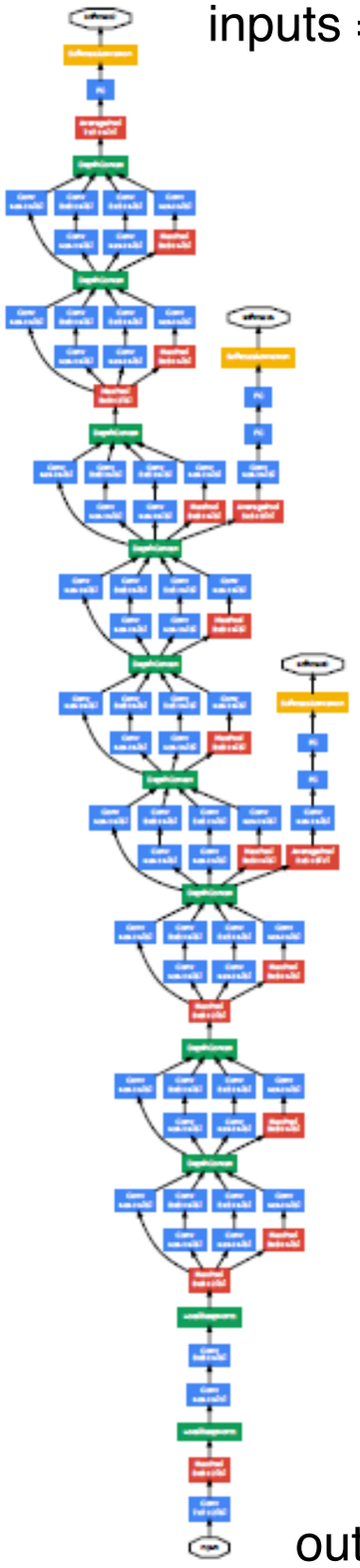
inputs = pixels



Deep network (from Google)
with 27 layers
for image recognition

outputs = P(class I pixels)

Figure from Szegedy et al, CVPR, 2015



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Rube Goldberg machine

From www.cartoonaday.com

Figure from Szegedy et al, CVPR, 2015

We need principled approaches…

https://xkcd.com/1838/

Outline of Remainder of Talk

1. Neural Networks and Generalized Linear Models
2. Model Fitting via Gradient-Based Optimization
3. Autoencoders and Factor Analysis
4. Recurrent Networks and State-Space Models
5. Open Problems and Summary

Building Neural Nets from GLMs

Generalized Linear Models (GLMs)

$$\mathbf{x}_i \in \mathbb{R}^d, \mathbf{w} \in \mathbb{R}^d, b \in \mathbb{R}$$

Link Function

$$g^{-1}(\mathbf{x}_i^T \mathbf{w} + b) = \mathbb{E}[\mathbf{y}_i | \mathbf{x}_i]$$

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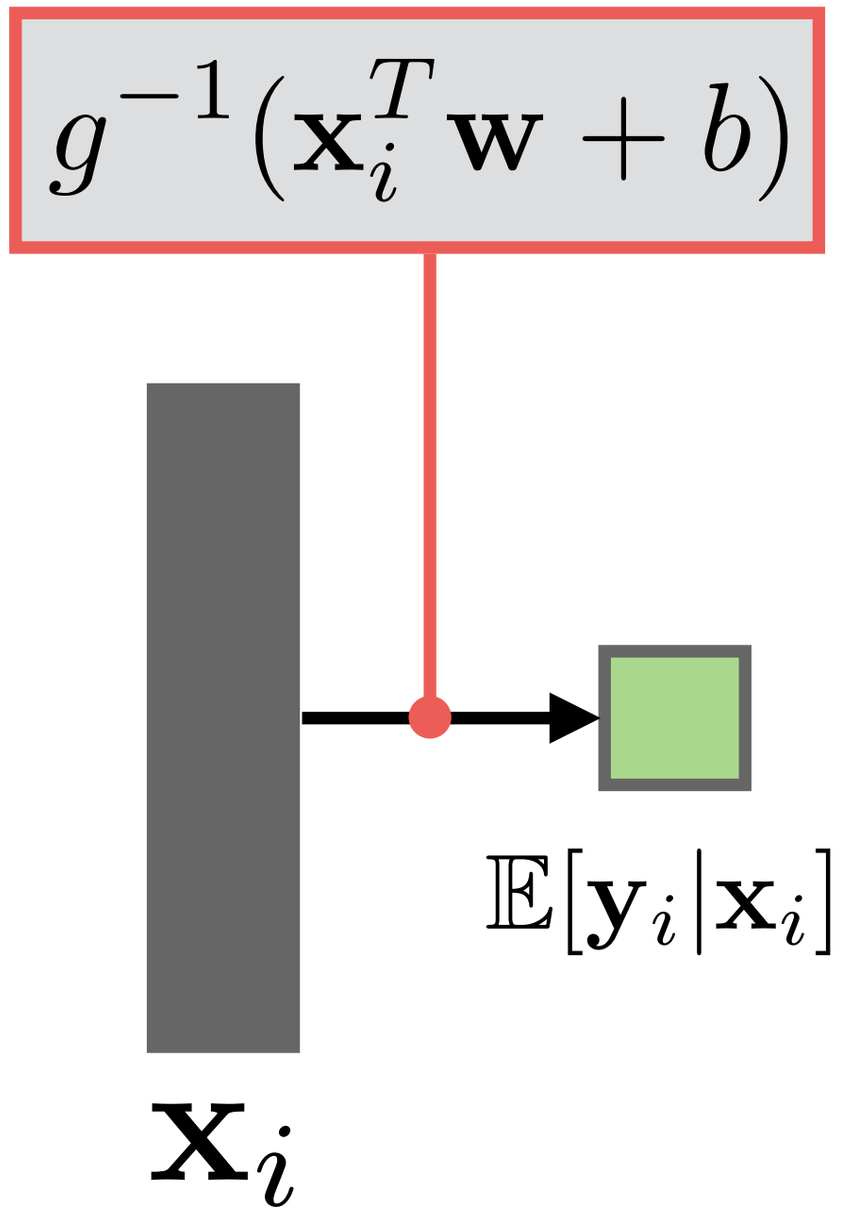
Example: Logistic Regression

$$\mathbf{y}_i \in \{0, 1\} \qquad g^{-1}(z) = \frac{1}{1 + e^{-z}}$$

THE LOGISTIC FUNCTION

Generalized Linear Models (GLMs)



Recursive GLMs

Define a latent feature via a GLM:

$$g_1^{-1}(\mathbf{x}_i^T \mathbf{w}_1 + b_1) = h_i$$

[Mohamed, 2015]

Recursive GLMs

Define a latent feature via a GLM:

$$g_1^{-1}(\mathbf{x}_i^T \mathbf{w}_1 + b_1) = h_i$$

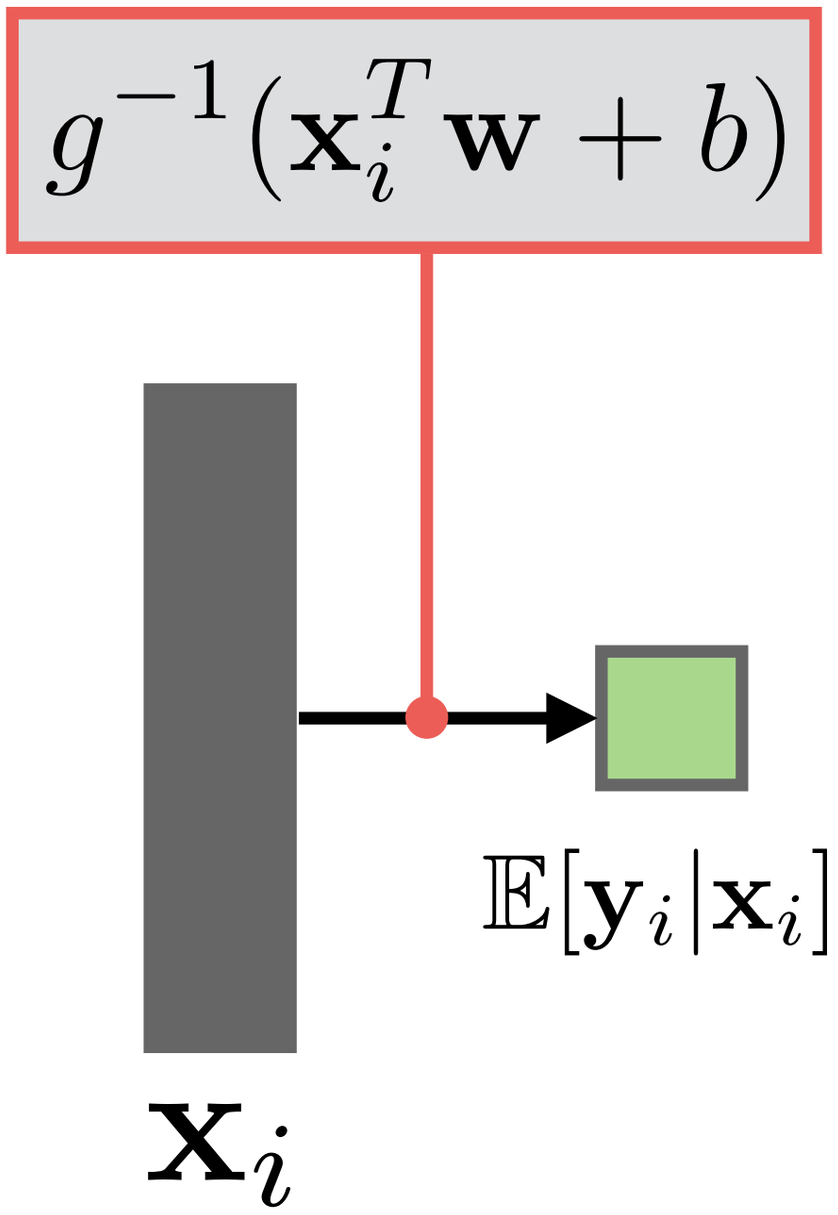
Define GLM on latent feature:

$$g_2^{-1}(h_i w_2 + b_2) = \mathbb{E}[\mathbf{y}_i | \mathbf{x}_i]$$

$$w_2 \in \mathbb{R}, b_2 \in \mathbb{R}$$

[Mohamed, 2015]

Recursive GLMs



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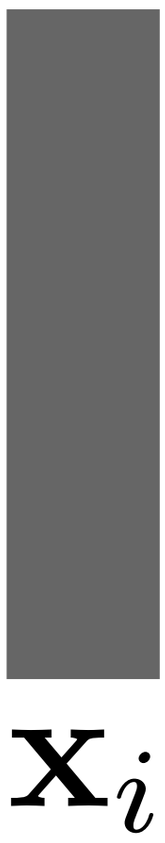

$\mathbf{x}_i$

$\mathbb{E}[\mathbf{y}_i|\mathbf{x}_i]$

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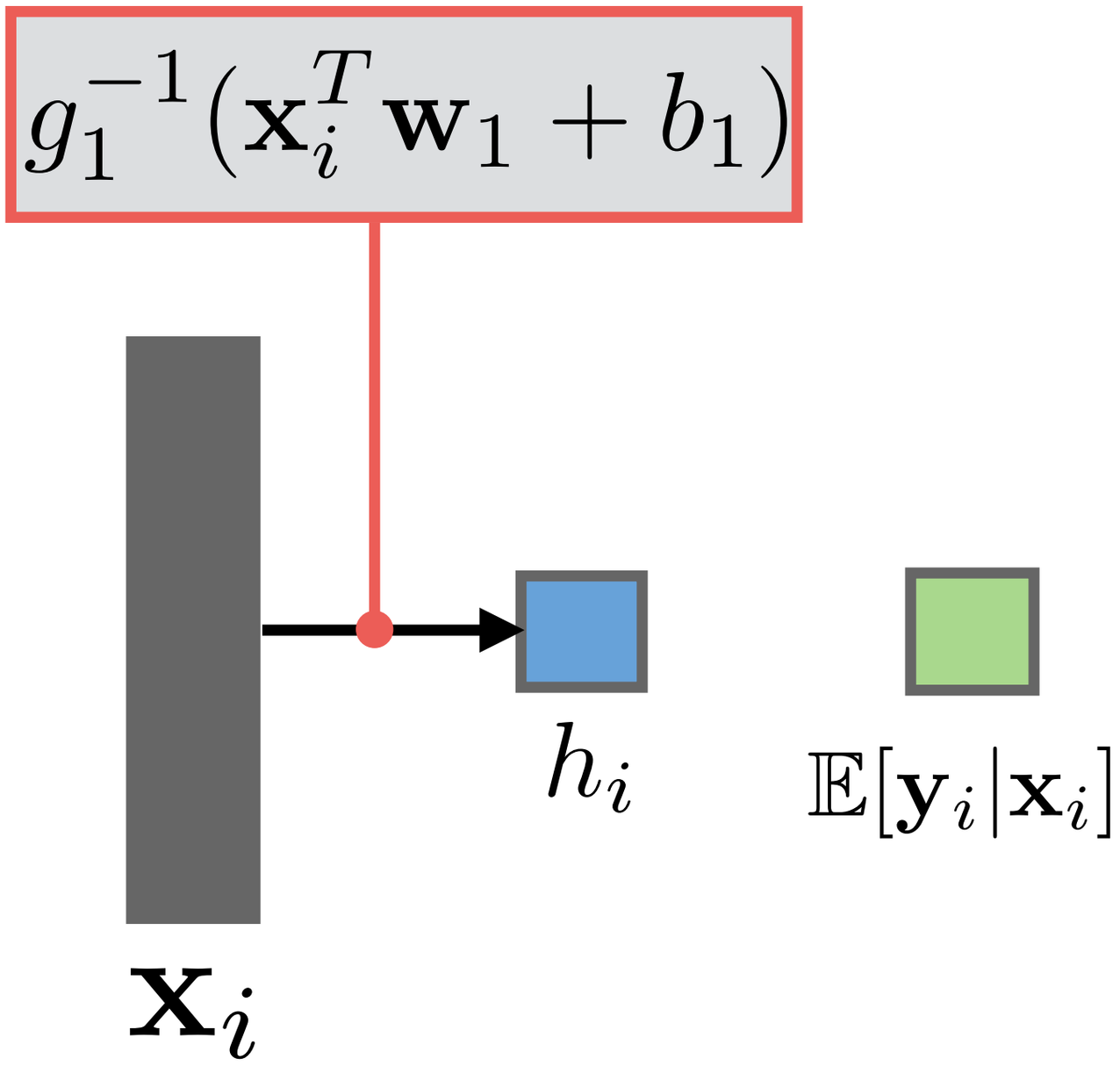

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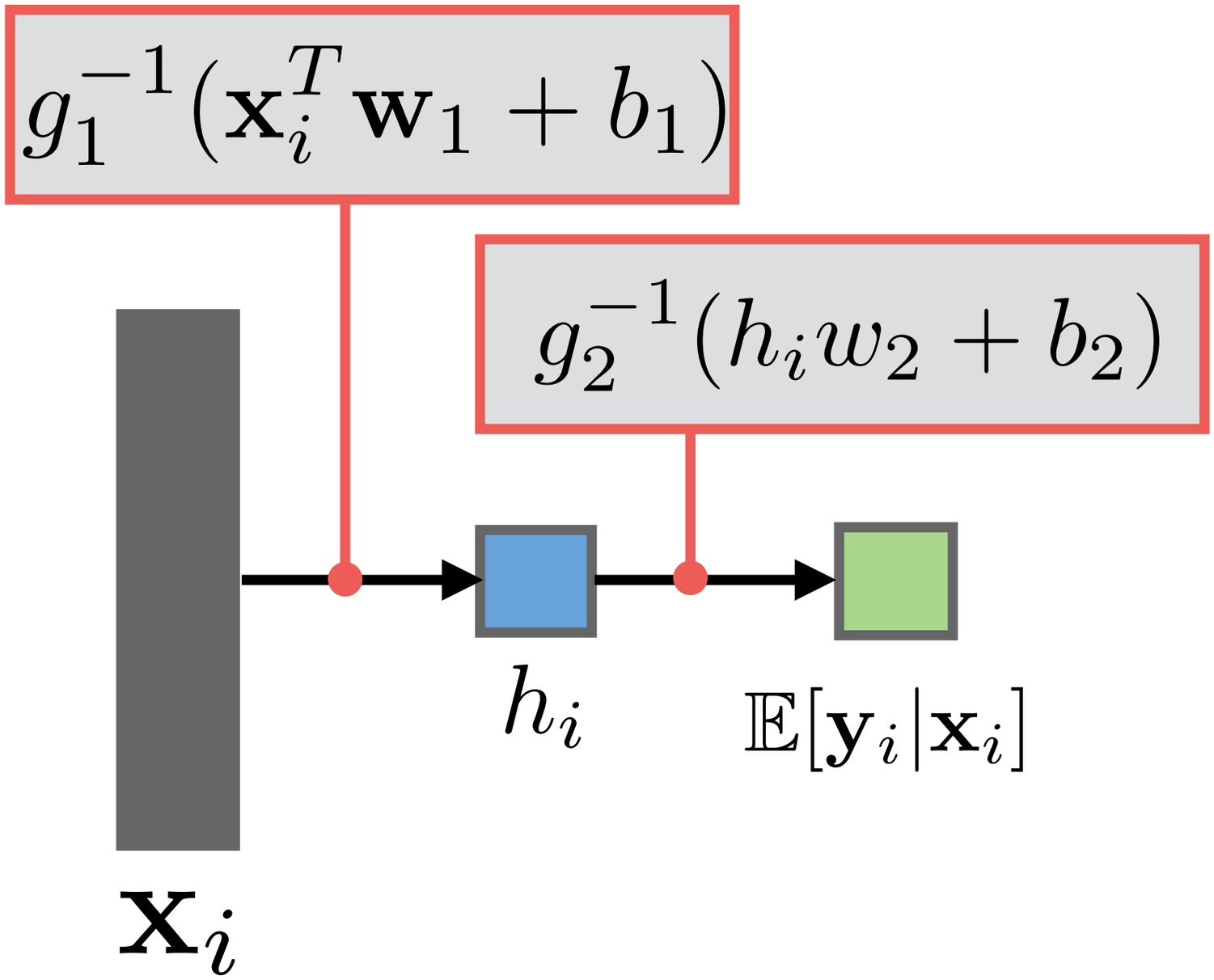

