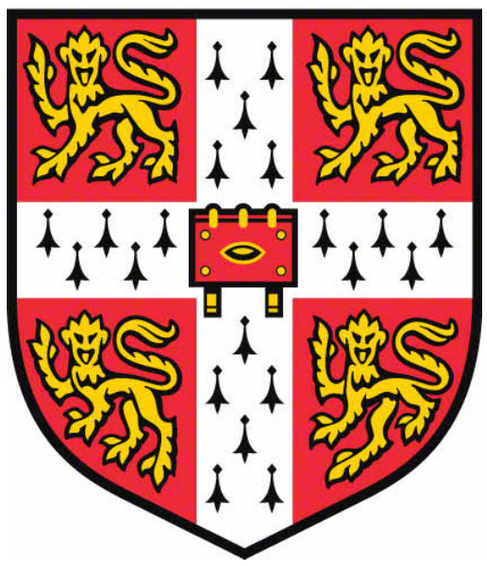
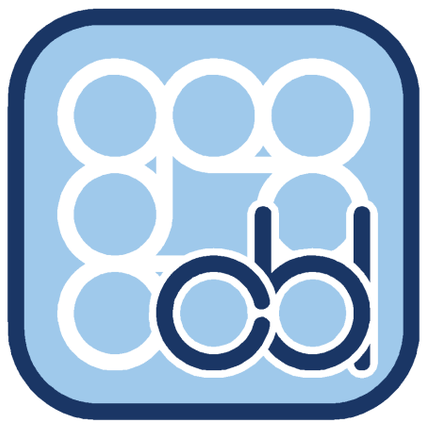
Structured Shrinkage Priors for Neural Networks

Eric Nalisnick

University of Cambridge





Computational and
Biological Learning
University of Cambridge

Outline

1 **Background:** Deep Learning and Modern Neural Networks

2 **Background:** Dropout Regularization

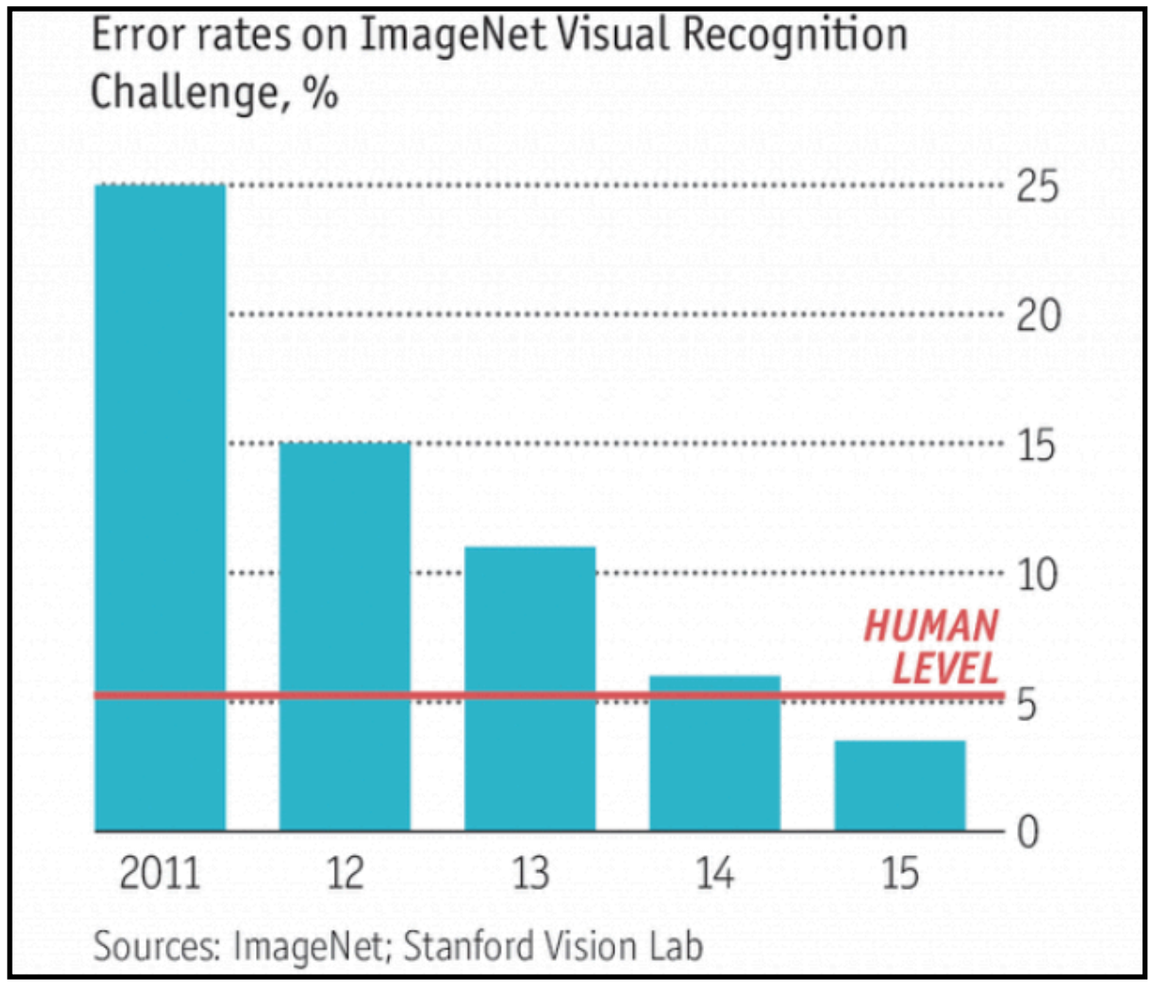
3 **Contribution:** Dropout as Bayesian Shrinkage

4 **Discussion:** Statistics and Deep Learning

Deep Learning and Neural Networks

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

Deep Learning Results

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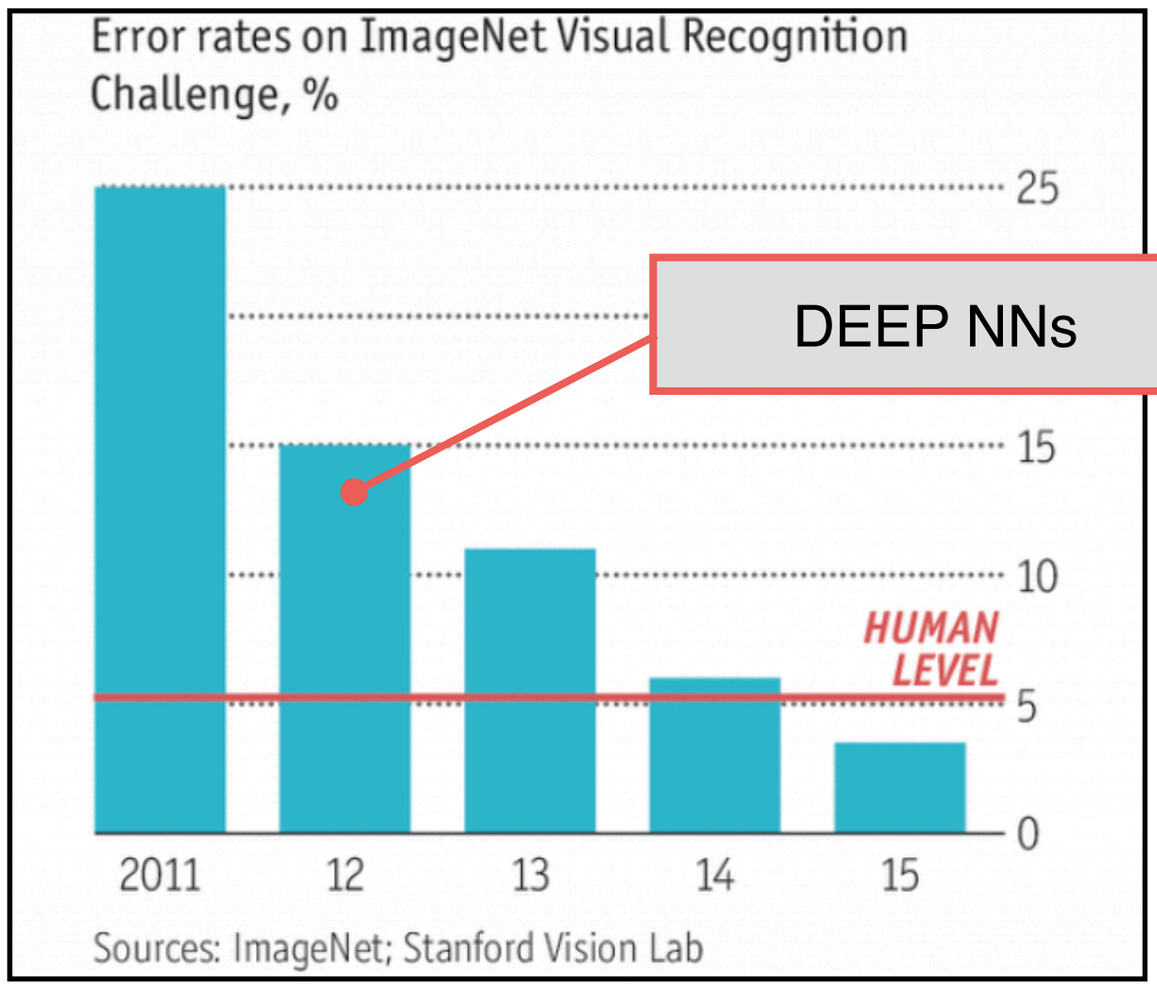