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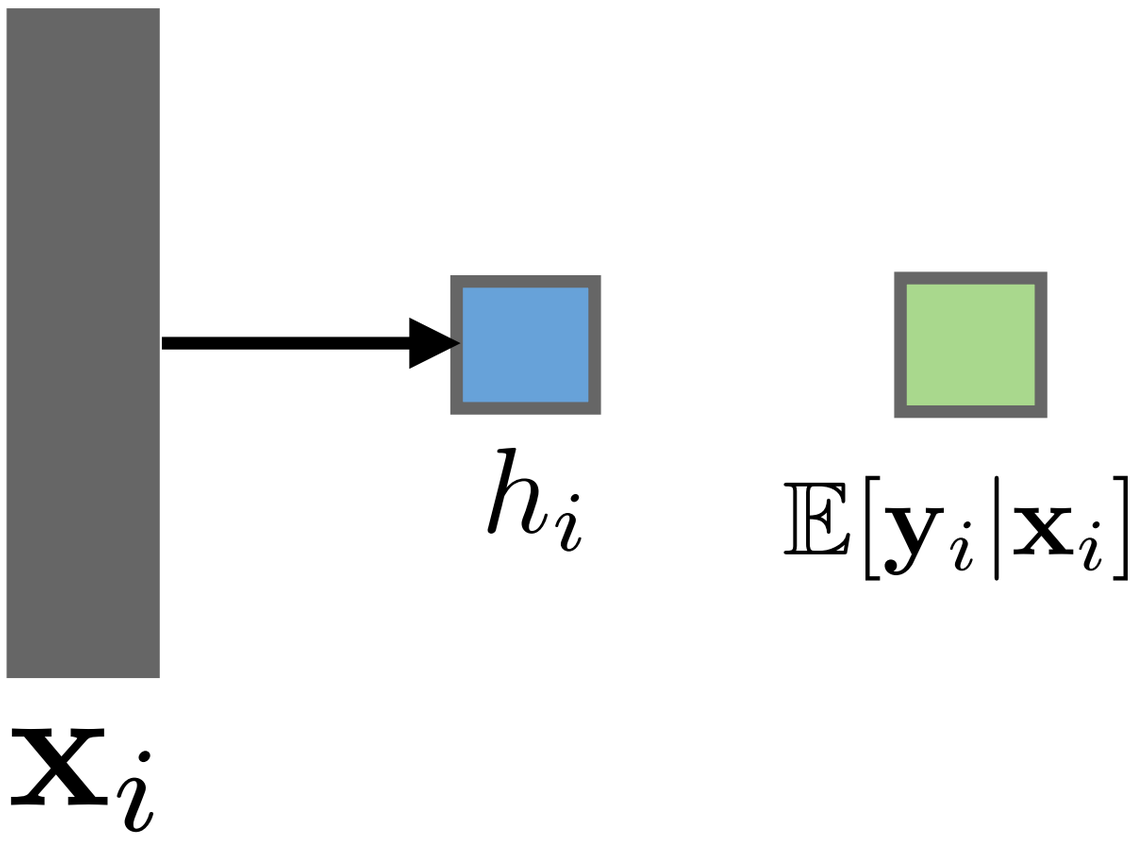
Building Neural Nets from Recursive GLMs



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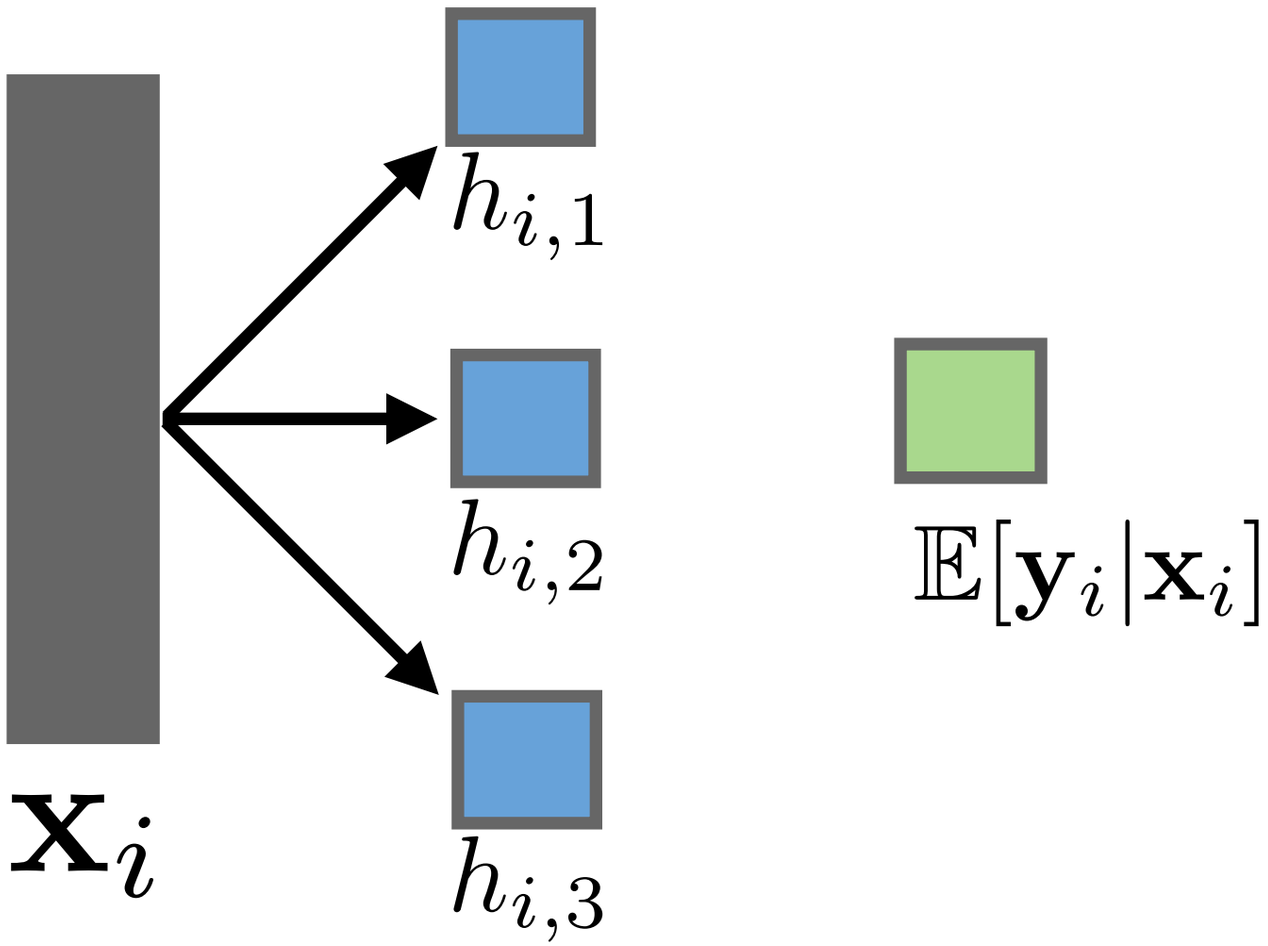

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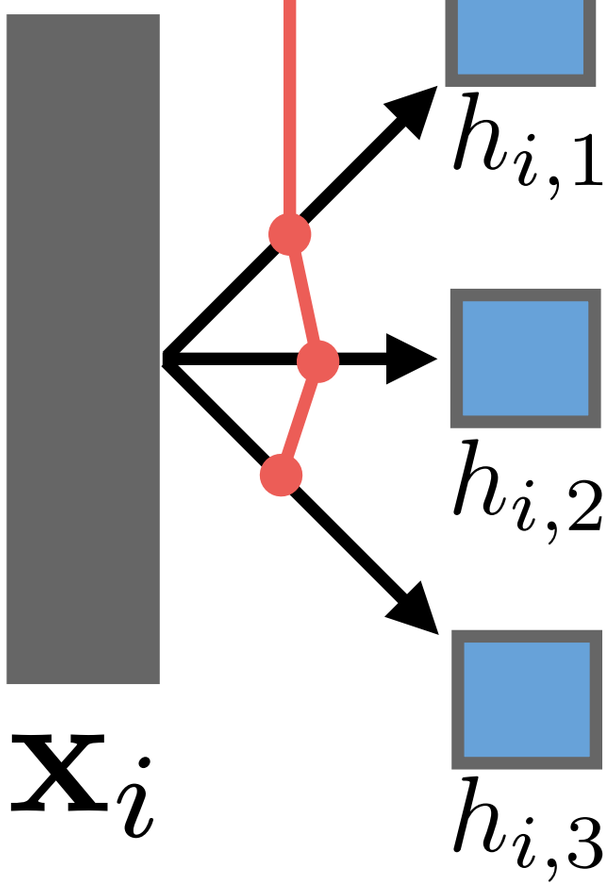

$\mathbb{E}[\mathbf{y}_i|\mathbf{x}_i]$

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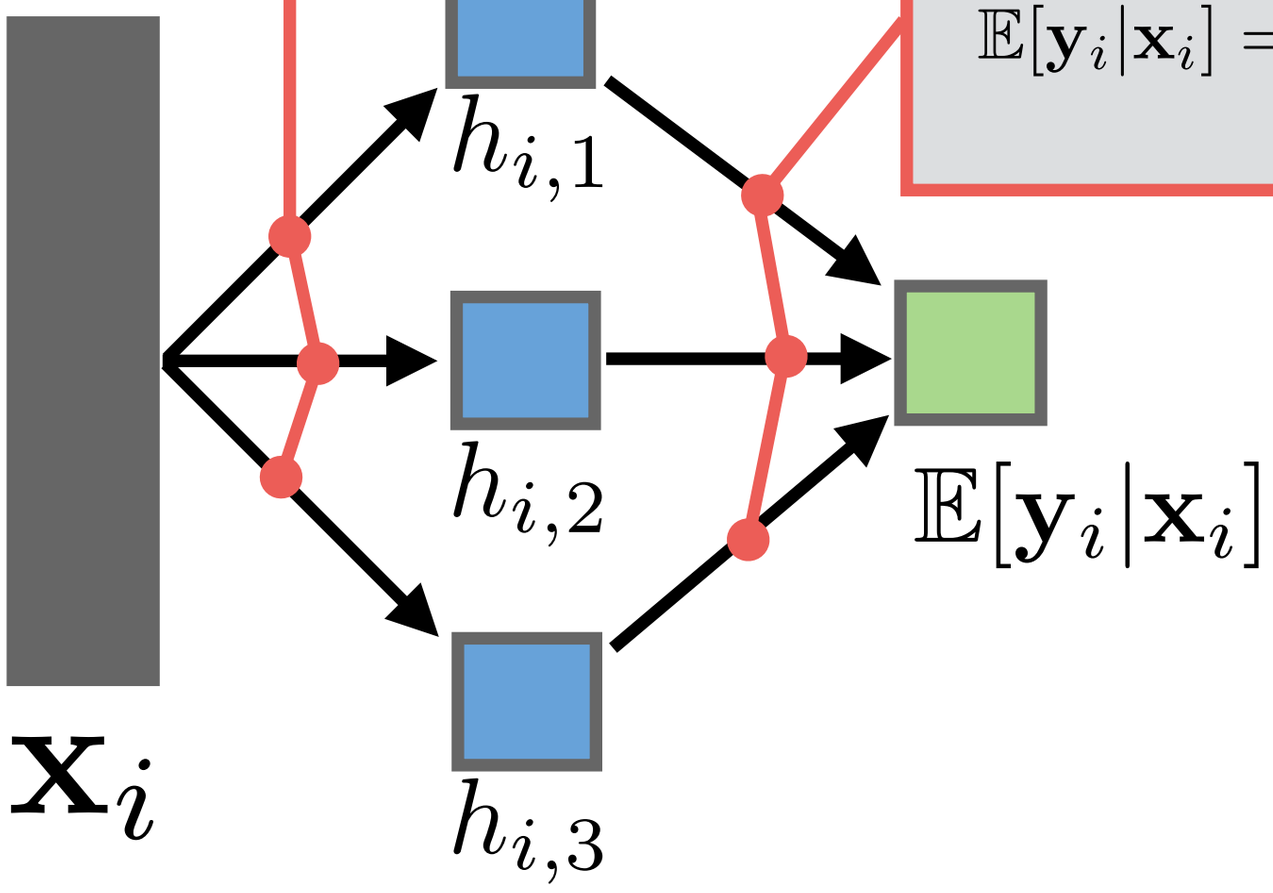


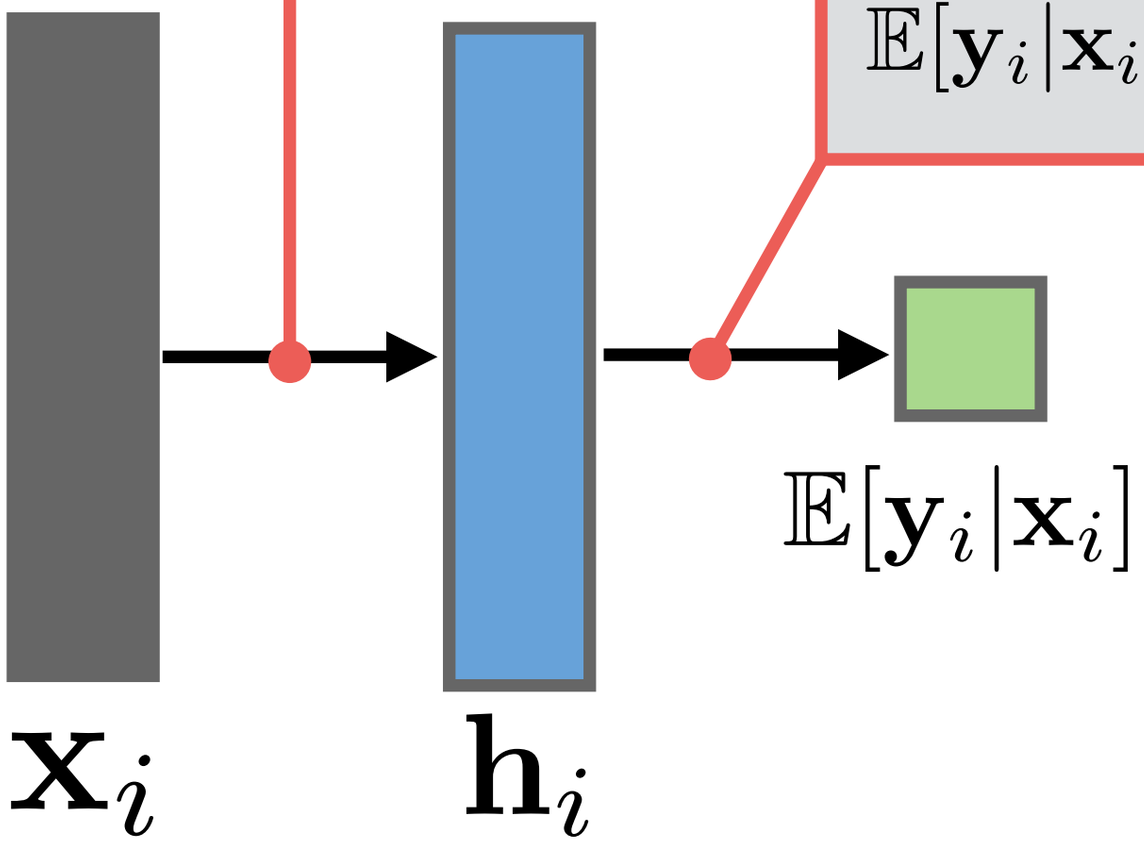
[Mohamed, 2015]

Building Neural Nets from Recursive GLMs

$\mathbf{h}_i \in \mathbb{R}^H, \mathbf{W}_1 \in \mathbb{R}^{d \times H}, \mathbf{b}_1 \in \mathbb{R}^H$