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Deep Learning Results

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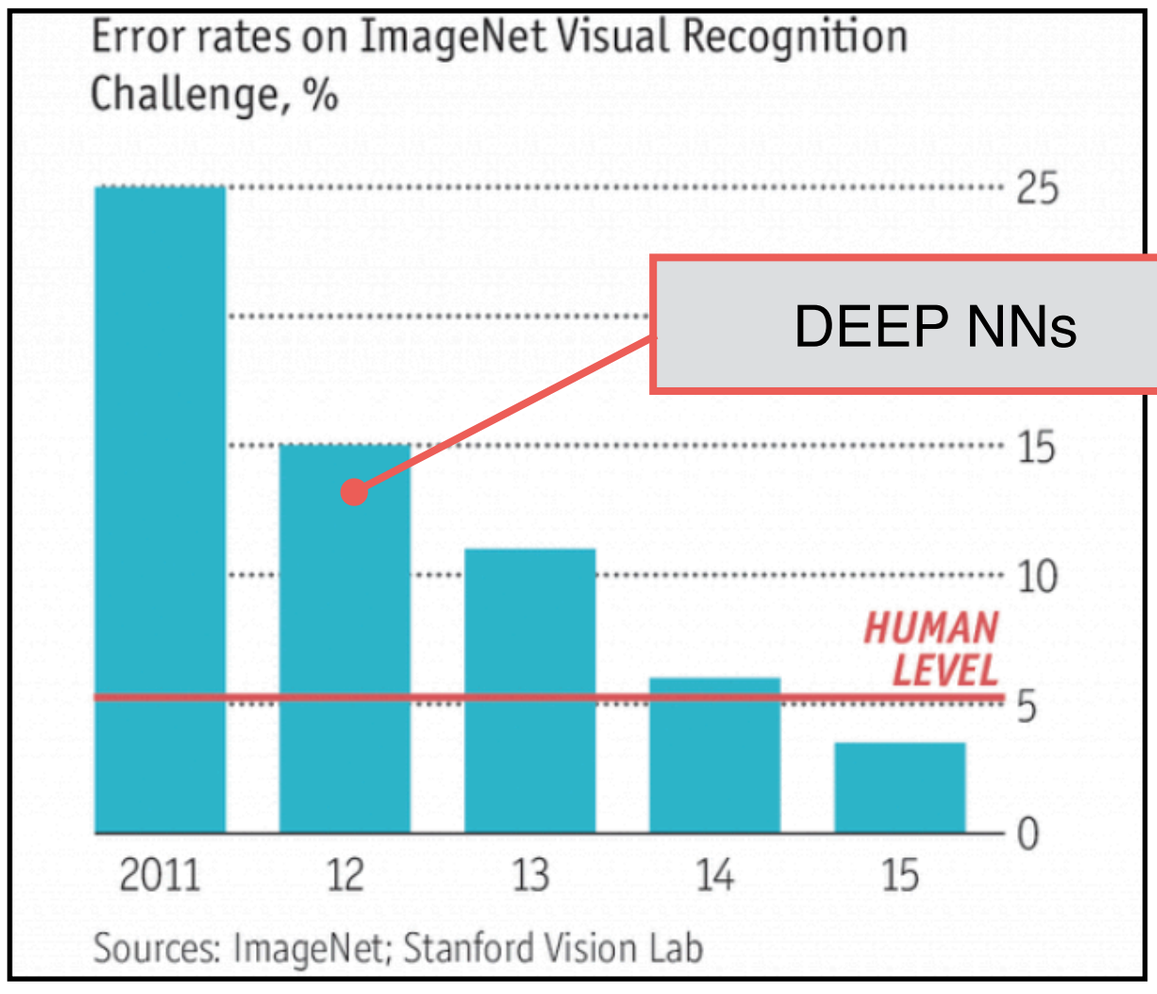
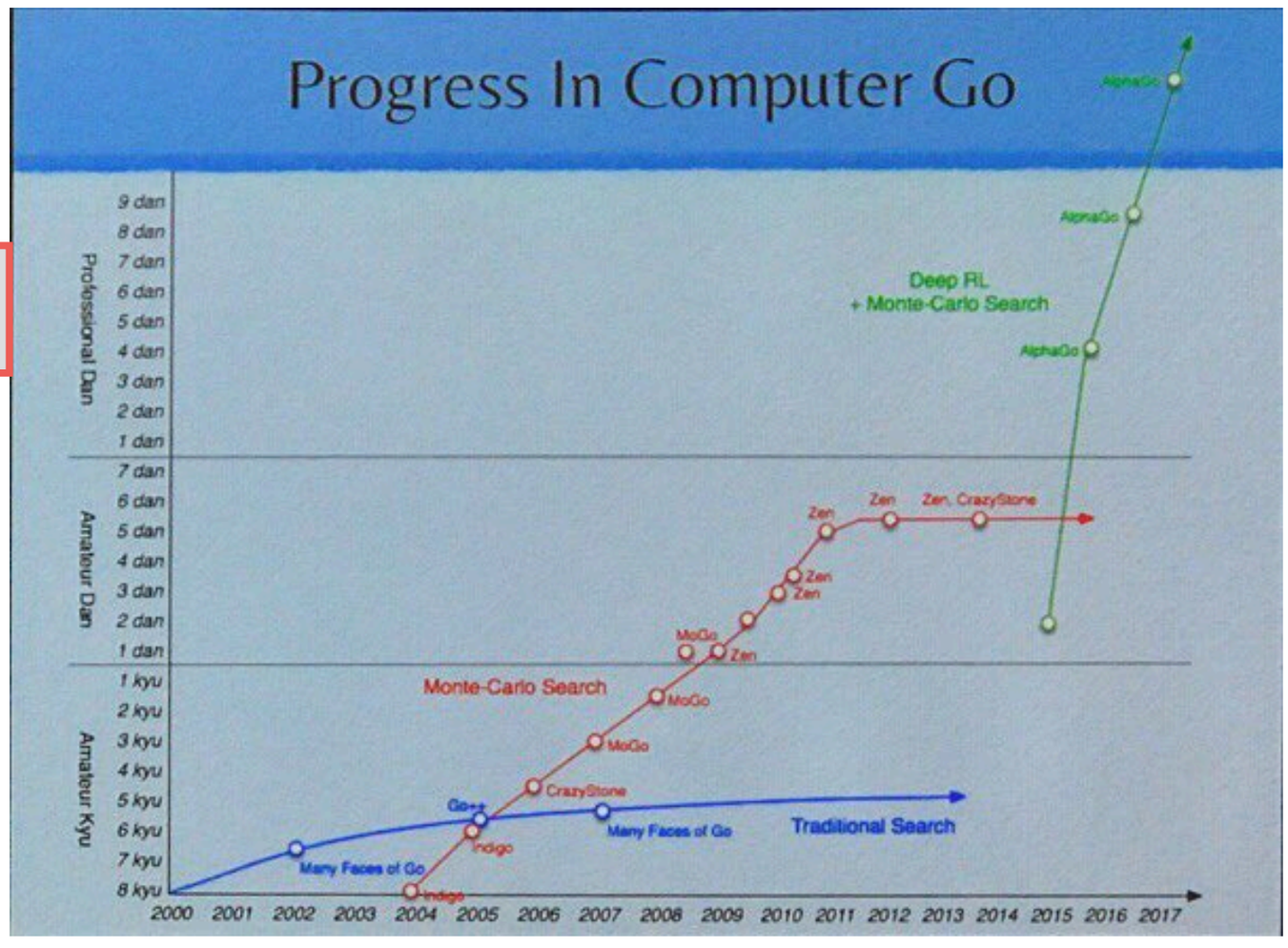
- **Reinforcement Learning**: Results in playing Go.