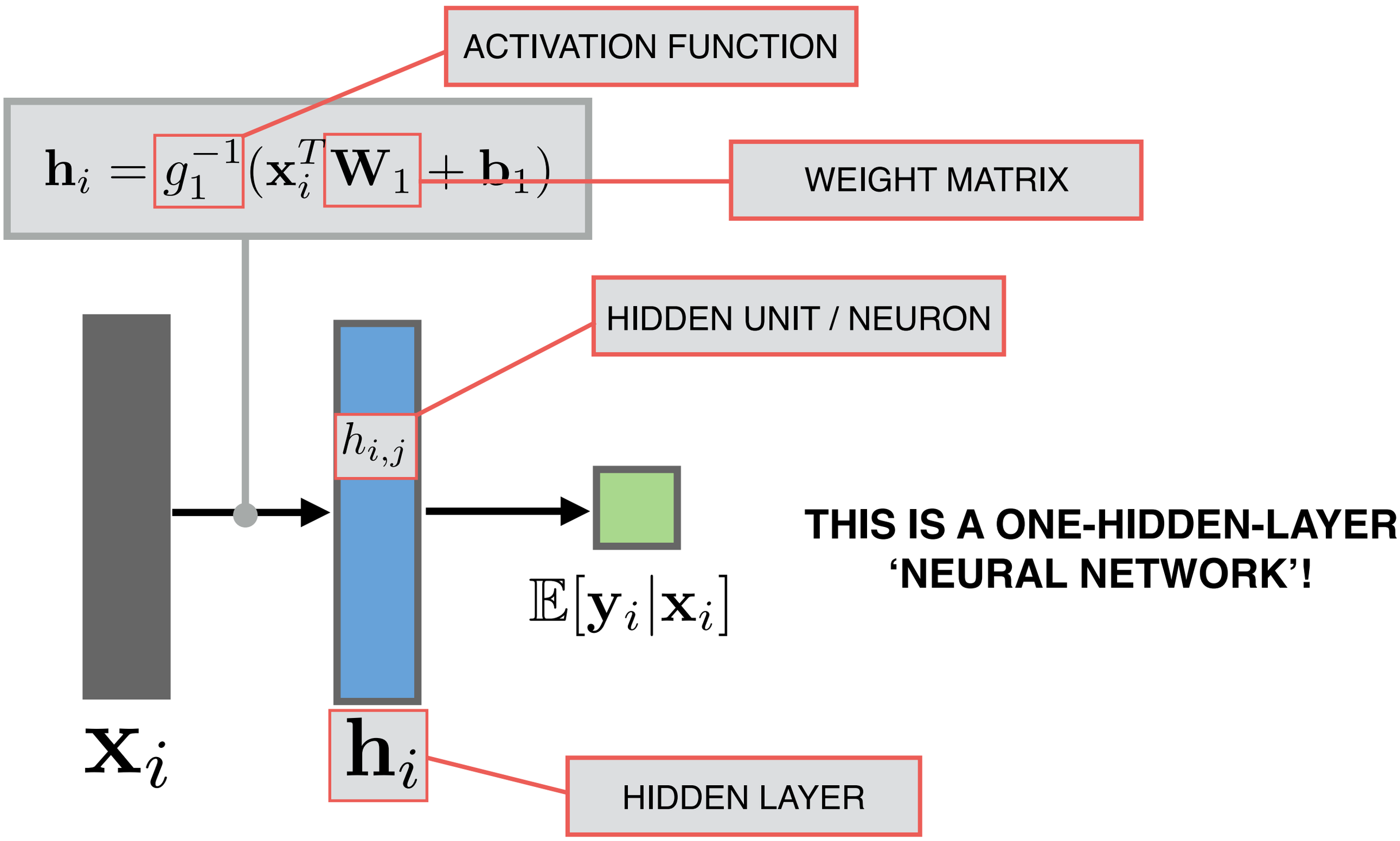
$$\mathbf{h}_i = g_1^{-1}(\mathbf{x}_i^T \mathbf{W}_1 + \mathbf{b}_1)$$

$$\mathbb{E}[\mathbf{y}_i|\mathbf{x}_i] = g_2^{-1}(\mathbf{h}_i \mathbf{w}_2 + b_2)$$



THIS IS A ONE-HIDDEN-LAYER ‘NEURAL NETWORK’!

Building Neural Nets from Recursive GLMs



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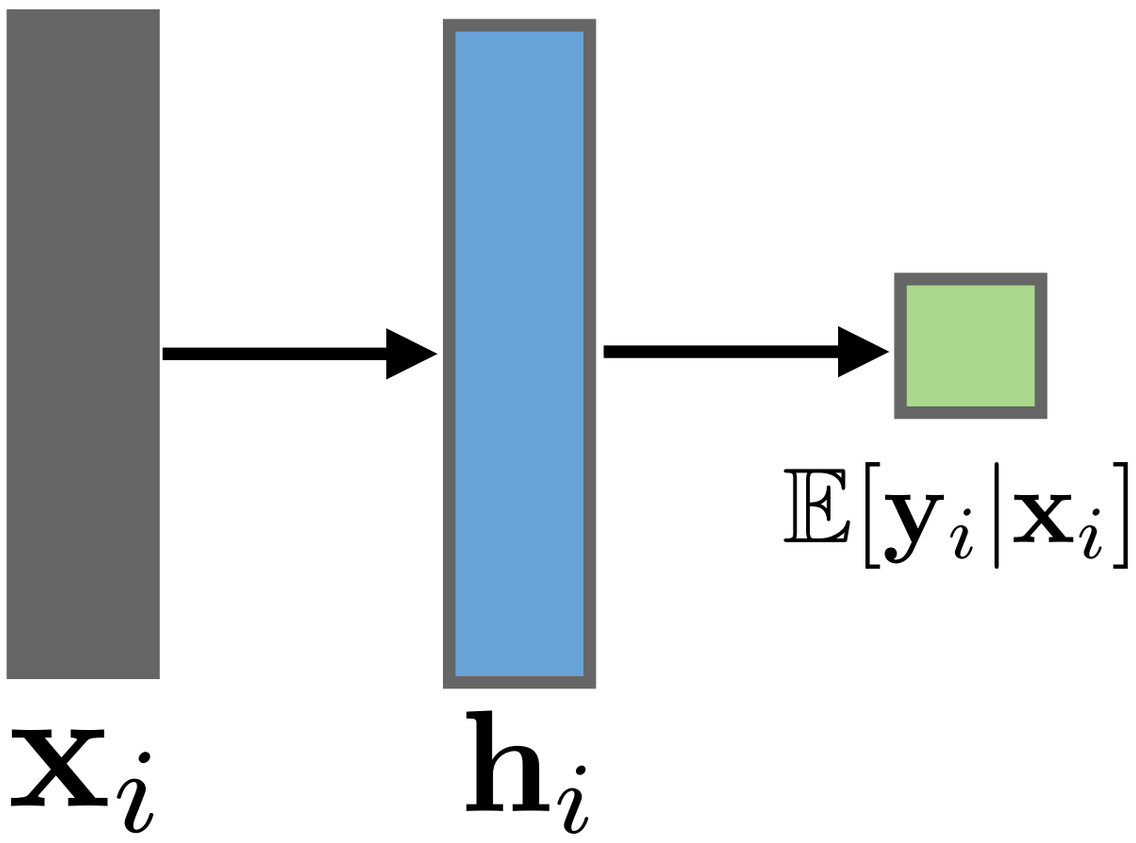
Deep Neural Networks



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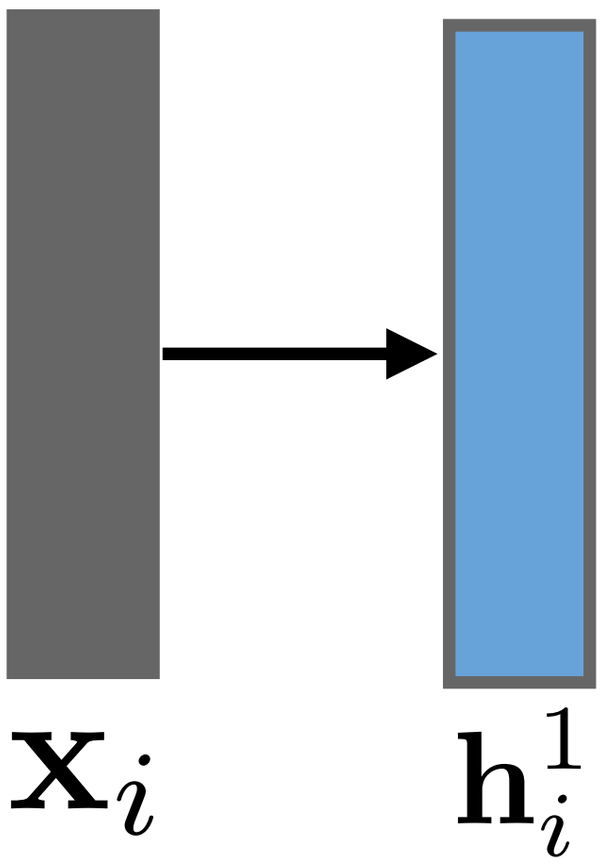

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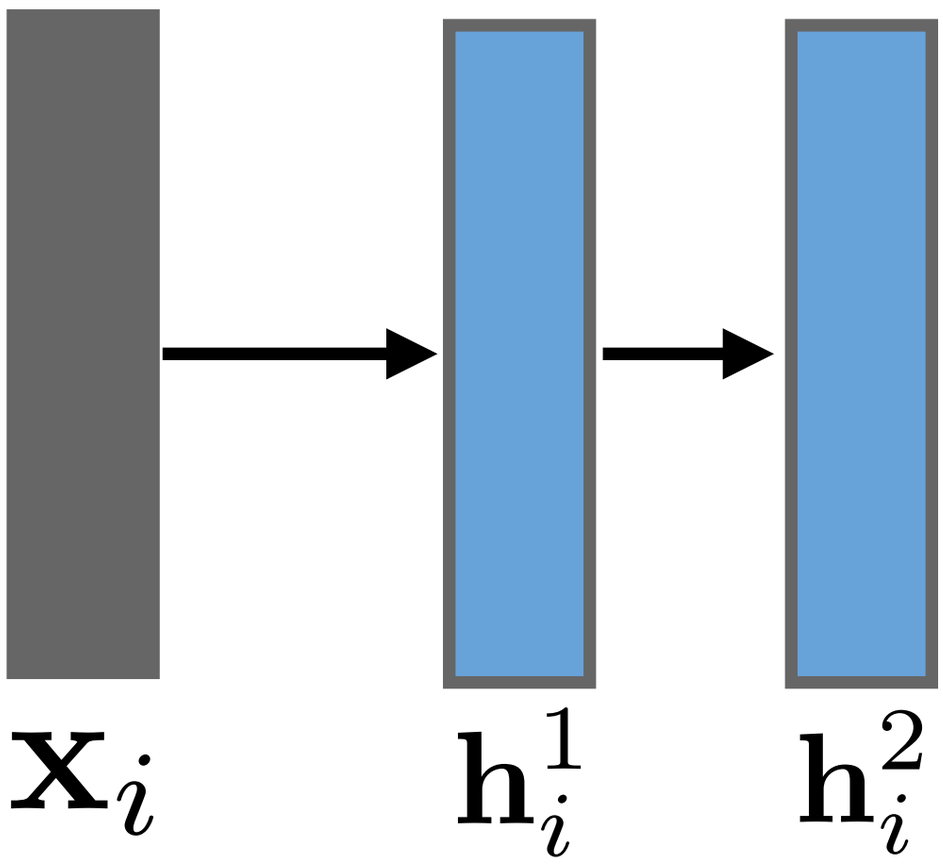

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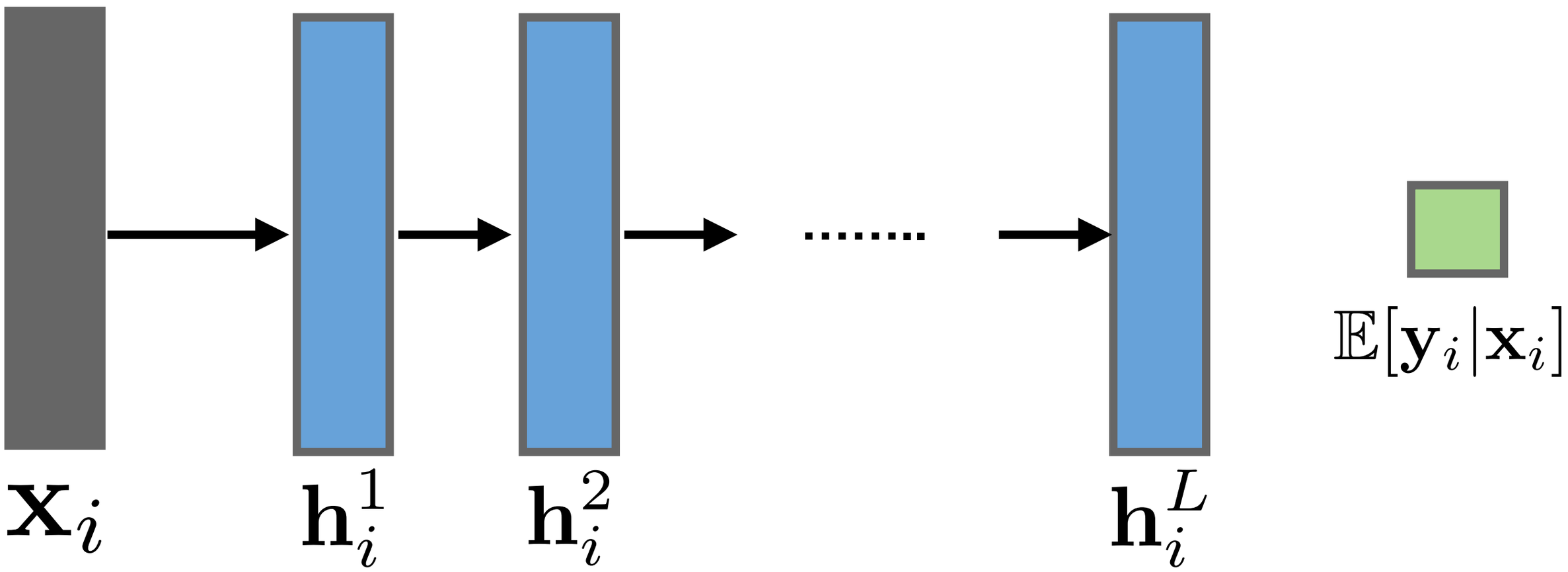
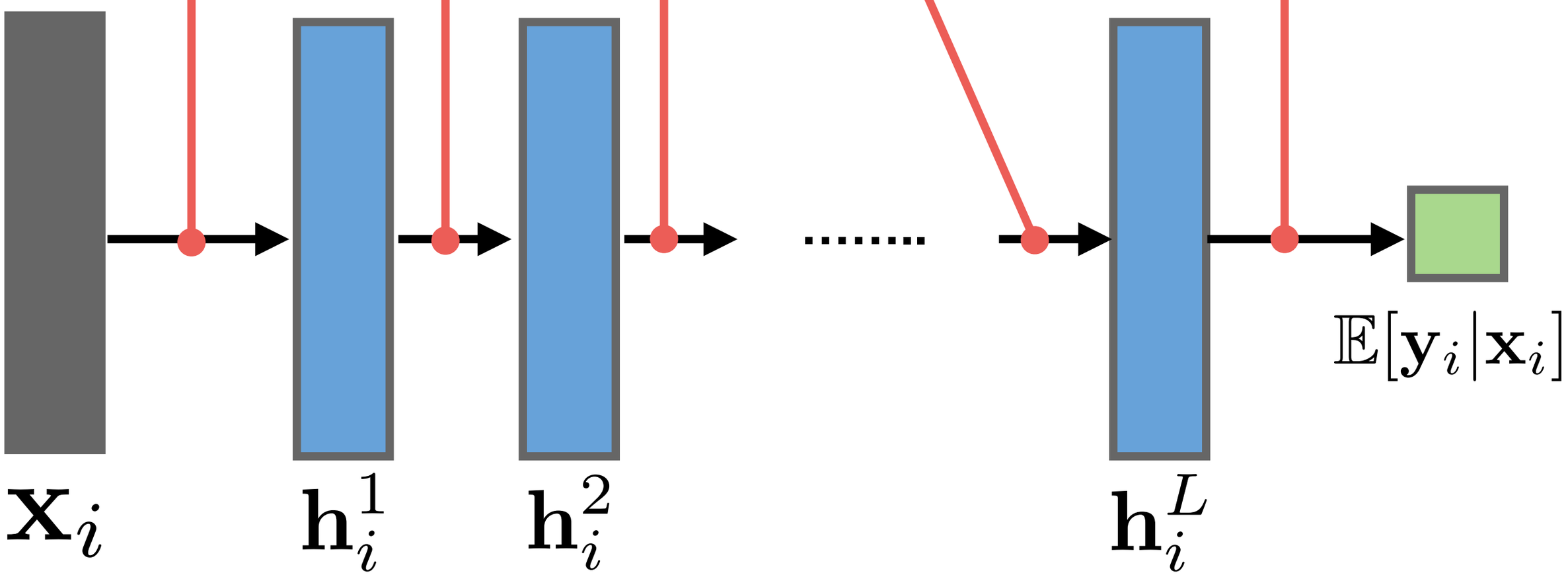


Deep Neural Networks

$$\mathbf{h}_i^l = f_l(\mathbf{h}_i^{l-1}\mathbf{W}_l + \mathbf{b}_l), \quad \mathbf{h}_i^0 = \mathbf{x}_i$$

$$\mathbb{E}[\mathbf{y}_i|\mathbf{x}_i] = g^{-1}(\mathbf{h}_i^L\mathbf{w}_o + b_o)$$



Deep Neural Networks

Adaptive Basis Function Regression: Neural networks are just performing regression with adaptive basis functions.