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Deep Learning Results

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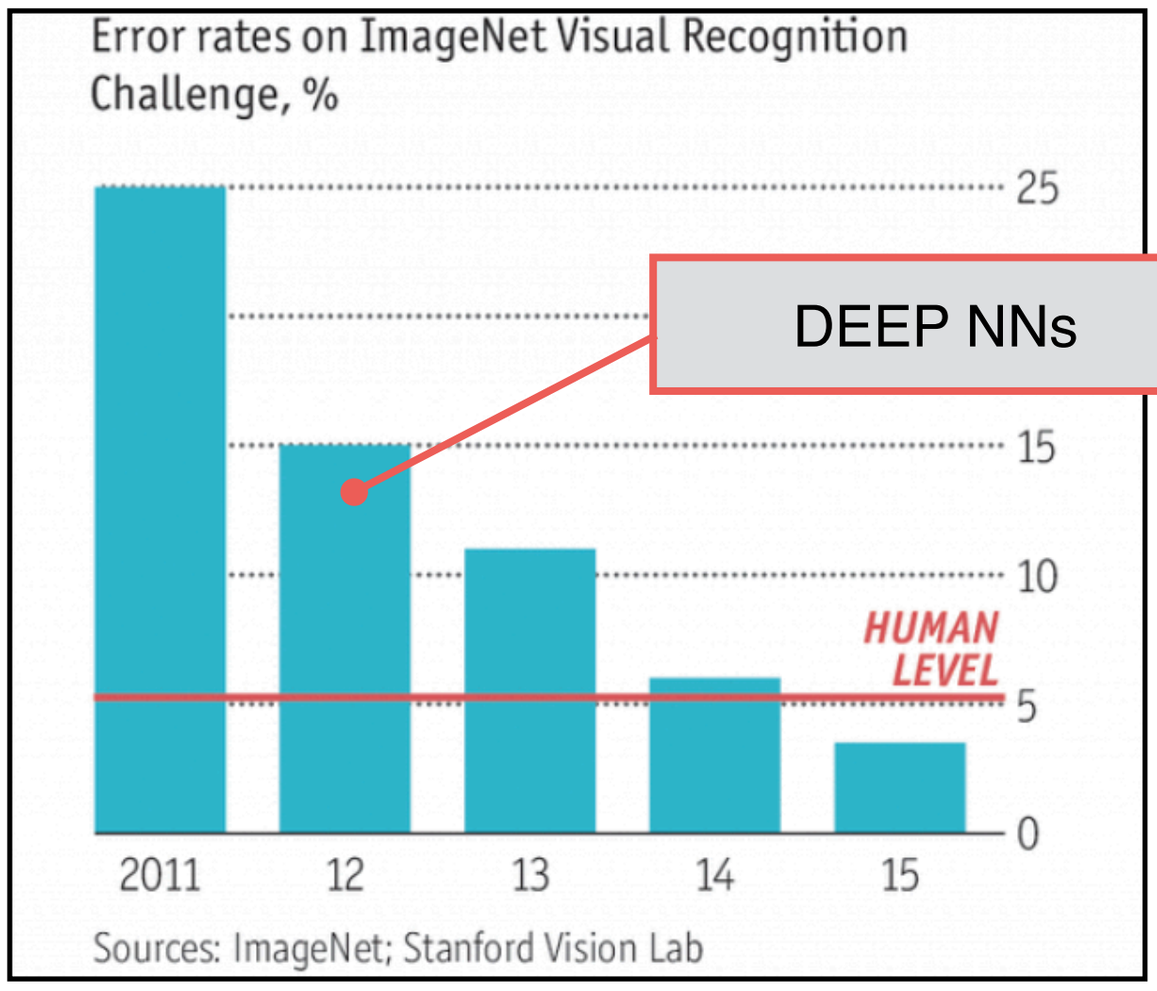
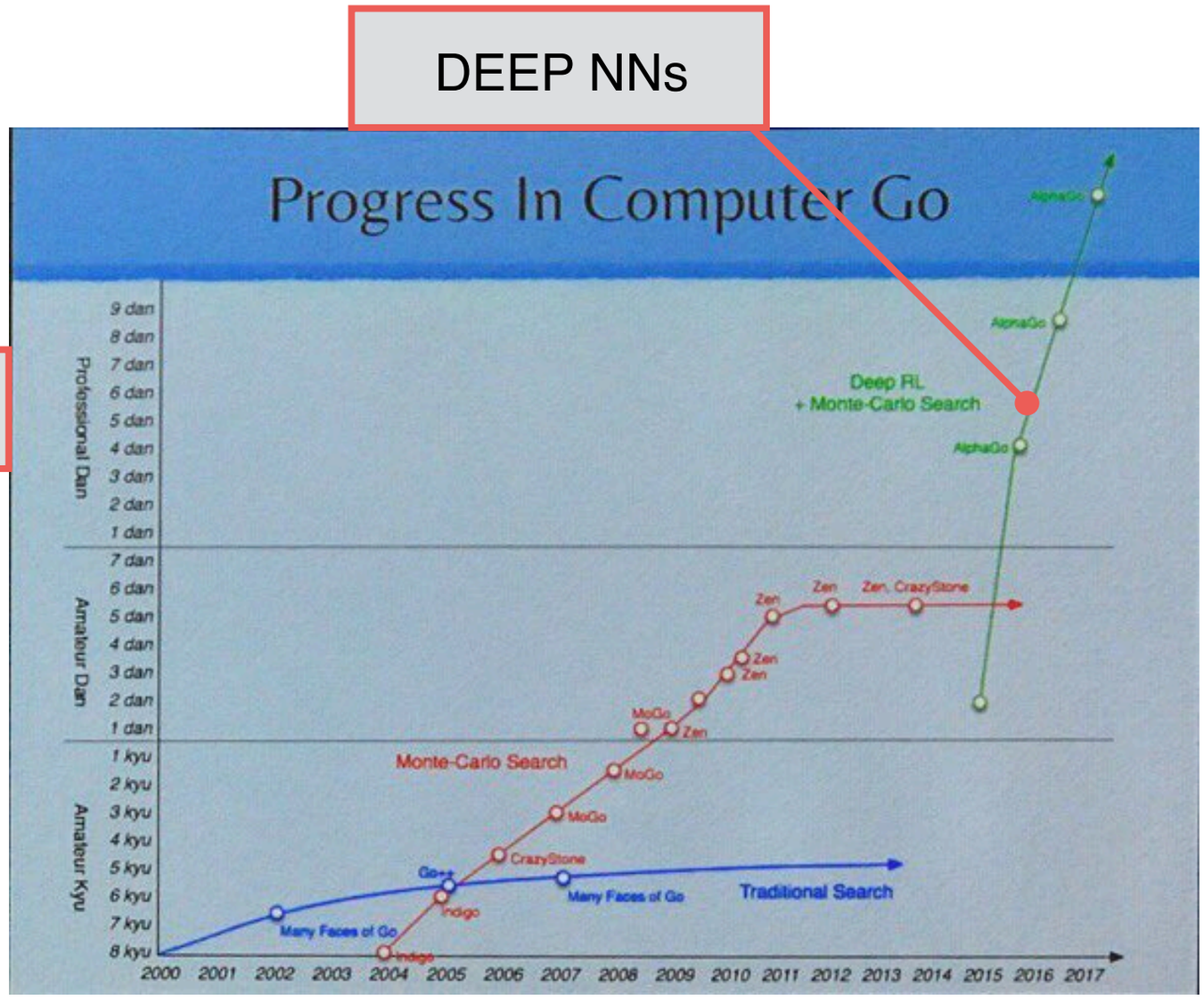


- **Reinforcement Learning**: Results in playing Go.