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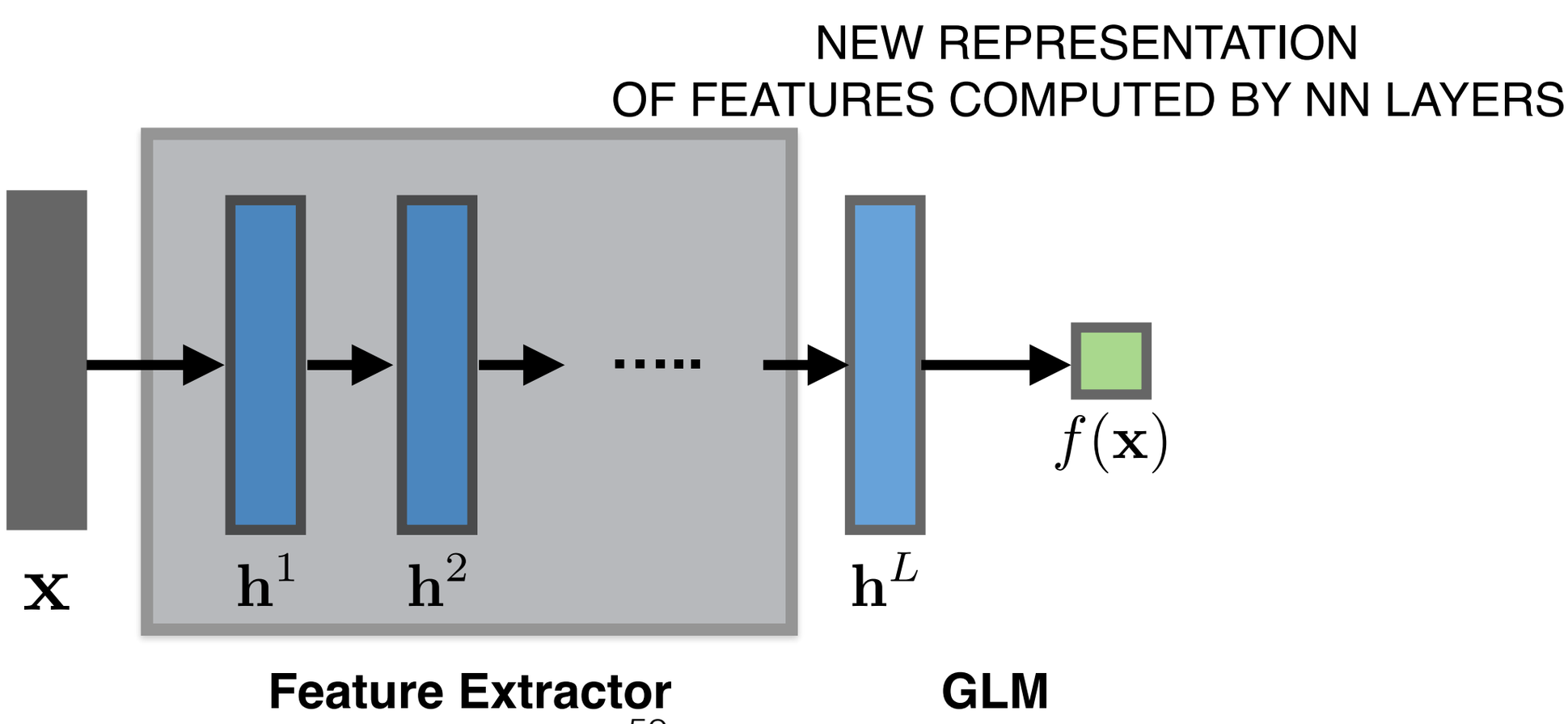

Gradient-Based Optimization

Model Fitting

Parameter Estimation: All parameters are estimated via gradient ascent on the log likelihood.

LOG LIKELIHOOD

$$\mathcal{L}(\mathbf{X}, \mathbf{Y}, \{\mathbf{W}_l\}_1^{L+1}, \{\mathbf{b}_l\}_1^{L+1}) = \sum_{i=1}^{N} \log p(\mathbf{y}_i | \mathbf{x}_i, \{\mathbf{W}_l\}_1^{L+1}, \{\mathbf{b}_l\}_1^{L+1})$$

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learning rate / step size.

Usually estimated with a subsample (i.e. 'stochastic gradient')

$$\nabla_{\mathbf{W}_l} \mathcal{L}(\mathbf{X}, \mathbf{Y}, \{\mathbf{W}_l\}_1^{L+1}, \{\mathbf{b}_l\}_1^{L+1}) \approx \nabla_{\mathbf{W}_l} \sum_{k=1}^{K} \log p(\mathbf{y}_k | \mathbf{x}_k, \{\mathbf{W}_l\}_1^{L+1}, \{\mathbf{b}_l\}_1^{L+1})$$

for $K << N$

Model Fitting

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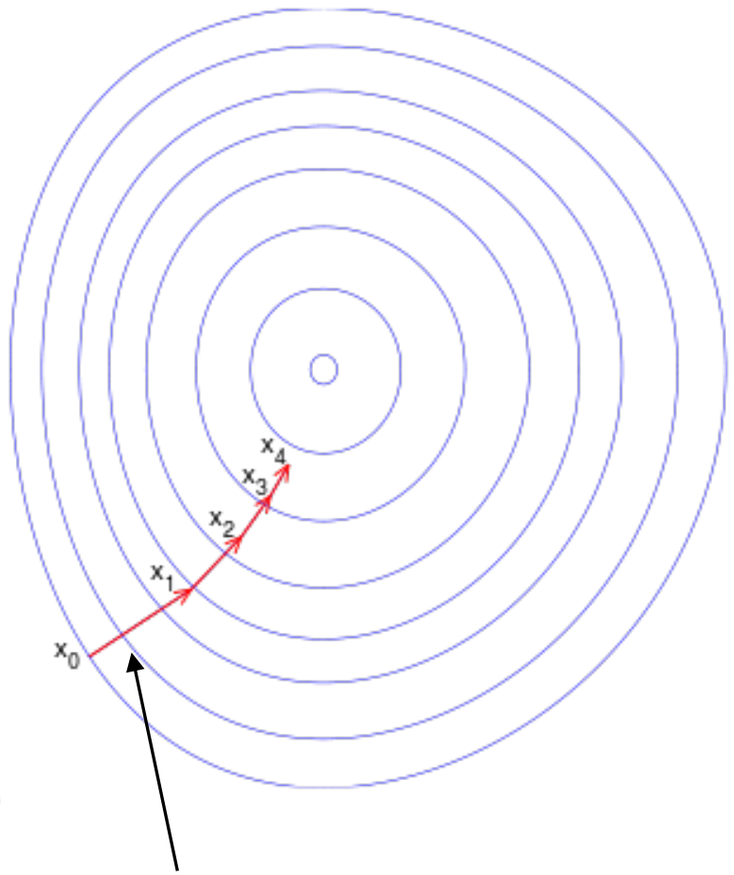

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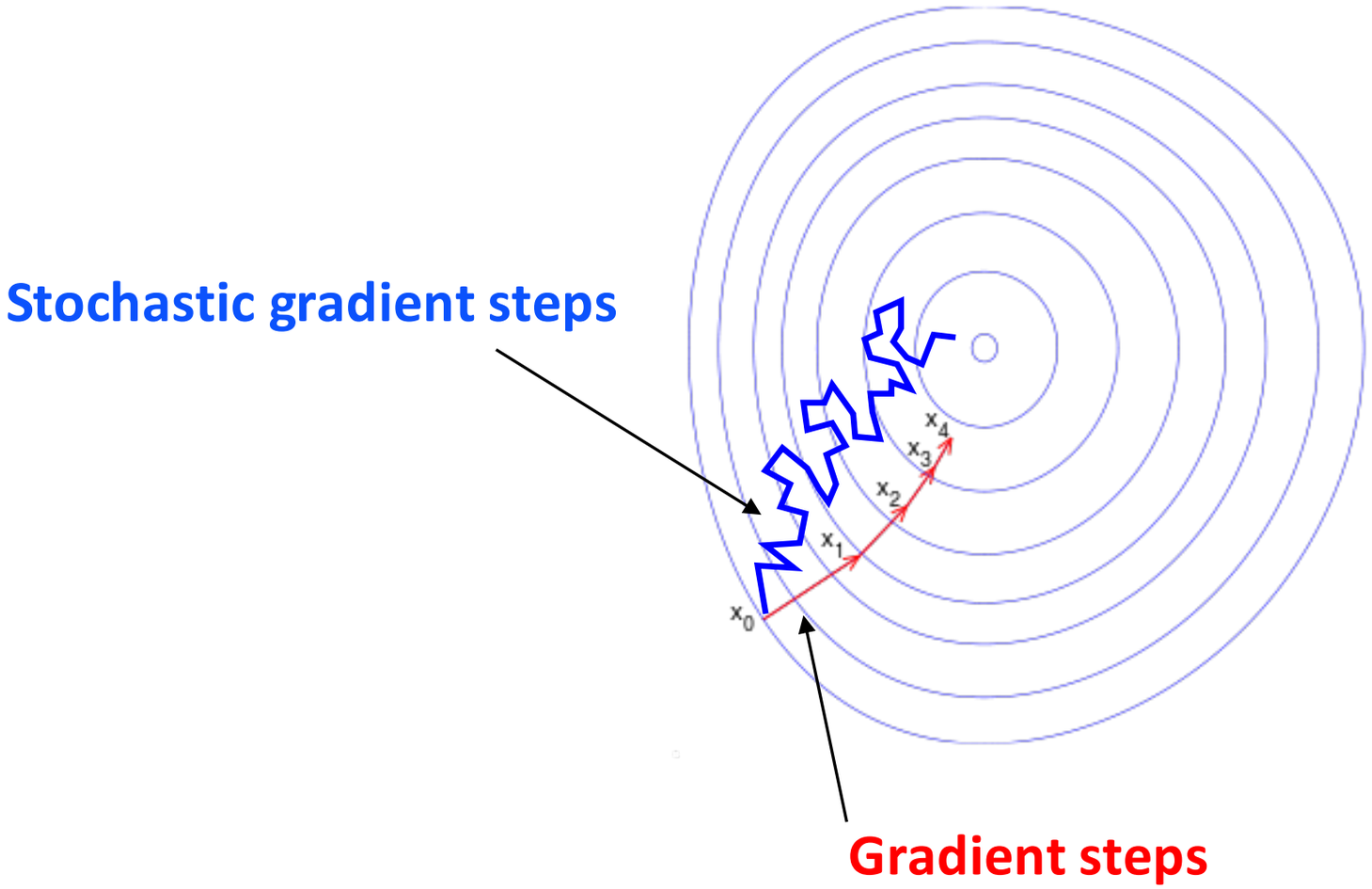
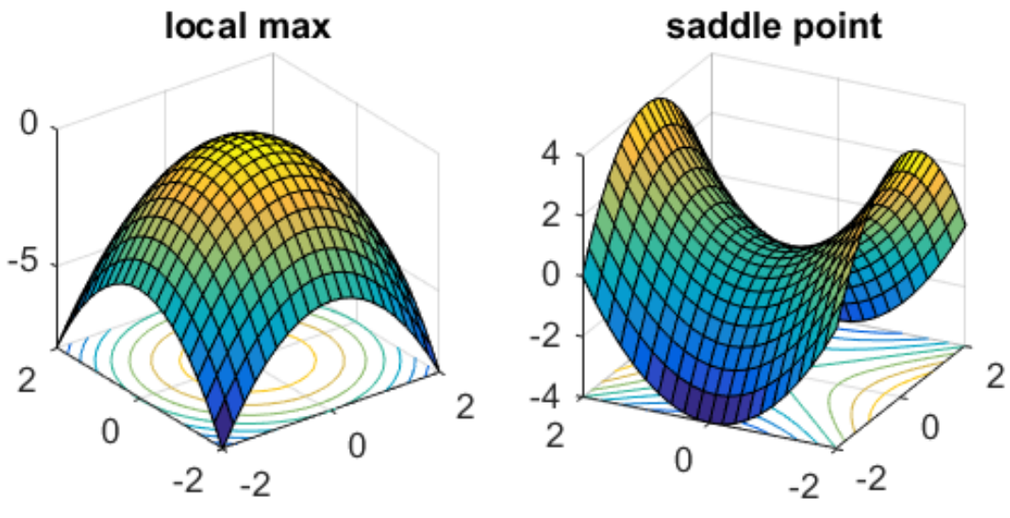


Optimization Landscape

- Previously, optimization of deep NNs was thought to be hopelessly non-convex. However, many of the critical points are not maxima but rather ***saddle points***. [Dauphin et al., 2014]



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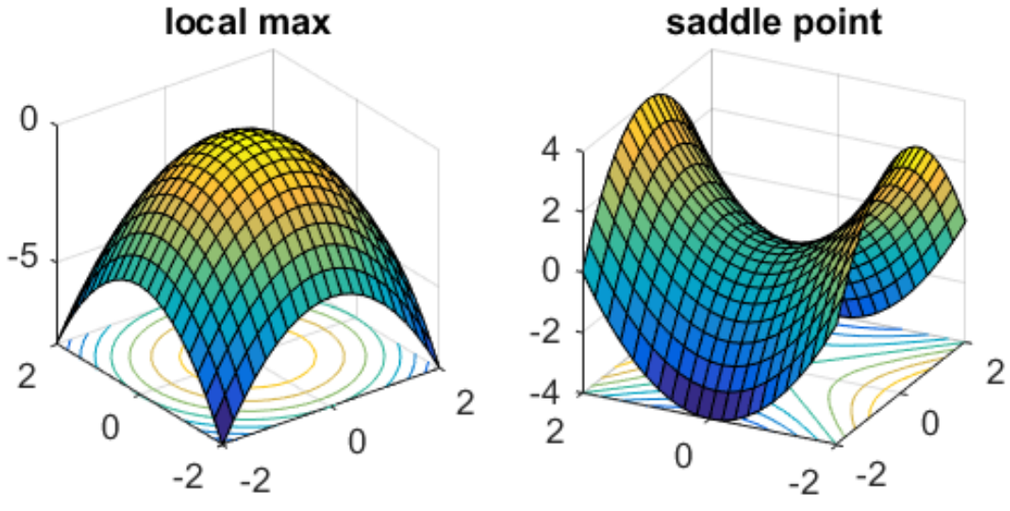

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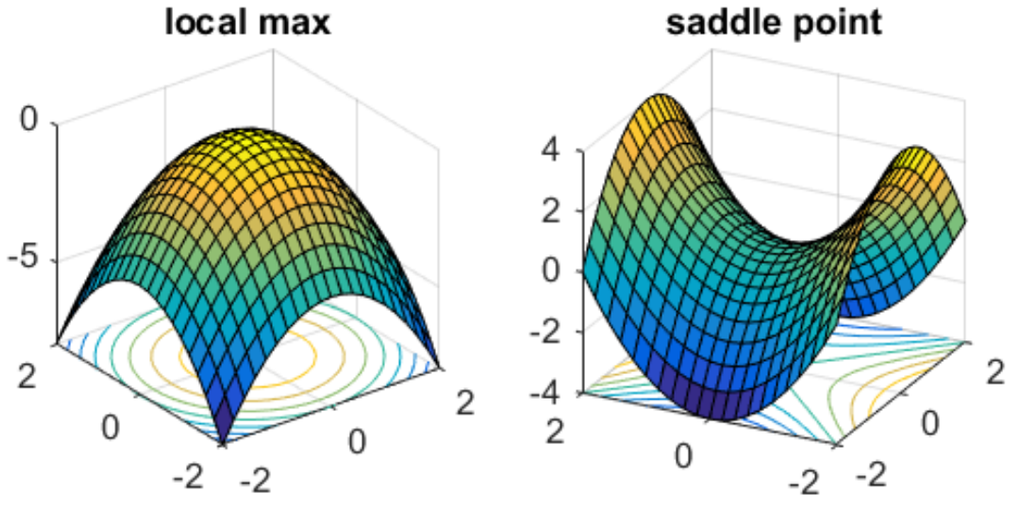
- **Stochastic Gradient:** [Hardt et al., 2016] (+ others) suggest the noise from stochastic gradient regularizes, improving model generalization.



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Model Fitting

- **Backpropagation**: The *backpropagation* algorithm [Rumelhart et al., 1986] is just an efficient way to compute the chain rule through the network.

$$\frac{\partial}{\partial\ \mathbf{W}_l}\mathcal{L} = \frac{\partial}{\partial\ \mathbf{h}_i^L}\log p(\mathbf{y}_i|\mathbf{h}_i^L, \mathbf{w}_o, b_o)\ \frac{\partial\ \mathbf{h}_i^L}{\partial\ \mathbf{h}_i^{L-1}}\cdots\frac{\partial\ \mathbf{h}_i^{l+1}}{\partial\ \mathbf{h}_i^l}\ \frac{\partial}{\partial\ \mathbf{W}_l}f_l(\mathbf{h}_i^{l-1}\mathbf{W}_l + \mathbf{b}_l)$$

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- **Automatic Differentiation**: Various 'autodiff' software libraries can compute these gradients for you, just needing definition of the forward model.

torch	theano	TensorFlow	PYTORCH
RONAN COLLOBERT (2000)	UNIVERSITY OF MONTREAL (2011)	GOOGLE BRAIN (2009/2015)	FACEBOOK AI (2016)

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MOST POPULAR TODAY

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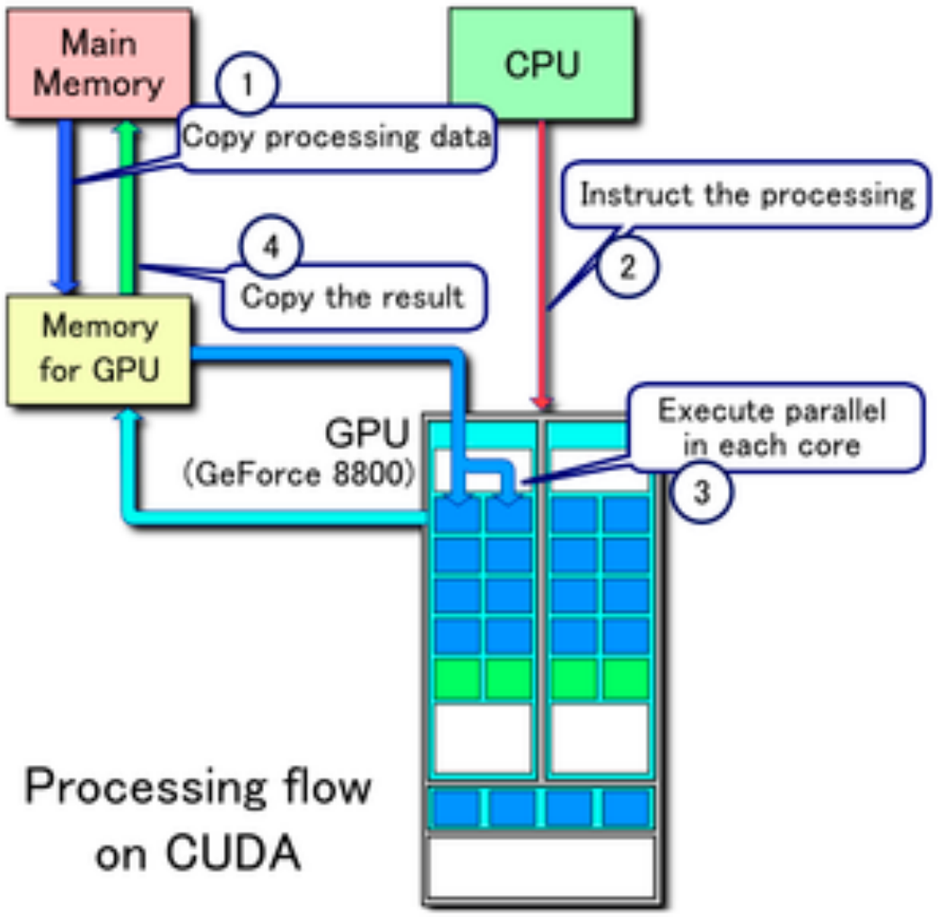
Graphics Processing Unit (GPU)



- GPU cards have been essential to scaling deep learning models.
- Perform fast matrix multiplications via parallel, but low precision, computation

Hyperparameter Tuning

- [ ] Tuning the network architecture (e.g. number of hidden units, layers) and optimization parameters (e.g. step size) is needed for best performance.

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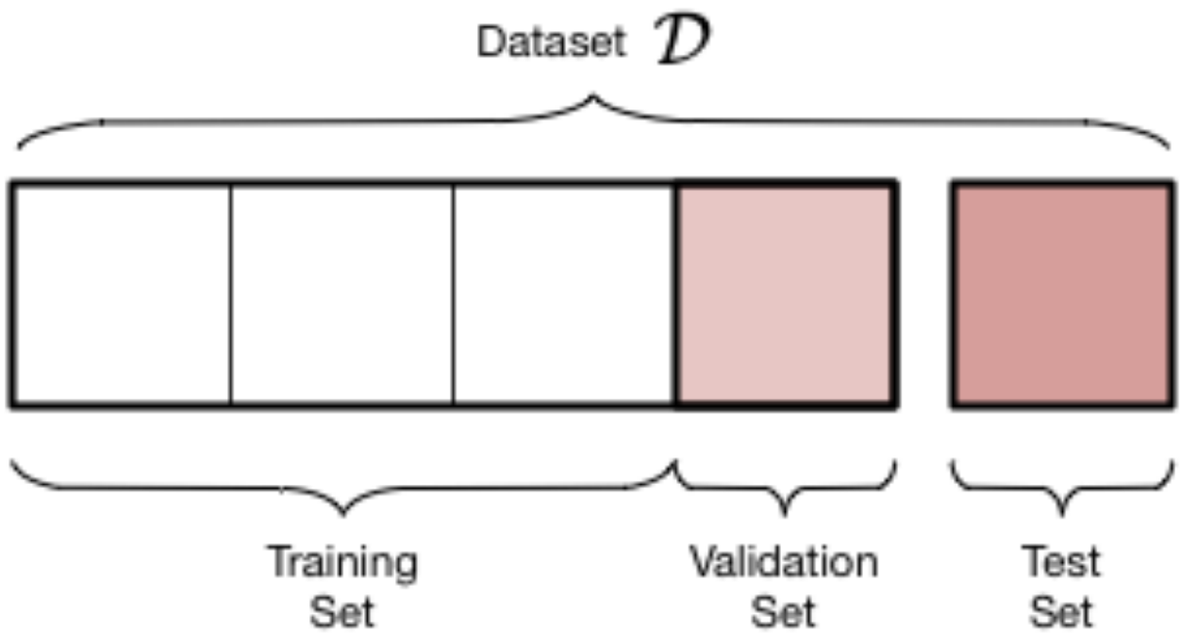

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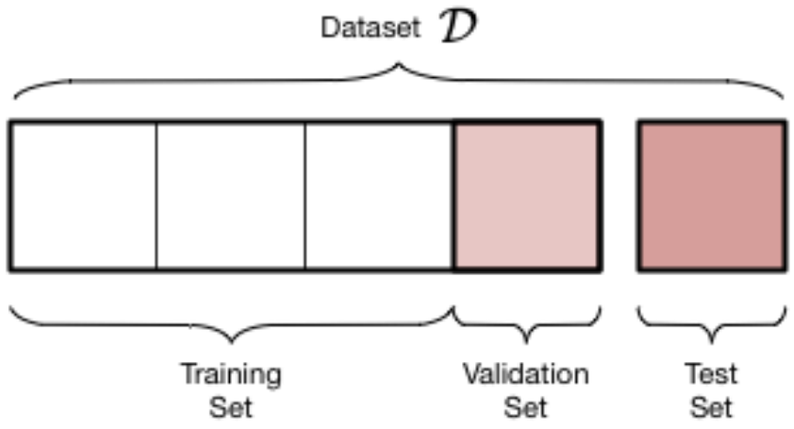
- Improving the model selection process is an on-going area of research. Bayesian optimization, bandit algorithms, and reinforcement learning methods have been proposed.

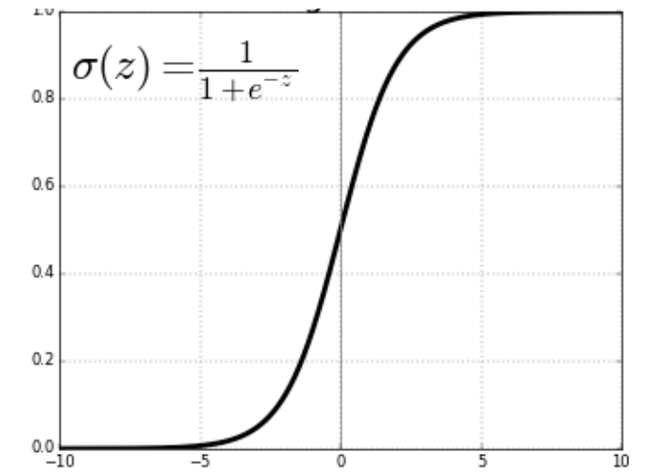


So What's Changed Since the 90's?

IN TERMS OF THE NN MODEL

Model Changes

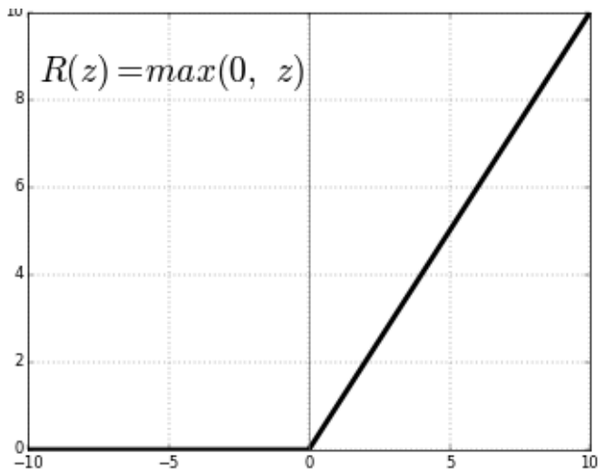
1. **ReLU Activations**: Scale-free non-linearities [Nair and Hinton, 2010].



LOGISTIC FUNCTION

OLD

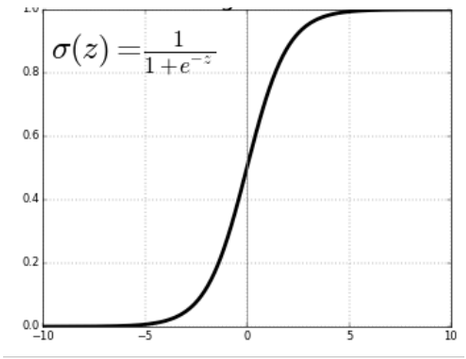
VS



RECTIFIED LINEAR UNIT (ReLU)

NEW

Model Changes



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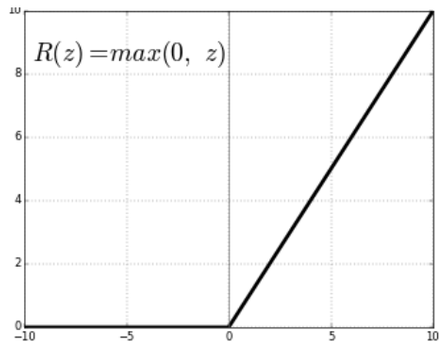


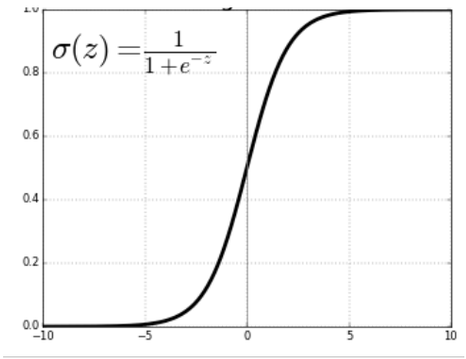
RECTIFIED LINEAR UNIT (ReLU)

CONNECTION

ReLUs are essentially the 'hockey stick' function used in piecewise linear spline regression:

$$\gamma(\mathbf{x}; \boldsymbol{\beta}, \{\boldsymbol{\xi}\}_H) = \sum_{m=1}^{H} \beta_h (\mathbf{x} - \boldsymbol{\xi}_m)_+$$

Model Changes



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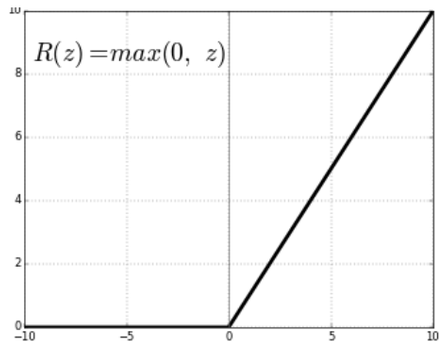

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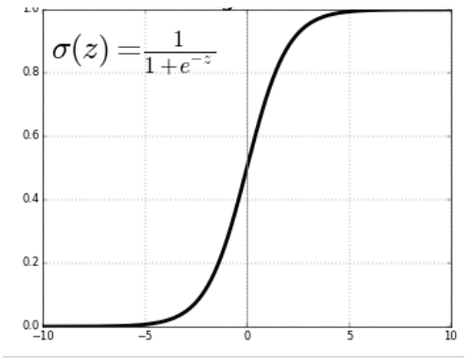
We can think of ReLU units in neural networks as having angular knots:

$$\mathbf{x} > \xi_m \quad \text{VS} \quad \cos(\mathbf{x}, \boldsymbol{\beta}_{1,m}) > \frac{\xi_m}{||\mathbf{x}||\ ||\boldsymbol{\beta}_{1,m}||}$$

Model Changes



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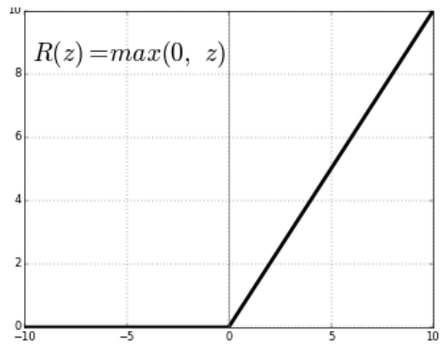

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BIAS VARIABLES = KNOTS

Model Changes

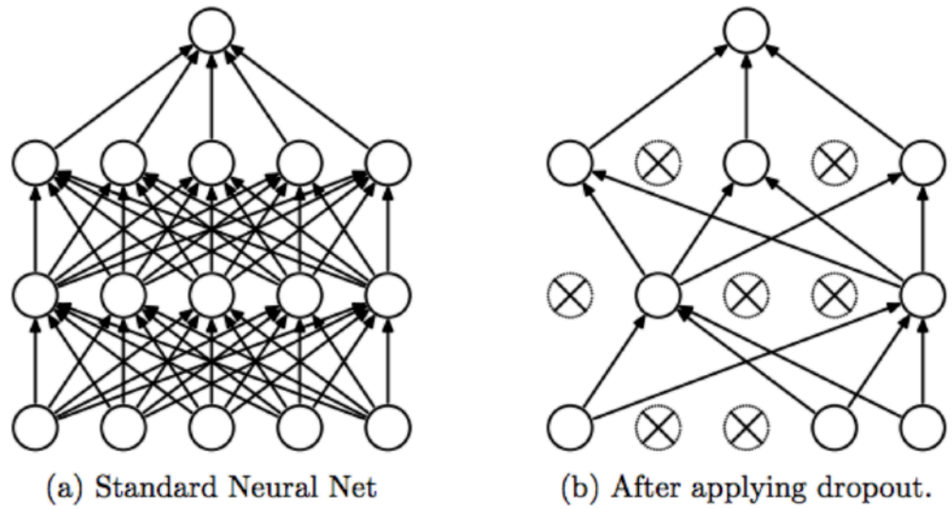
2. Better Regularization: Stochastic regularization strategies [Srivastava et al., 2014].

$$\sum_{l=1}^{L+1} ||\mathbf{W}_l||_2^2$$

RIDGE PENALTY

OLD

VS



(a) Standard Neural Net

(b) After applying dropout.

DROPOUT

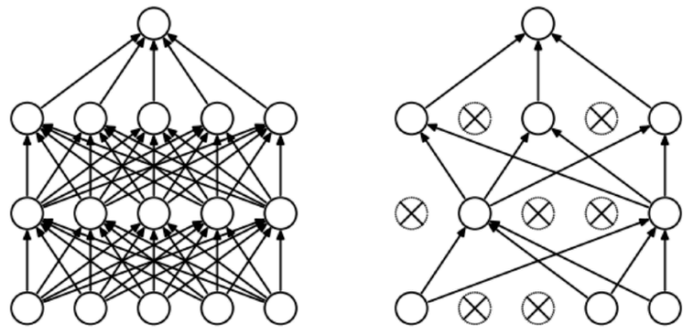
NEW

Model Changes

$$\sum_{l=1}^{L+1} ||\mathbf{W}_l||_2^2$$

RIDGE PENALTY

VS



(a) Standard Neural Net (b) After applying dropout.

DROPOUT

CONNECTION

Can think of dropout as spike and slab variable selection

[Kuo and Mallick, 1998]:

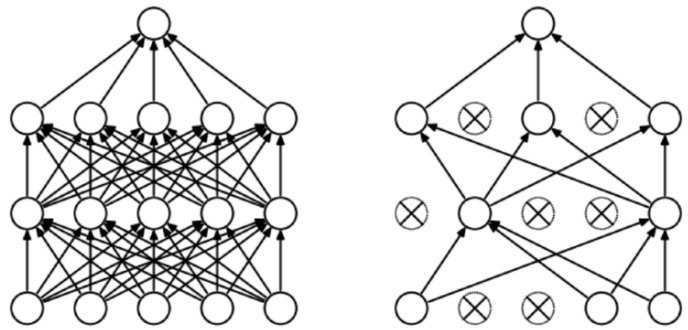
$$\mathbf{h}_i^l = f_l\left((\mathbf{h}_i^{l-1} \odot \boldsymbol{\xi})\mathbf{W}_l + \mathbf{b}_l\right), \boldsymbol{\xi} \sim \text{Bernoulli}(p)$$

Model Changes

$$\sum_{l=1}^{L+1} ||\mathbf{W}_l||_2^2$$

RIDGE PENALTY

vs



(a) Standard Neural Net (b) After applying dropout.