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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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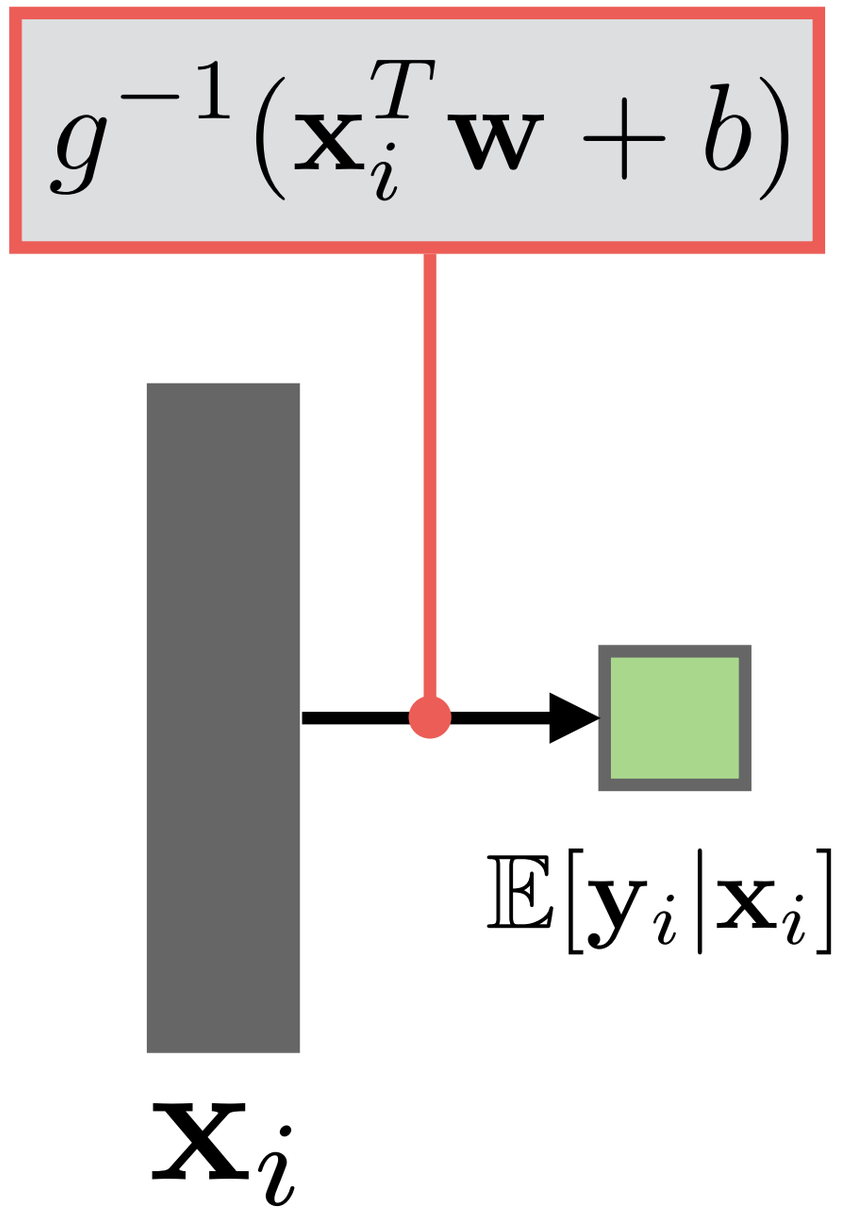
Example: Logistic Regression

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

THE LOGISTIC FUNCTION

Generalized Linear Models (GLMs)



Recursive GLMs

Define a latent feature via a GLM:

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

Recursive GLMs

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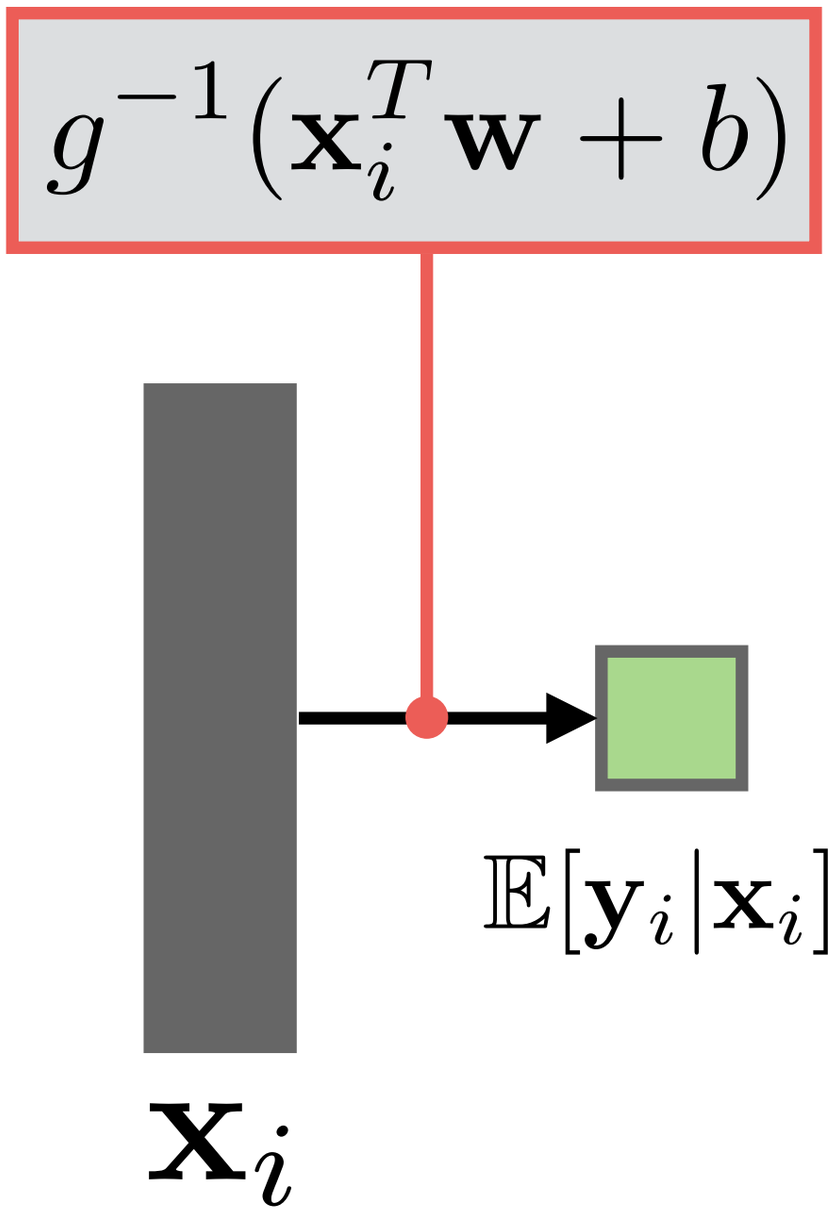
$$g_1^{-1}(\mathbf{x}_i^T \mathbf{w}_1 + b_1) = h_i$$

Define GLM on latent feature:

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

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

Recursive GLMs



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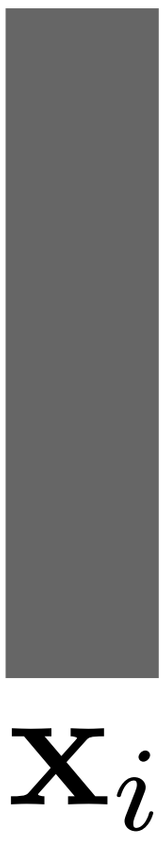
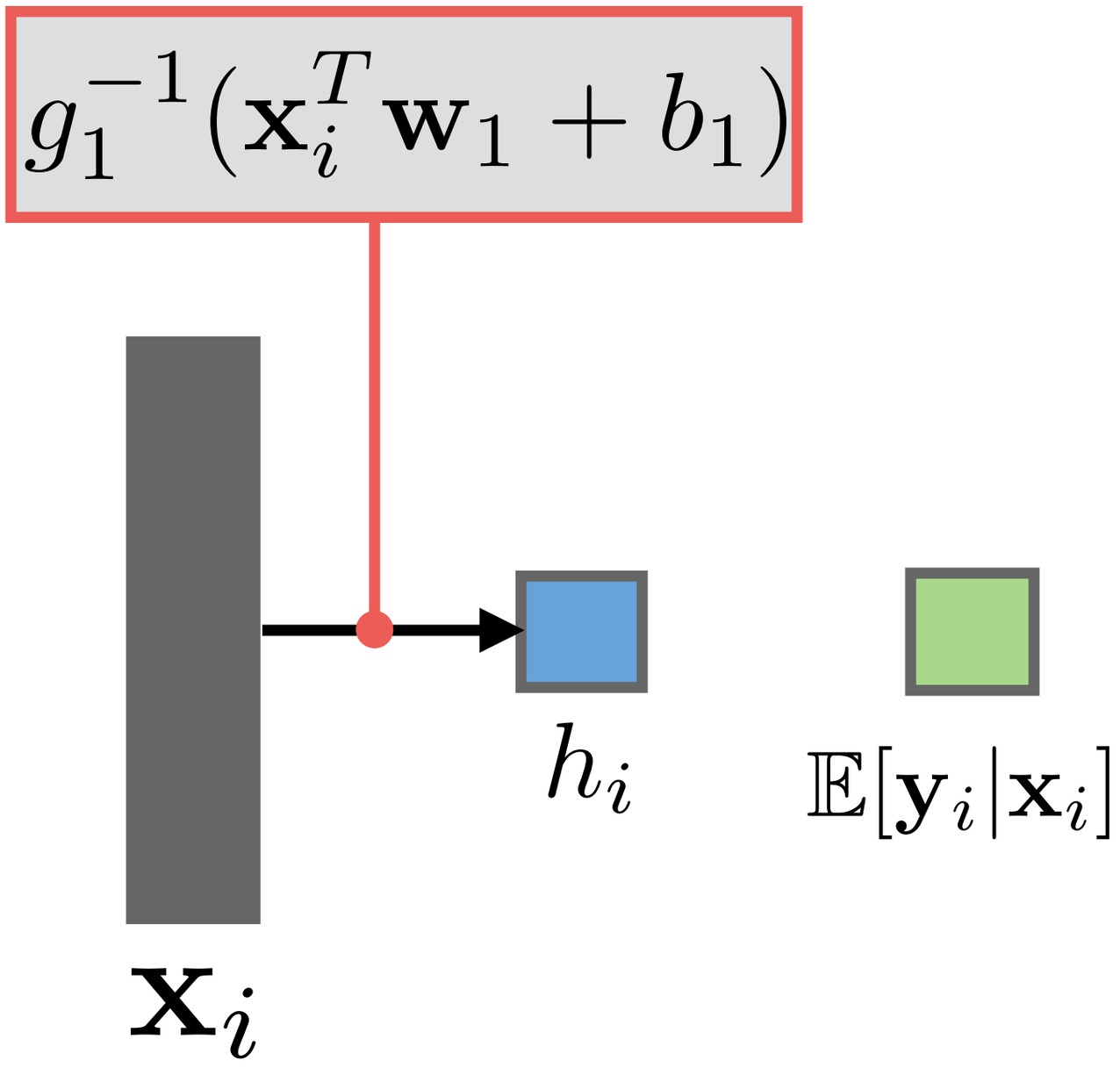