DROPOUT

CONNECTION

Can think of dropout as spike and slab variable selection

[Kuo and Mallick, 1998]:

$$\mathbf{h}_i^l = f_l\left((\mathbf{h}_i^{l-1} \odot \boldsymbol{\xi})\mathbf{W}_l + \mathbf{b}_l\right), \boldsymbol{\xi} \sim \text{Bernoulli}(p)$$

Noise Model $p(\lambda)$	Variance Prior $p(\lambda^2)$	Marginal Prior $p(w)$
Bernoulli	Bernoulli	Spike-and-Slab
Gaussian	χ^2	Unnamed
Rayleigh	Exponential	Laplace
Inverse Nagakami	Γ^{-1}	Student-t
Half-Cauchy	Unnamed	Horseshoe

[Nalisnick et al., 2015]

Model Changes

3. Skip Connections: Identity connections to previous layer [He et al., 2015].

$$\mathbf{h}_i^l = f_l(\mathbf{h}_i^{l-1}\mathbf{W}_l + \mathbf{b}_l)$$

NONLINEAR TRANSFORM

OLD

VS

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SKIP CONNECTION

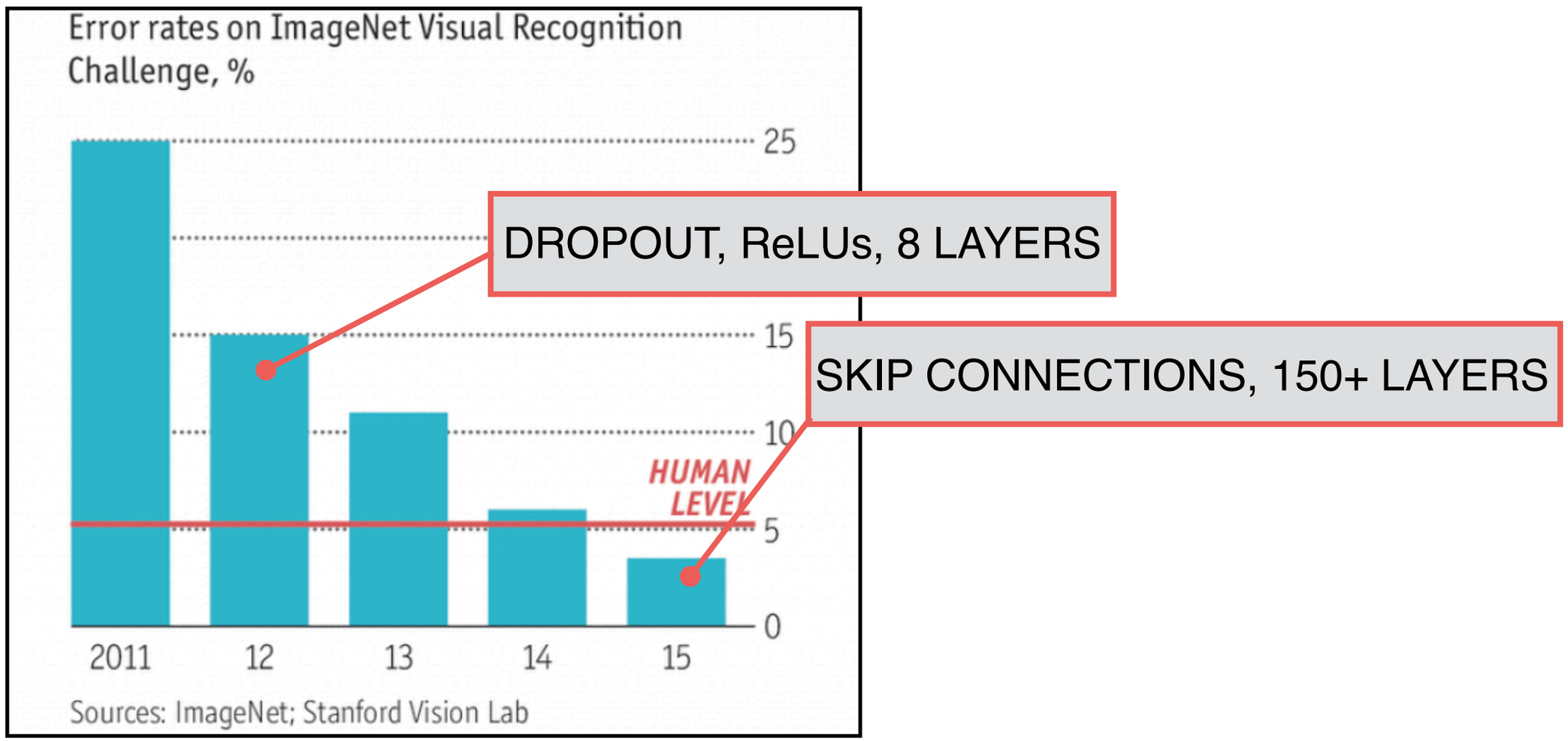
NEW

Can think of skip-connections as modeling the residual transformation:

$$\mathbf{h}_i^l - \mathbf{h}_i^{l-1} = f_l(\mathbf{h}_i^{l-1}\mathbf{W}_l + \mathbf{b}_l)$$

Deep Learning Results

Computer Vision: Results on ImageNet object classification dataset.



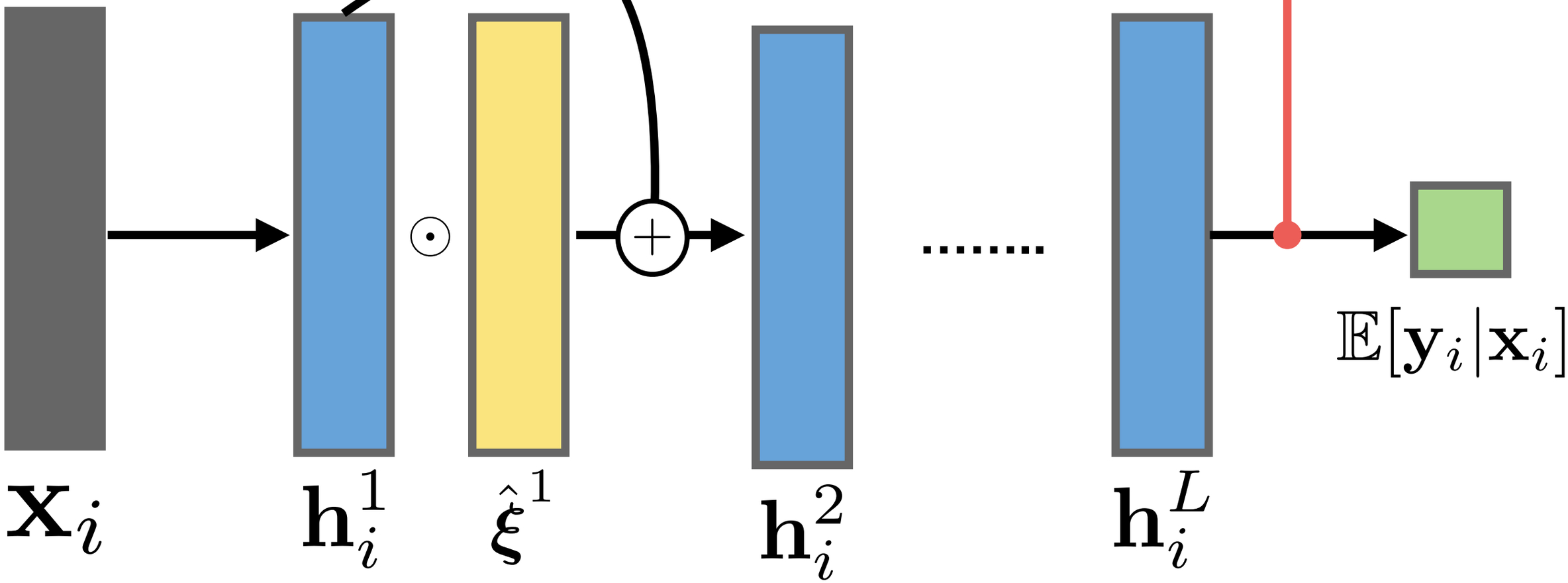
https://www.economist.com/news/special-report/21700756-artificial-intelligence-boom-based-old-idea-modern-twist-not

Modern Deep Neural Networks

ReLU

$$\mathbf{h}_i^l = f_l\left((\mathbf{h}_i^{l-1} \odot \hat{\boldsymbol{\xi}}^l)\mathbf{W}_l + \mathbf{b}_l\right) + \mathbf{h}_i^{l-1}$$

$$\mathbb{E}[\mathbf{y}_i|\mathbf{x}_i] = g^{-1}(\mathbf{h}_i^L \mathbf{w}_o + b_o)$$



$\hat{\boldsymbol{\xi}}^1 \sim \text{Bernoulli}(p)$

Factor Analysis and Autoencoders

Factor Analysis and Autoencoders

- **Factor Analysis**:

$$\mathbf{x}_i = \mathbf{z}_i \mathbf{A} + \mathbf{b} + \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathrm{N}(\mathbf{0}, \boldsymbol{\Sigma}_0)$$

loading matrix

Factor Analysis and Autoencoders

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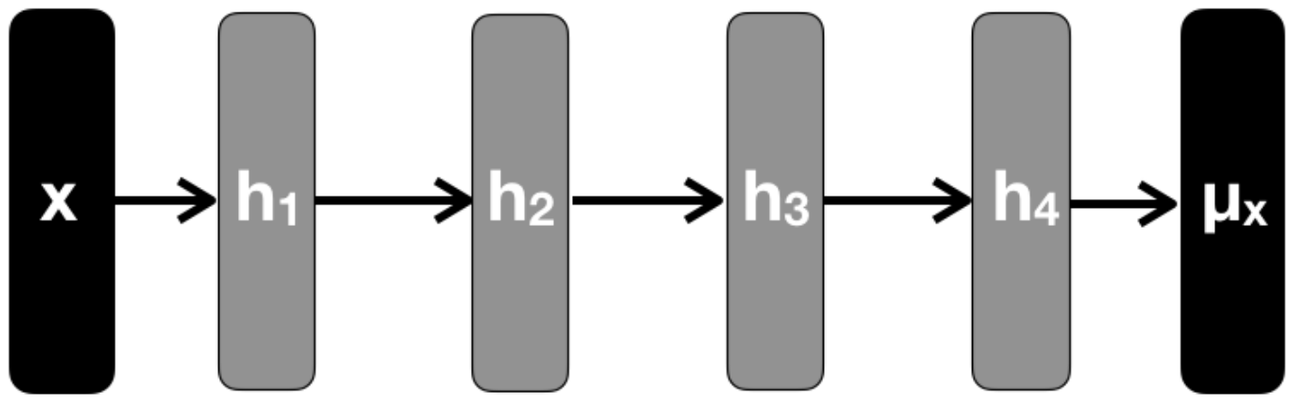
loading matrix

Autoencoder:



$$\mathbb{E}[\mathbf{x}_i|\mathbf{x}_i] = g^{-1}(\mathbf{h}_{i,L}\mathbf{W}_{L+1} + \mathbf{b}_{L+1}), \quad \mathbf{h}_{i,l} = f_L(\mathbf{h}_{i,l-1}\mathbf{W}_l + \mathbf{b}_l), \quad \mathbf{h}_{i,0} = \mathbf{x}_i$$

Equivalence

- **Principal Components Analysis (PCA):** Both models can be shown equivalent to PCA under certain modifications. [Tipping & Bishop, 1999] [Baldi & Hornik, 1989]

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- **Nonlinear Factor Analysis:** Factor analysis can be made non-linear in the factors and parameters [Amemiya, 1993].

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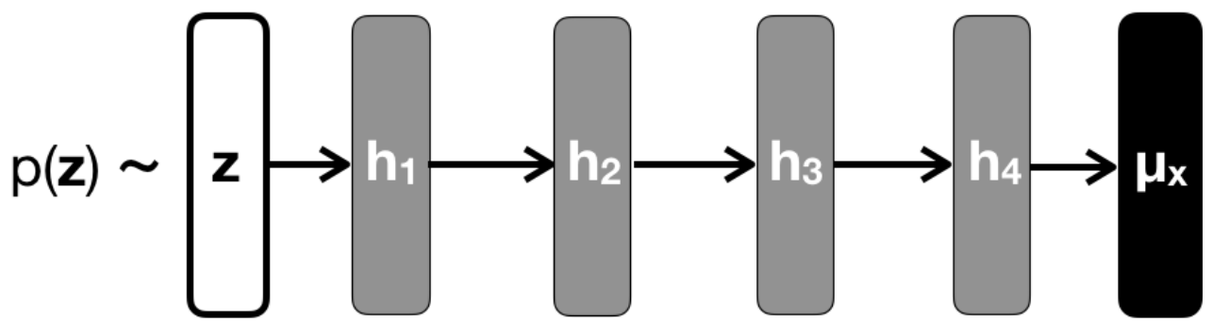
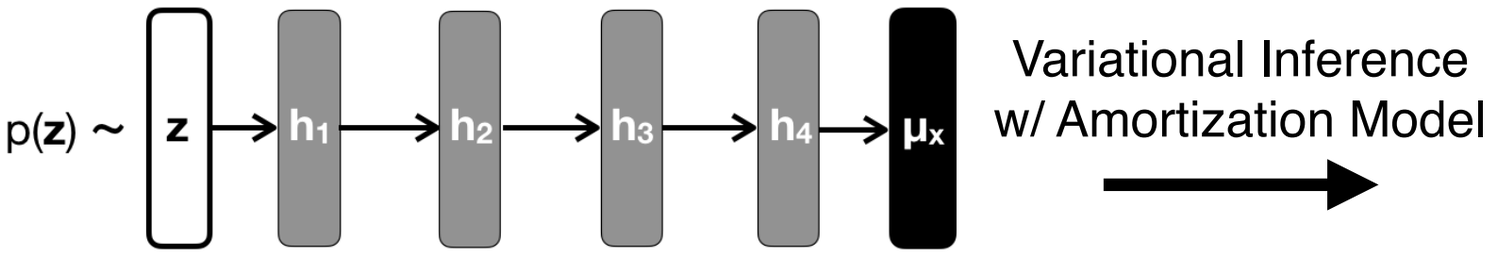
If we assume the non-linearity is defined by a neural network, then we have what's known as a **density network** [MacKay & Gibbs, 1999].



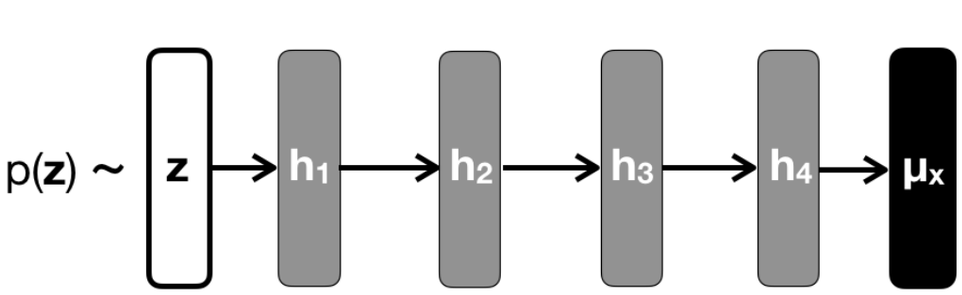
Equivalence



Variational Inference
w/ Amortization Model

Nonlinear Factor Analysis /
Density Network

Equivalence



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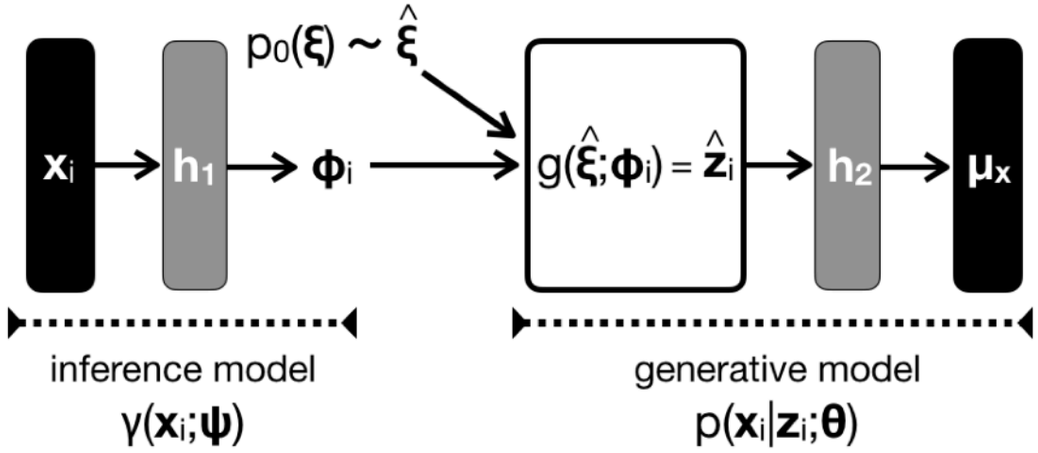

Nonlinear Factor Analysis /
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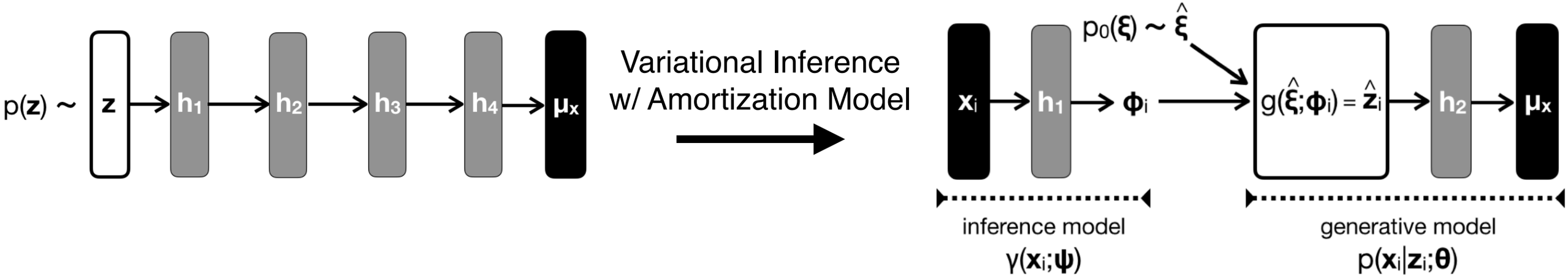
Variational Autoencoder
[Kingma & Welling, 2014]