$\mathbf{x}_i$

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

Recursive GLMs



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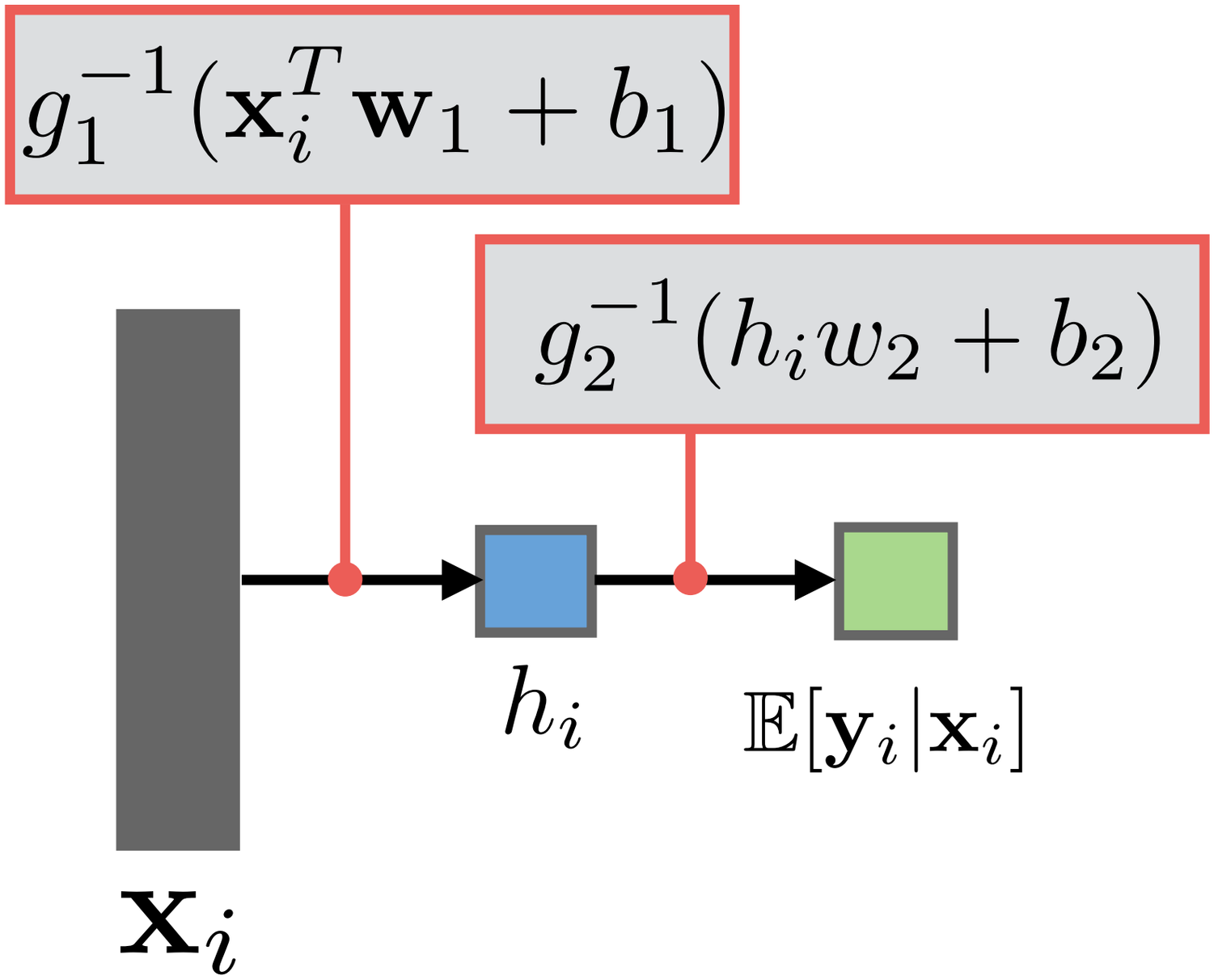
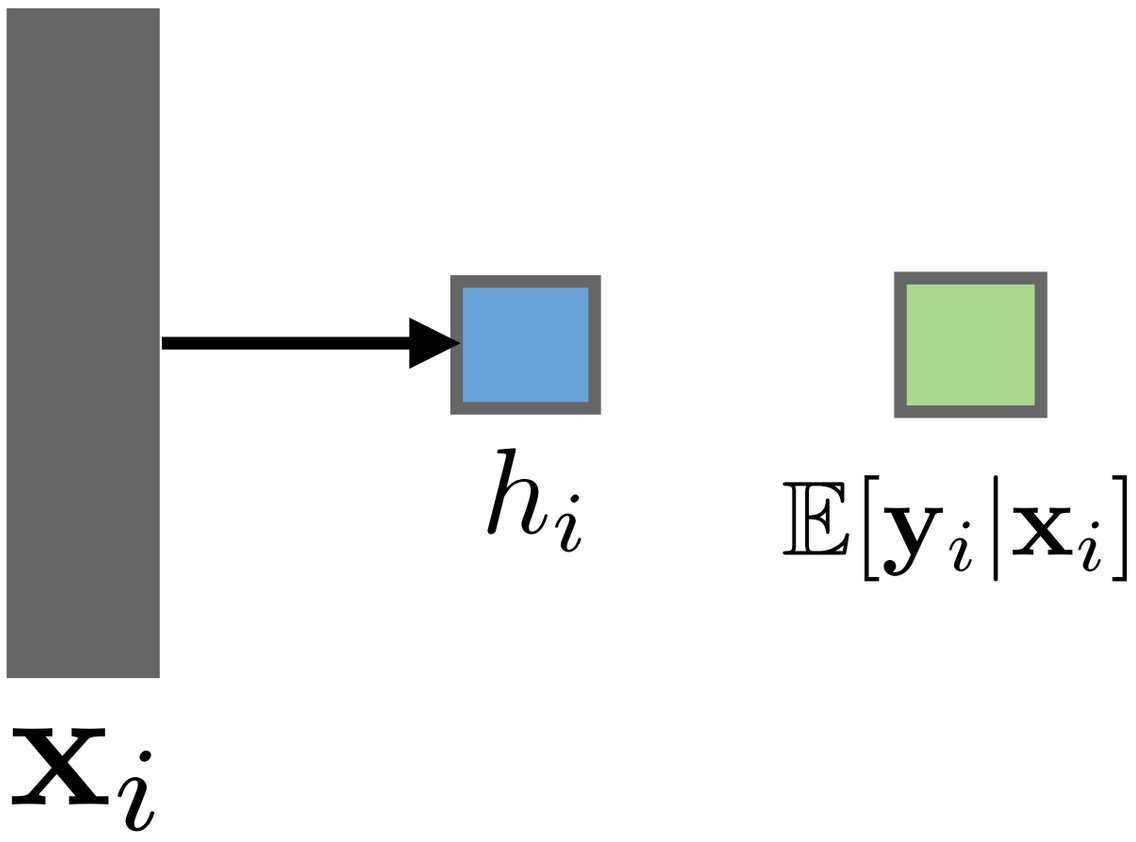