Equivalence



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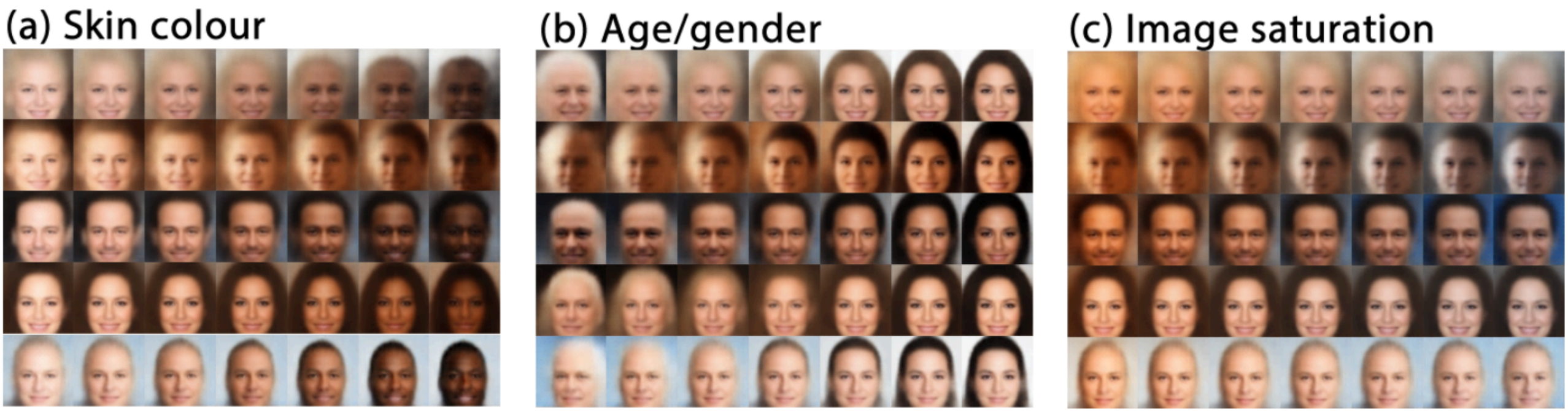
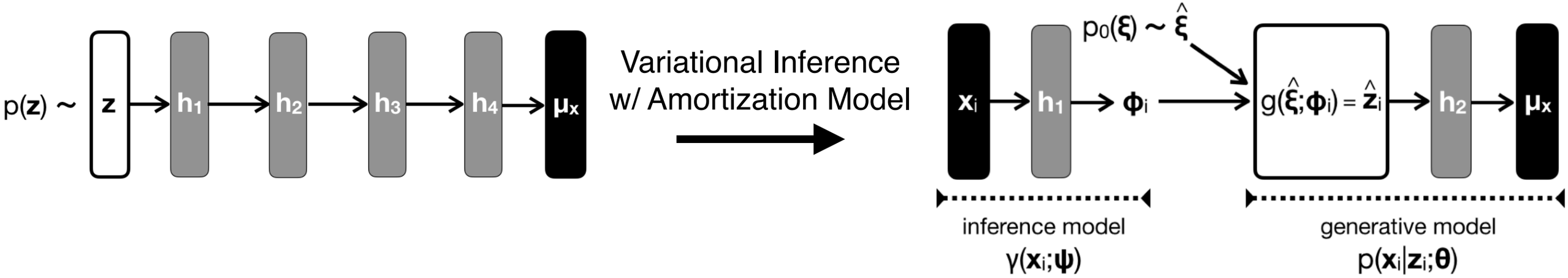


[Higgins et al., 2017]

Equivalence



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Interpretable VAEs for nonlinear group factor analysis

Samuel K. Ainsworth[1], Nicholas J. Foti[1], Adrian KC Lee[2], and Emily B. Fox[1]

[1]School of Computer Science and Engineering, University of Washington
[2]Institute for Learning & Brain Sciences, University of Washington

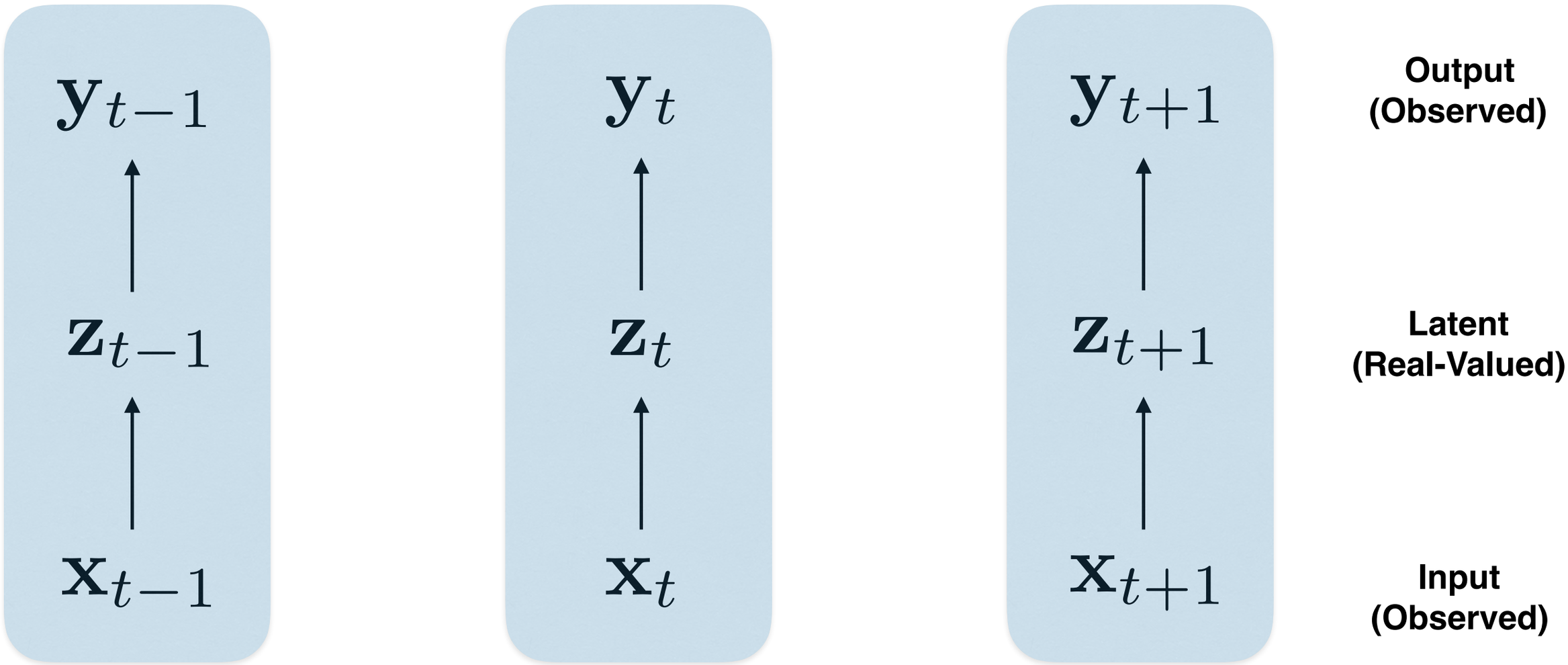
February 15, 2018

Abstract

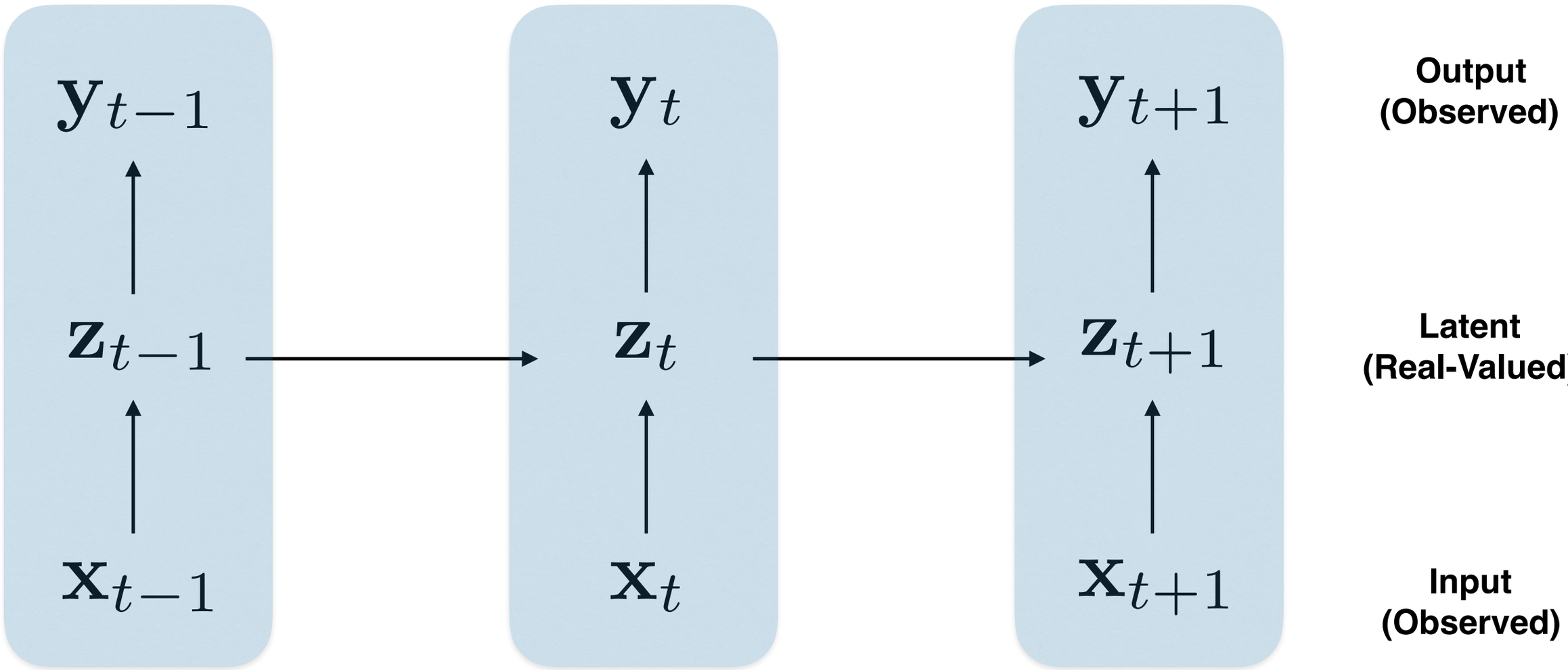
Deep generative models have recently yielded encouraging results in producing subjectively realistic samples of complex data. Far less attention has been paid to making these generative models interpretable. In many scenarios, ranging from scientific applications to finance, the observed variables have a natural grouping. It is often of interest to understand systems of interaction amongst these groups, and latent factor models (LFMs) are an attractive approach. However, traditional LFMs are limited by assuming a linear correlation structure. We present an output interpretable VAE (oi-VAE) for grouped data that models complex, nonlinear latent-to-observed relationships.

State-Space Models and Recurrent NNs

Prediction with Sequential Data

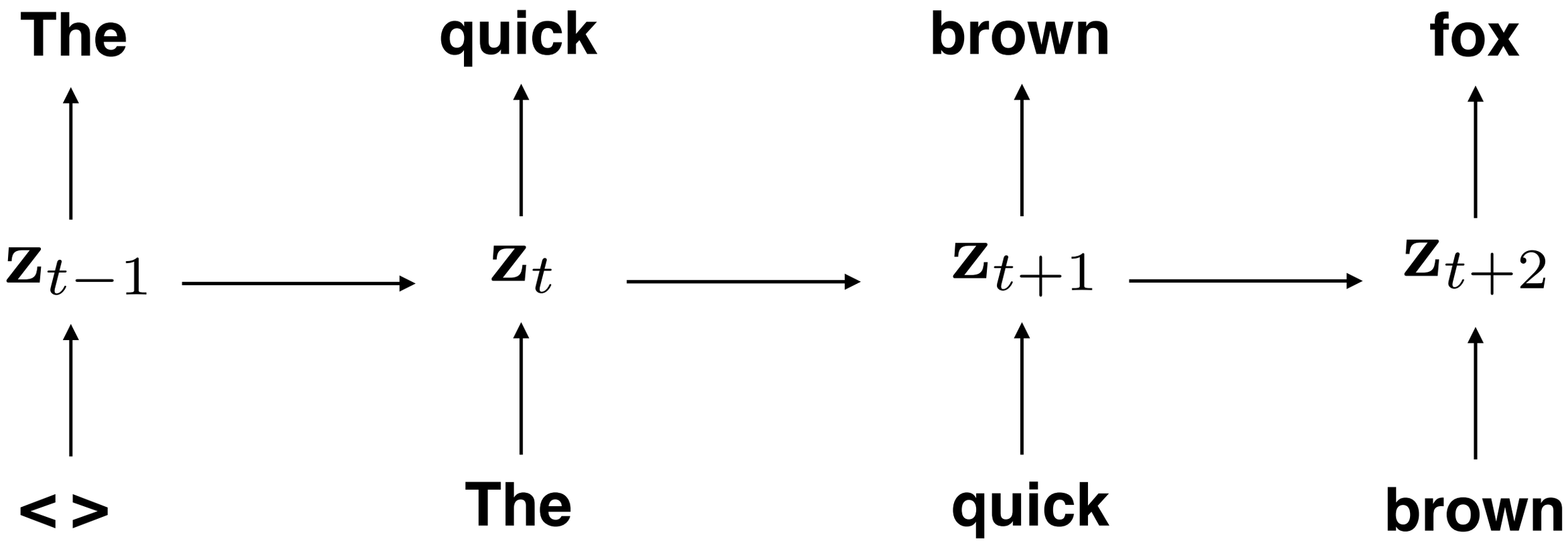


Recurrent Neural Network (RNN) Models



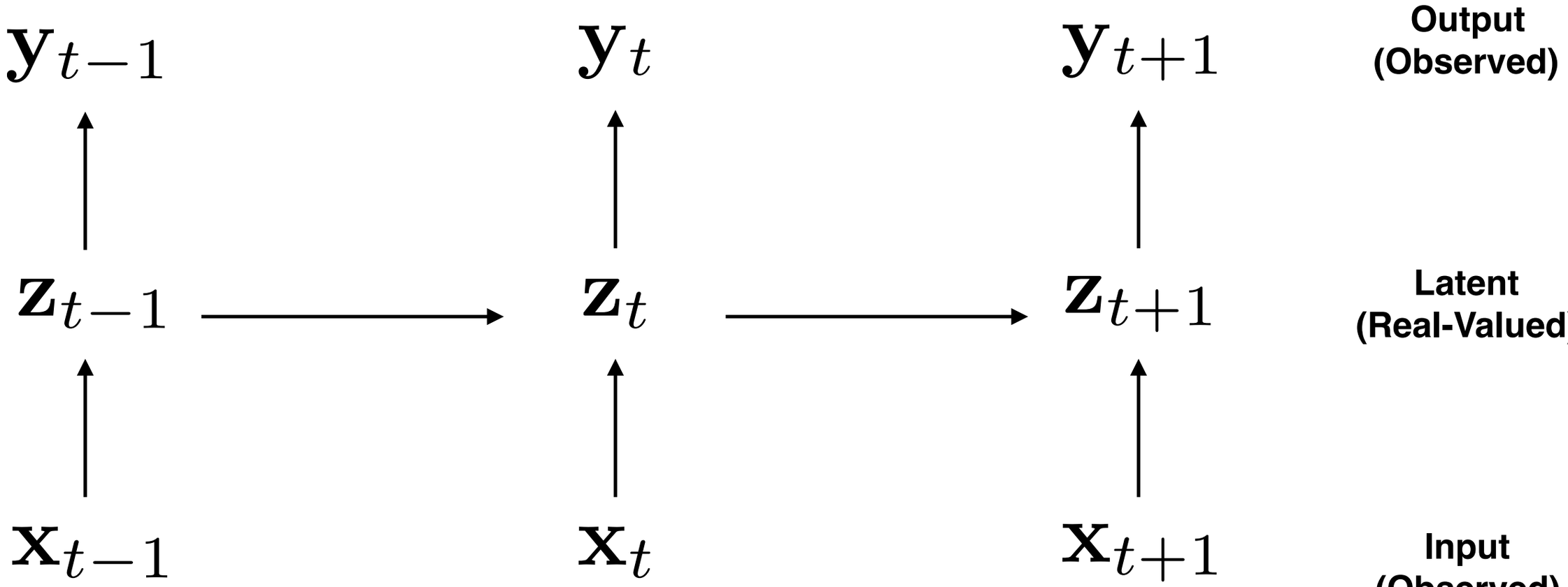
Each time-slice can be a deep network
….hidden (latent) vectors are coupled together over time

Language Modeling with RNNs



Many extensions, e.g,
Long-short-term-memory (LSTM) models for longer memory

State-Space Models in Statistics



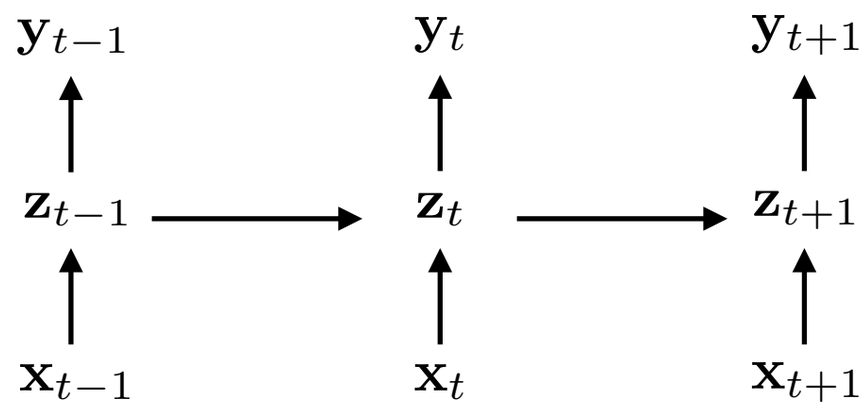
Kalman (1960)
Durbin and Koopman (2001)
Shumway and Stoffer (2016)

e.g., Linear-Gaussian assumptions
for dependencies in graph

Recurrent Neural Network (RNN) Models

State dynamics equation:

$$\mathbf{z}_t = f\Big(\mathbf{W}^{zz}\mathbf{z}_{t-1} \; + \; \mathbf{W}^{xz}\mathbf{x}_t \; + \; \mathbf{b}_z \Big)$$



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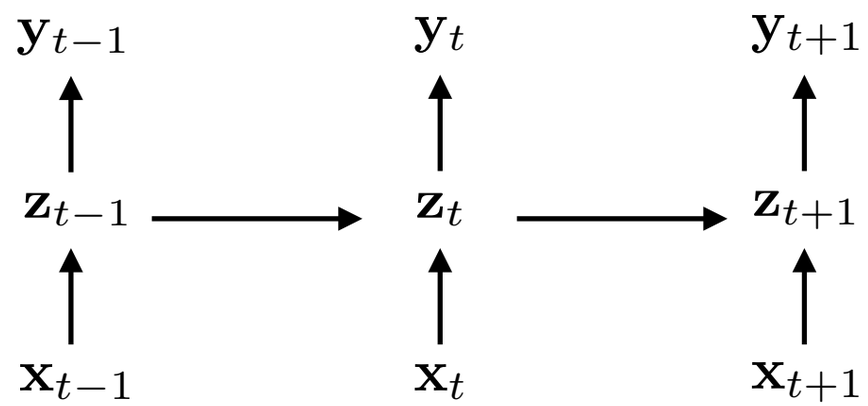

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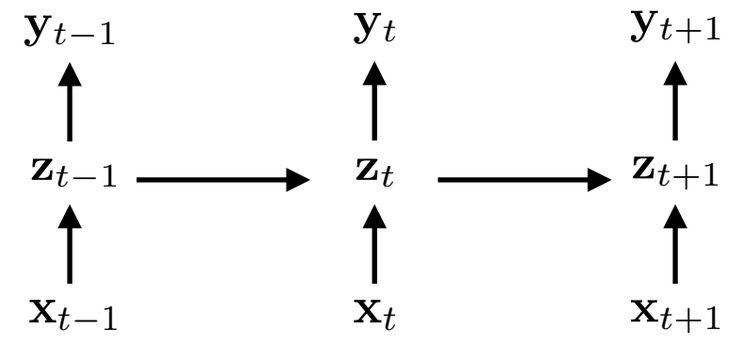
Key difference with state-space models:
Latent variables z are computed as deterministic (non-linear) functions
No distributional assumptions (e.g., Gaussian)
Both an advantage and a drawback

Comparing RNNs and State Space Models



Similarities:

Use of latent state representation (e.g., for dimensionality reduction)

Independence of output at time t, given state at time t

Parameter estimation with gradient methods

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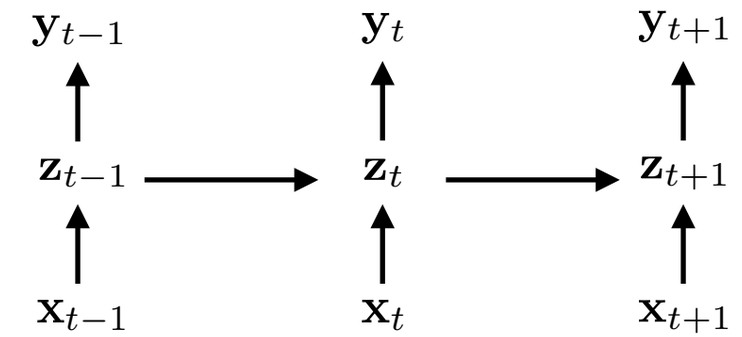

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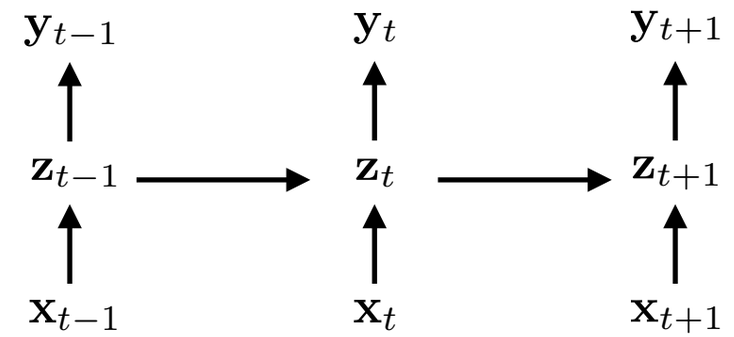

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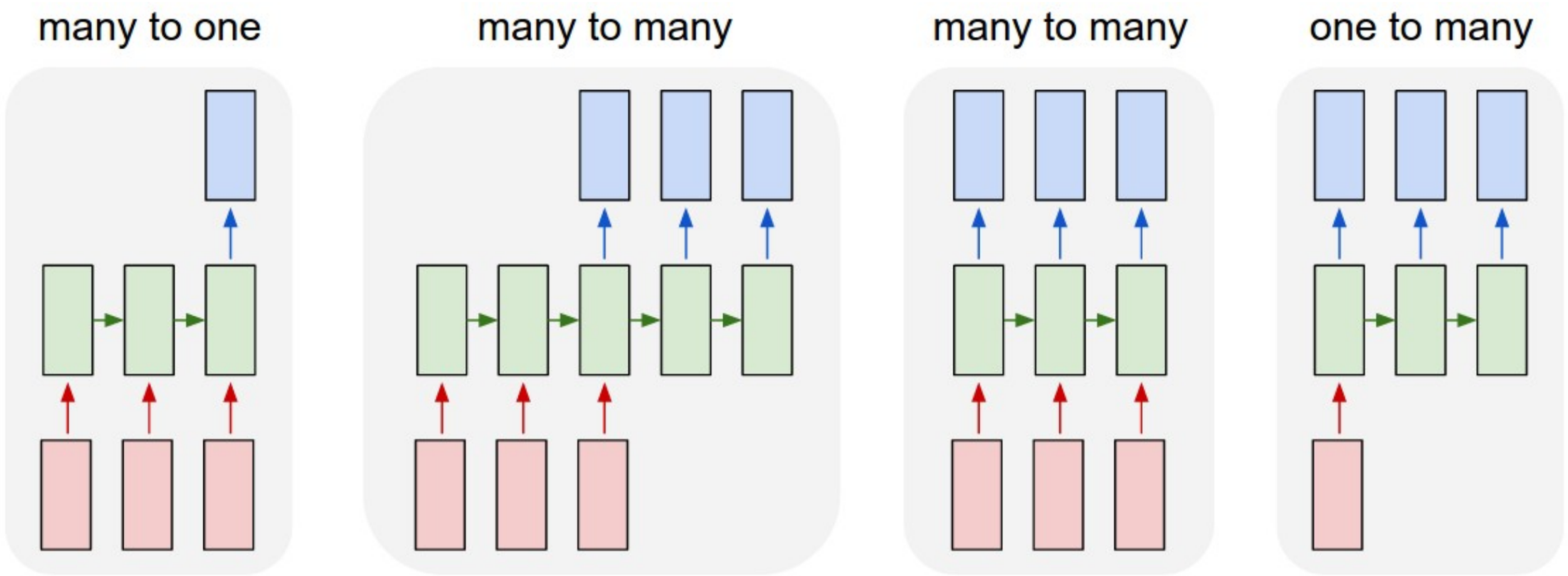
Exploration of hybrid RNN/state-space models: active area of research

e.g., see Fraccaro et al., 2016, Krishnan et al 2017, Zheng et al, 2017

The Many Variants of Recurrent Network Models



Figures from http://cs231n.stanford.edu/slides/2017/

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- **Model interpretation and uncertainty quantification:** *How can we understand what the model has learned? When will it fail? Can we get calibrated uncertainty estimates?*

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- [ ] **Uncertainty Quantification for Safe Automation:** [Gal & Ghahramani, 2016], [Li & Gal, 2017], [Louizos & Welling, 2017], [Lakshminarayanan et al., 2017]

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☐ **Using Deep Learning to Improve the Speed / Accuracy of Inference**

- **MCMC:** [Zhang et al., 2017], [L. Li et al., 2017], [Y. Li et al., 2017], [Levy et al., 2018]

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- **MCMC:** [Zhang et al., 2017], [L. Li et al., 2017], [Y. Li et al., 2017], [Levy et al., 2018]

- **Variational Inference:** [Kingma & Welling, 2014], [Burda et al., 2015], [Li & Turner, 2016], [Ranganath et al., 2016], [Mescheder et al., 2017], [Tran et al., 2017], [Feng & Liu, 2017] (+ many more)

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- [ ] **Rubin-Neyman Potential Outcomes:** [Johansson et al., 2016]

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- [ ] **Relational Data / Networks:** [Duvenaud et al., 2016], [Kipf & Welling, 2017] (+ many more)

Conclusions and Summary

PROBLEM: Prior to 2000's, NNs with 4+ layers were hard to train. SVMs worked just as well as shallow NNs.

SOLUTIONS:

- **More Data**: Many of the datasets being tested were too small, resulting in the NNs overfitting.
  - → **ImageNet Dataset**: 15 million images, 22,000 classes
- **Better Hardware**: And when the datasets were large, the hardware was not fast enough to make NN training practical.
  - → **Graphics Processing Units (GPUs)**: Can perform fast matrix multiplications (but with loss of precision).
- **Model Changes**: Small but crucial changes to the NN model architecture.
- **Better Understanding of Gradient Ascent**: Gradient-based optimization is better in non-convex settings than previously thought.

Summary: Key Points from This Talk

- [ ] Deep neural networks are very flexible non-linear models
- [ ] Models tend to be very complex, require lots of labeled data
- [ ] Focus is on prediction, not on model interpretation
- [ ] “Learning” is often regularized maximum likelihood via gradient methods

Many links to statistical thinking:

There is much that statistics can contribute to deep learning.

Statistics will benefit from an awareness about deep learning.

Further Reading from a Statistical Perspective

- [ ] L. Breiman
Statistical Modeling: The Two Cultures
Statistical Science, 2001

- [ ] B. Efron and T. Hastie
Chapter 18: Neural Networks and Deep Learning
Computer Age Statistical Inference
Cambridge University Press, 2016

- [ ] S. Mohamed
A Statistical View of Deep Learning
Blog post: http://blog.shakirm.com/wp-content/uploads/2015/07/SVDL.pdf, 2015

- [ ] E. Nalisnick, D. Tran, D. Blei, and P. Smyth
Deep Learning: A Synthesis from Probabilistic Foundations
coming soon…

Thank you. Questions?

SLIDES: `http://www.ics.uci.edu/~enalisni/DLforStats.pdf`

References

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Samuel Ainsworth, Nicholas J. Foti, Adrian K. C. Lee, and Emily B. Fox. Interpretable vaes for nonlinear group factor analysis. *ArXiv Preprint*, 2018.

Yasuo Amemiya. On nonlinear factor analysis. In *Proceedings of the ASA Social Statistics Section*, pages 290–294, 1993.

Pierre Baldi and Kurt Hornik. Neural networks and principal component analysis: Learning from examples without local minima. *Neural networks*, 2(1):53–58, 1989.

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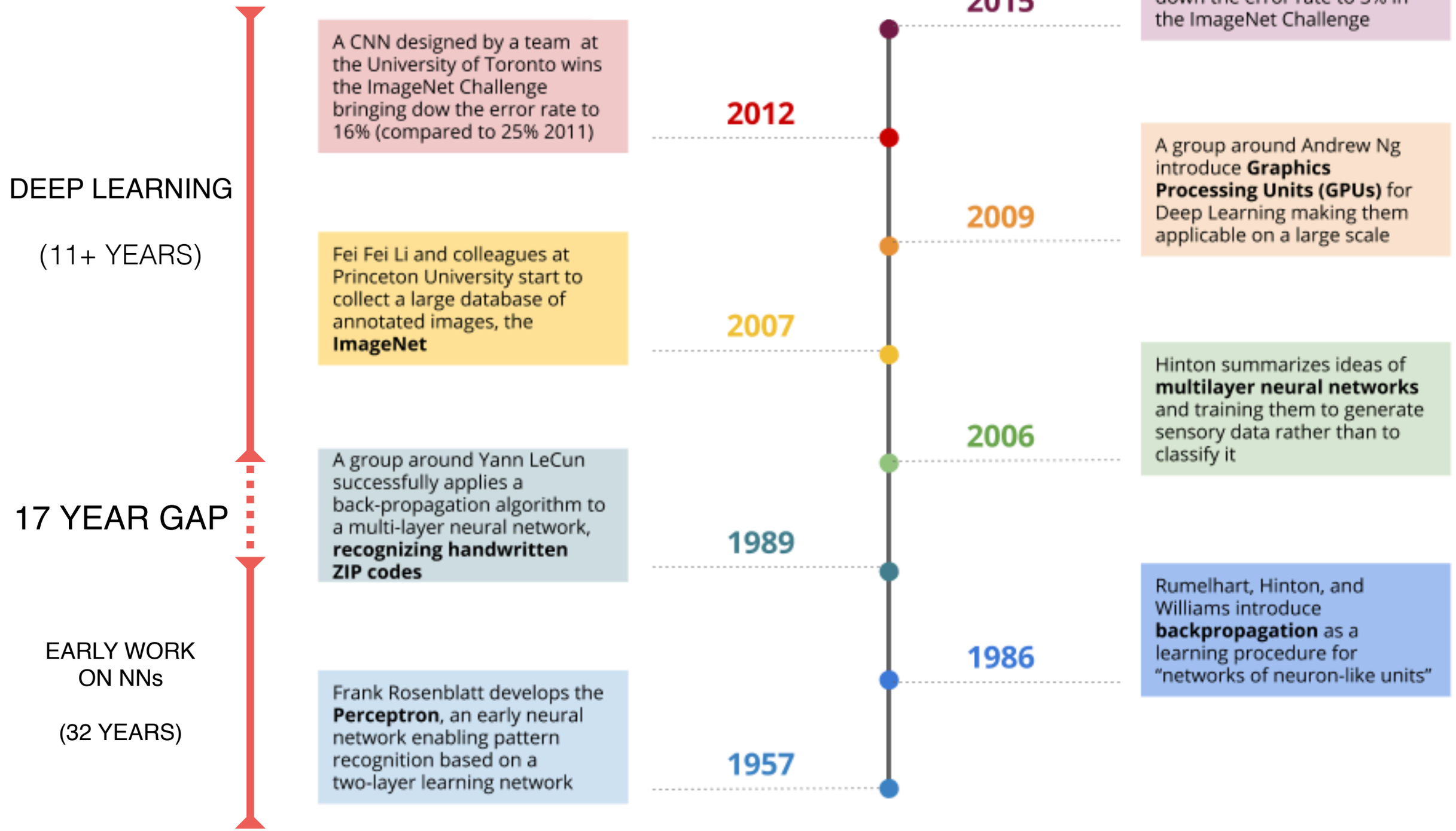
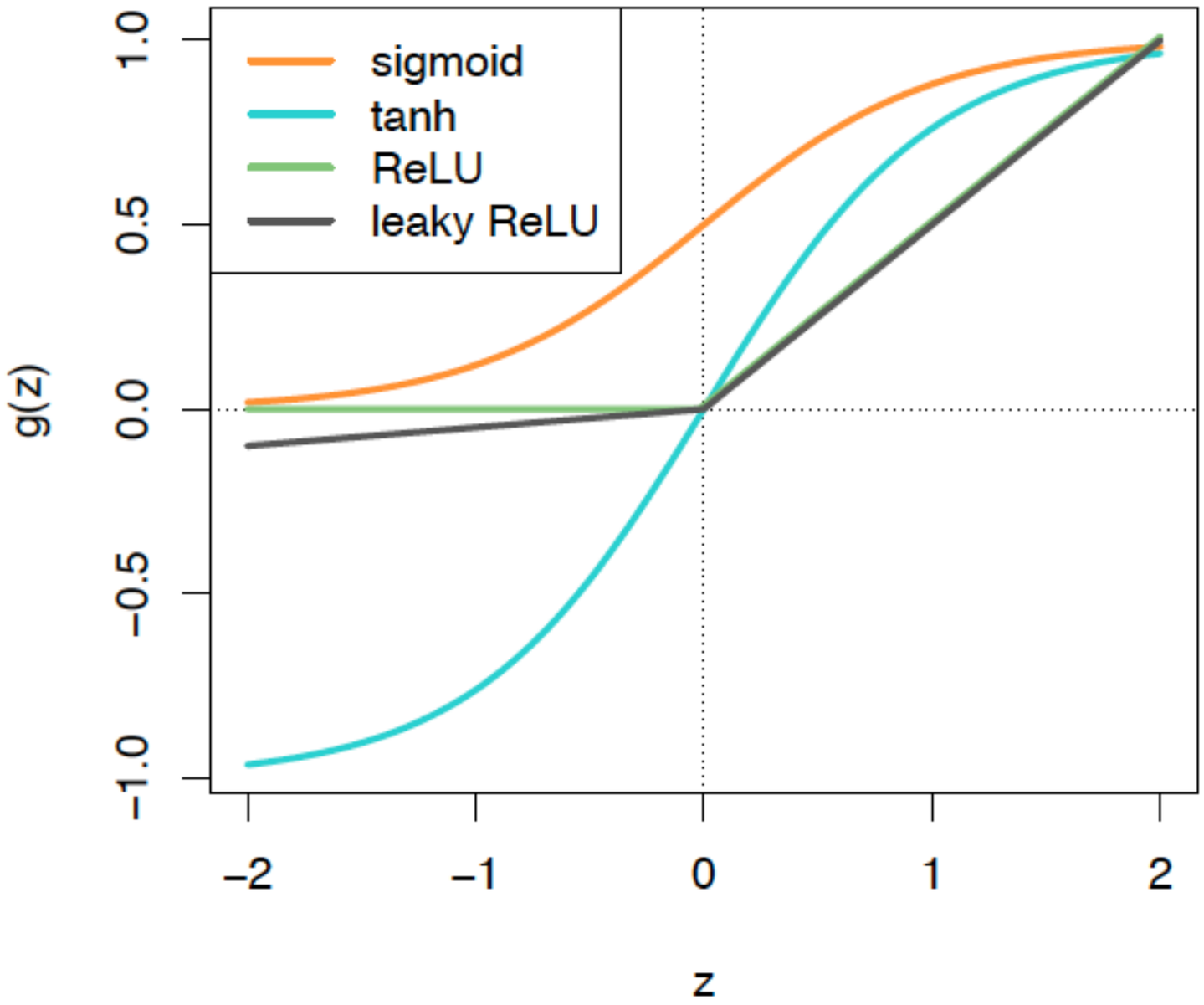
Appendix

Historical Perspective



https://micro-dimensions.com/blog/2017/2/13/whats-all-the-fuss-about-deep-learning-and-how-will-it-impact-pathology

Non-Linearities at Hidden Units



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