Building Neural Nets from Recursive GLMs



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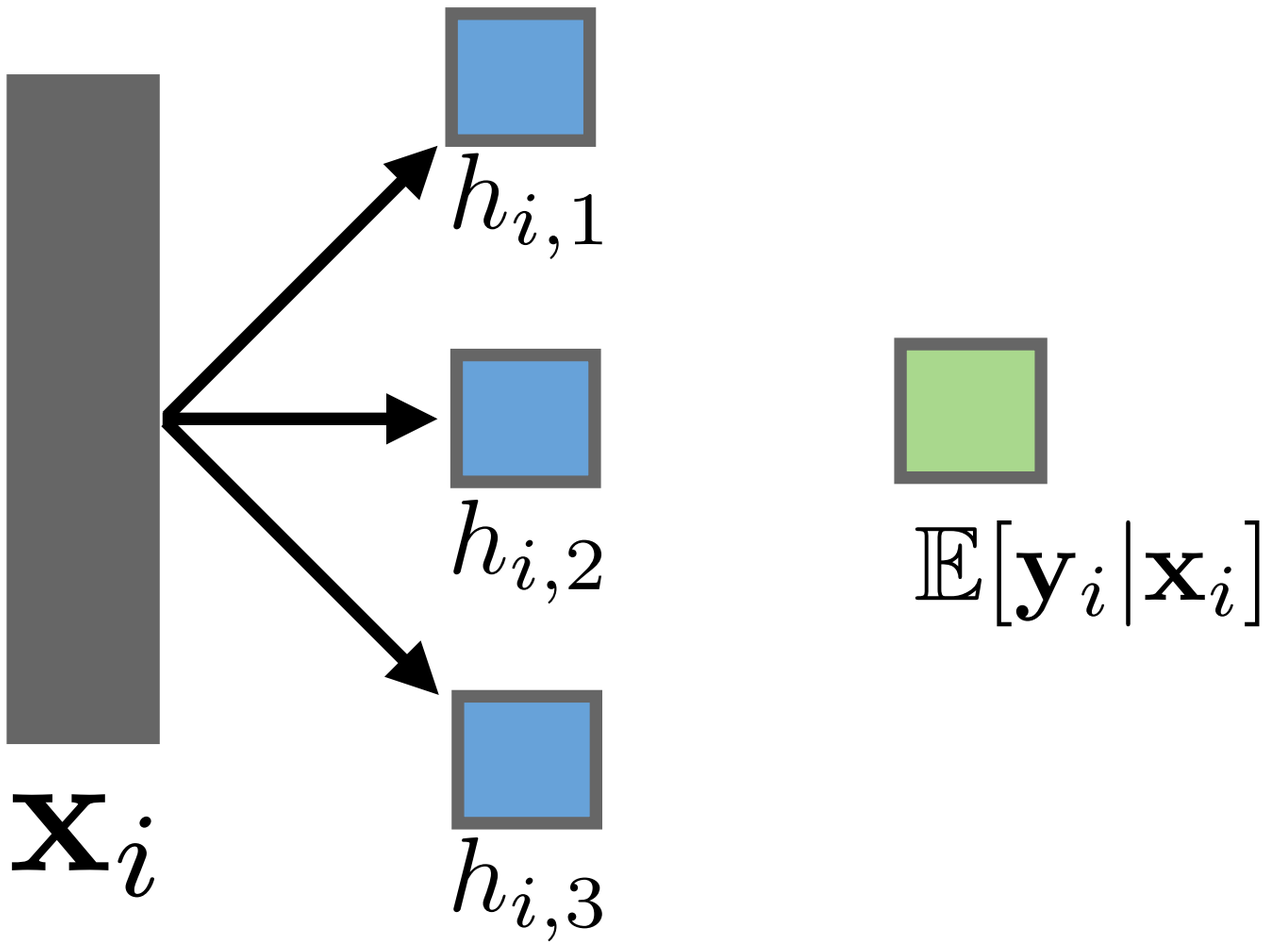
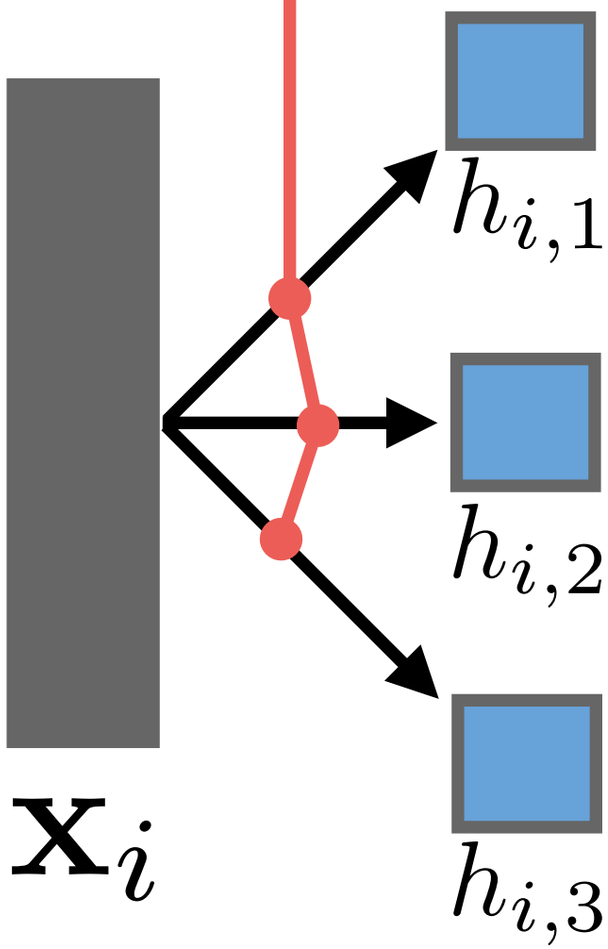


Building Neural Nets from Recursive GLMs

$$h_{i,j} = g_{1,j}^{-1}(\mathbf{x}_i^T \mathbf{w}_{1,j} + b_j)$$

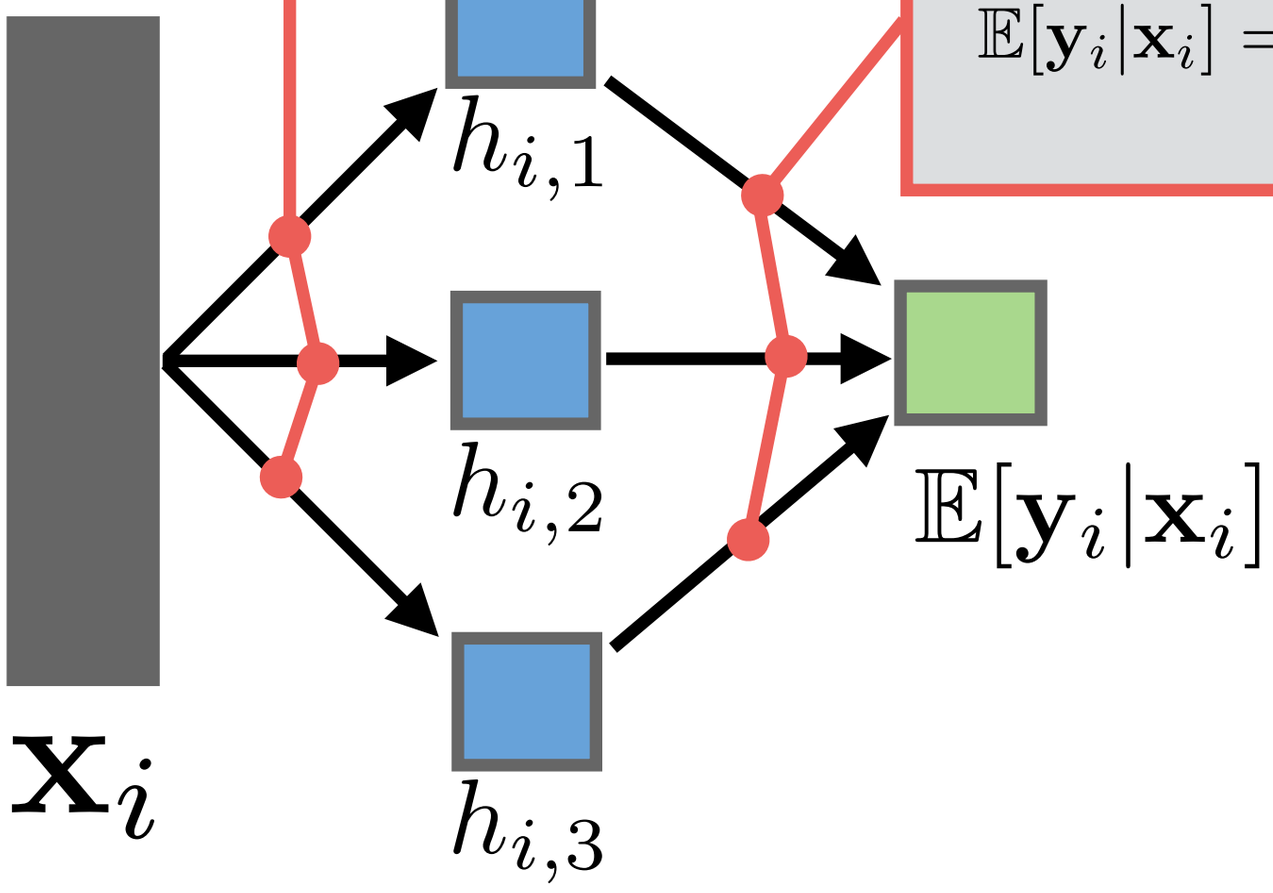


$\mathbb{E}[\mathbf{y}_i|\mathbf{x}_i]$

Building Neural Nets from Recursive GLMs

$$h_{i,j} = g_{1,j}^{-1}(\mathbf{x}_i^T \mathbf{w}_{1,j} + b_j)$$

$$\mathbb{E}[\mathbf{y}_i|\mathbf{x}_i] = g_2^{-1}\left(\sum_{j=1}^{H} h_{i,j} w_{2,j} + b_2\right)$$

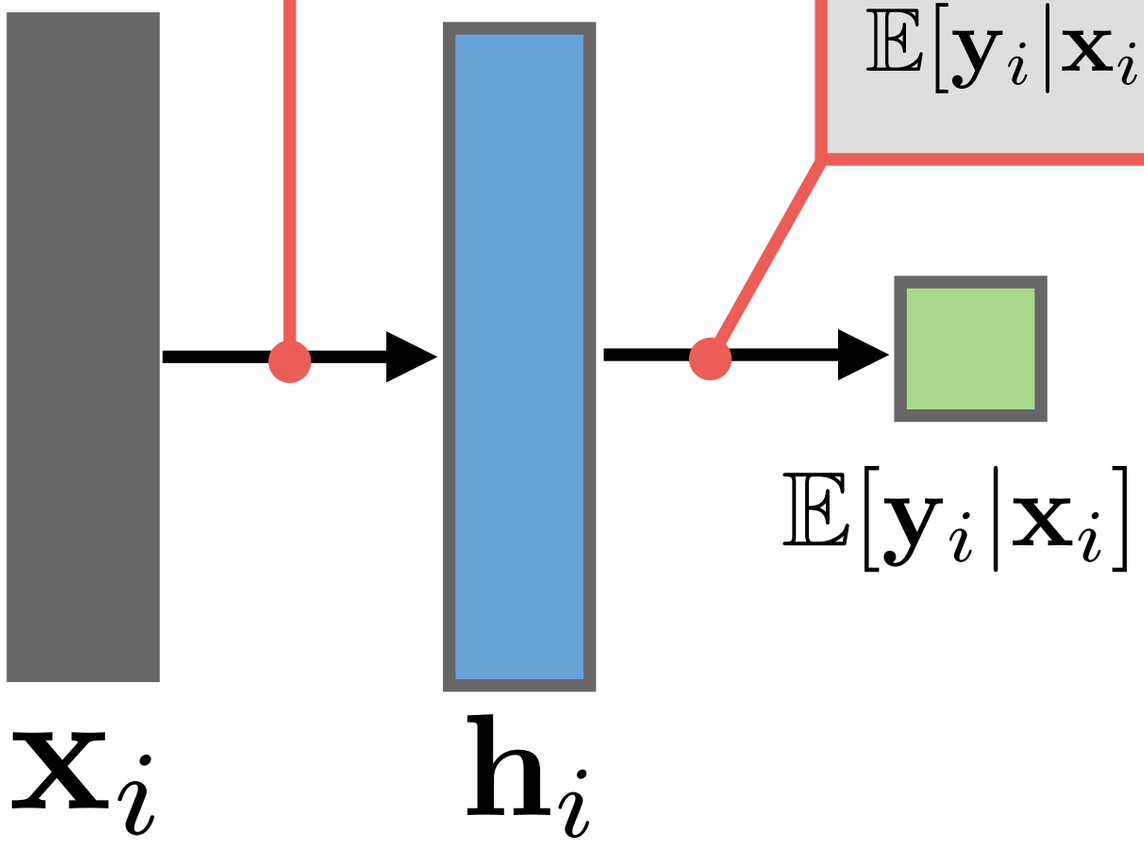


Building Neural Nets from Recursive GLMs

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

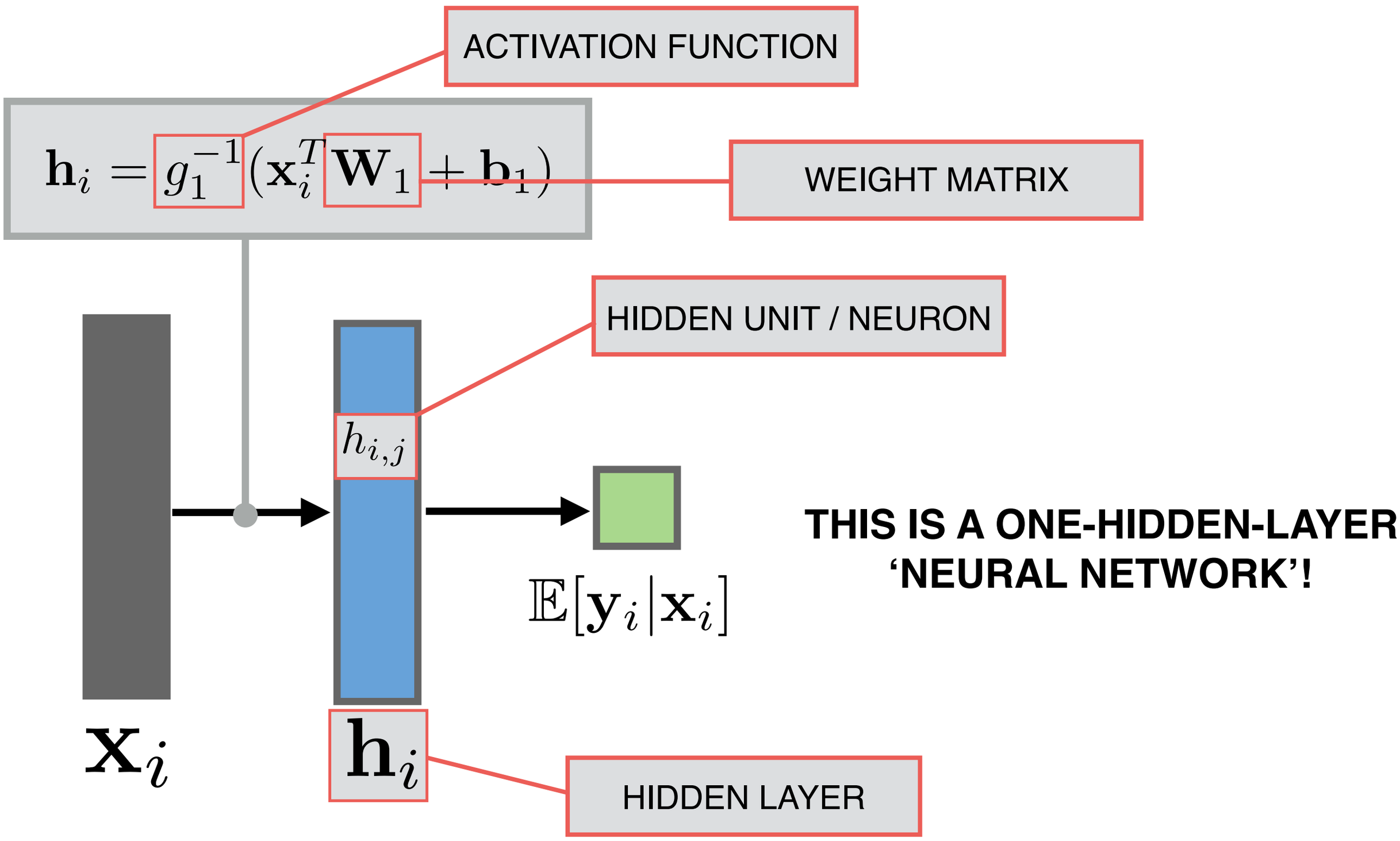
$$\mathbf{h}_i = g_1^{-1}(\mathbf{x}_i^T \mathbf{W}_1 + \mathbf{b}_1)$$

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



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

Building Neural Nets from Recursive GLMs



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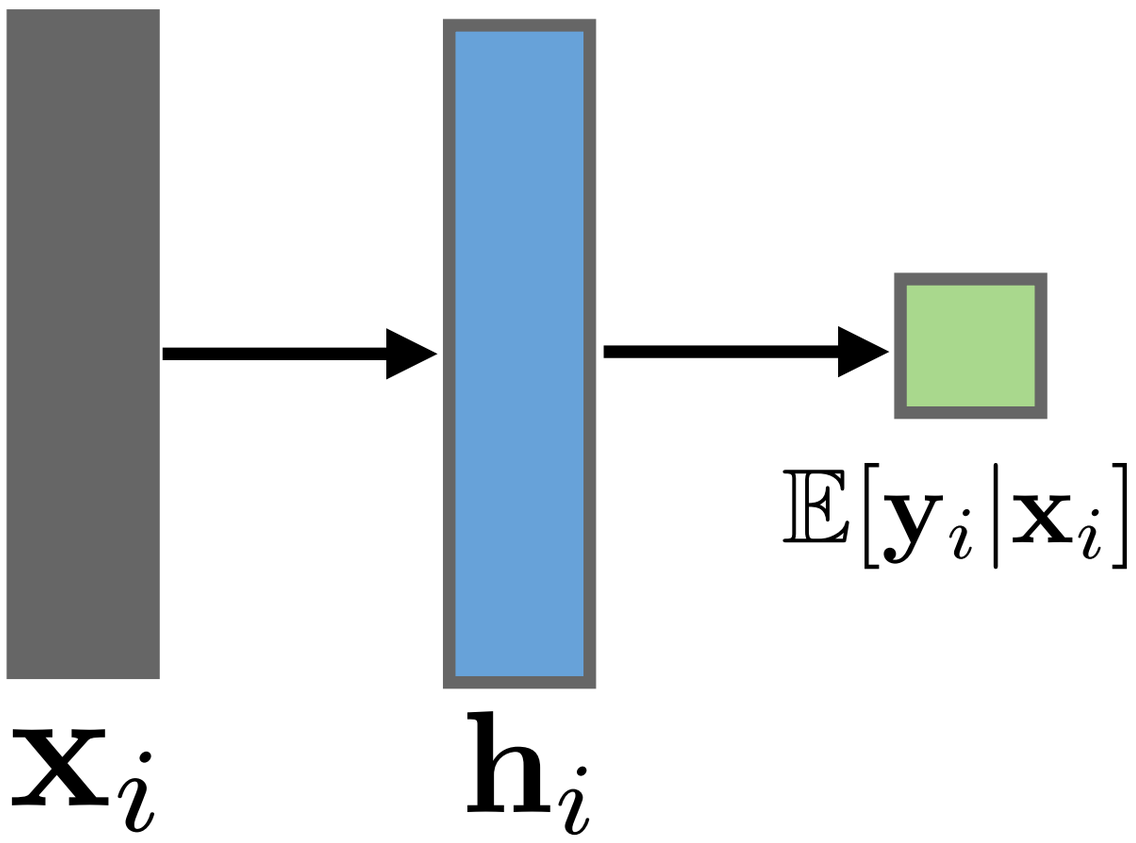
Deep Neural Networks



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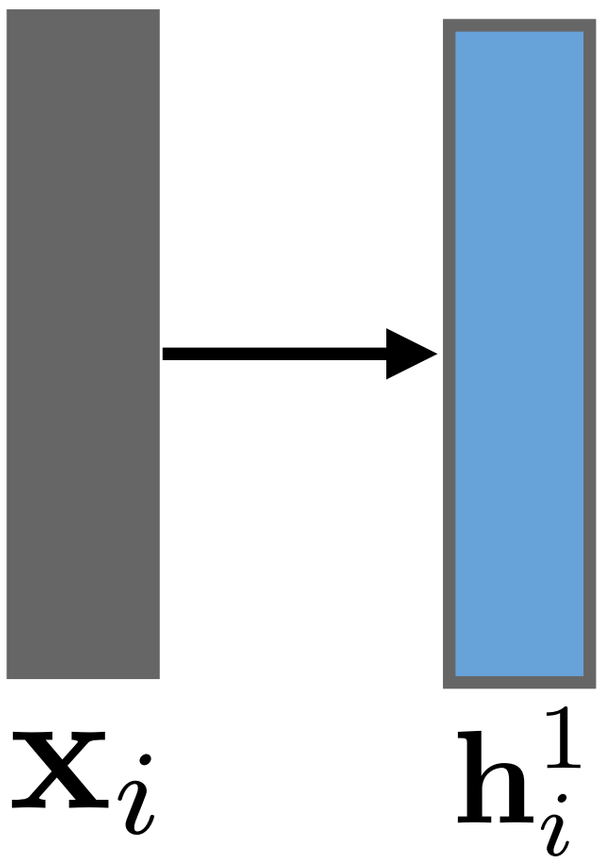
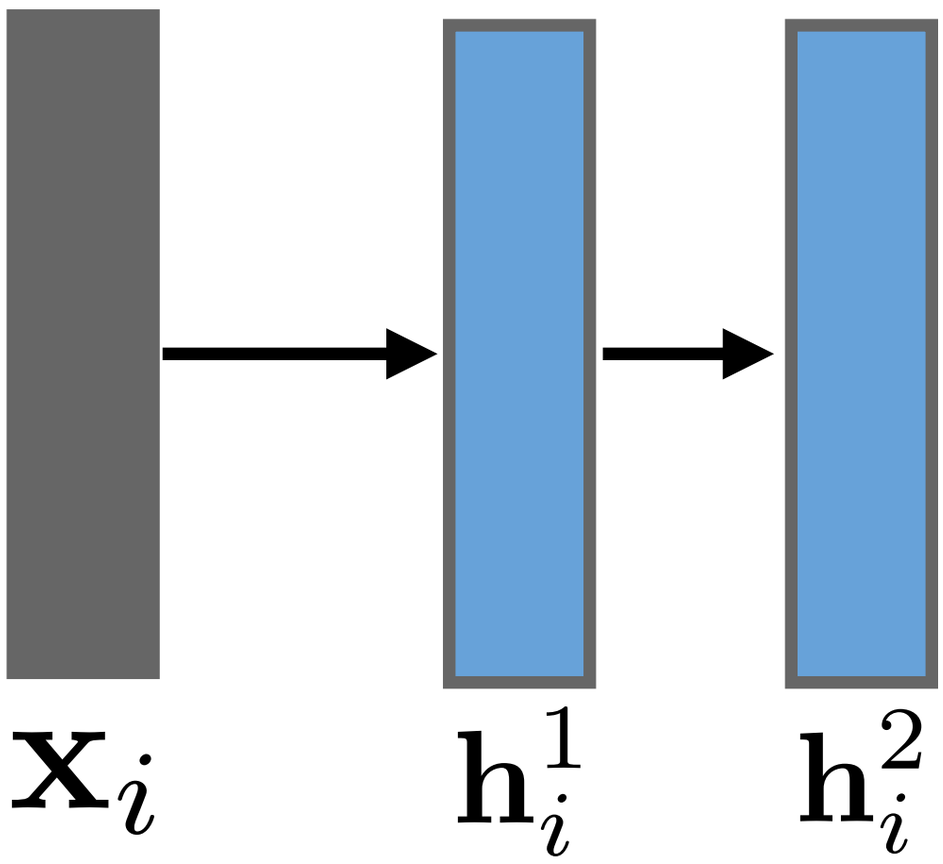
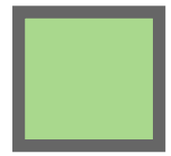


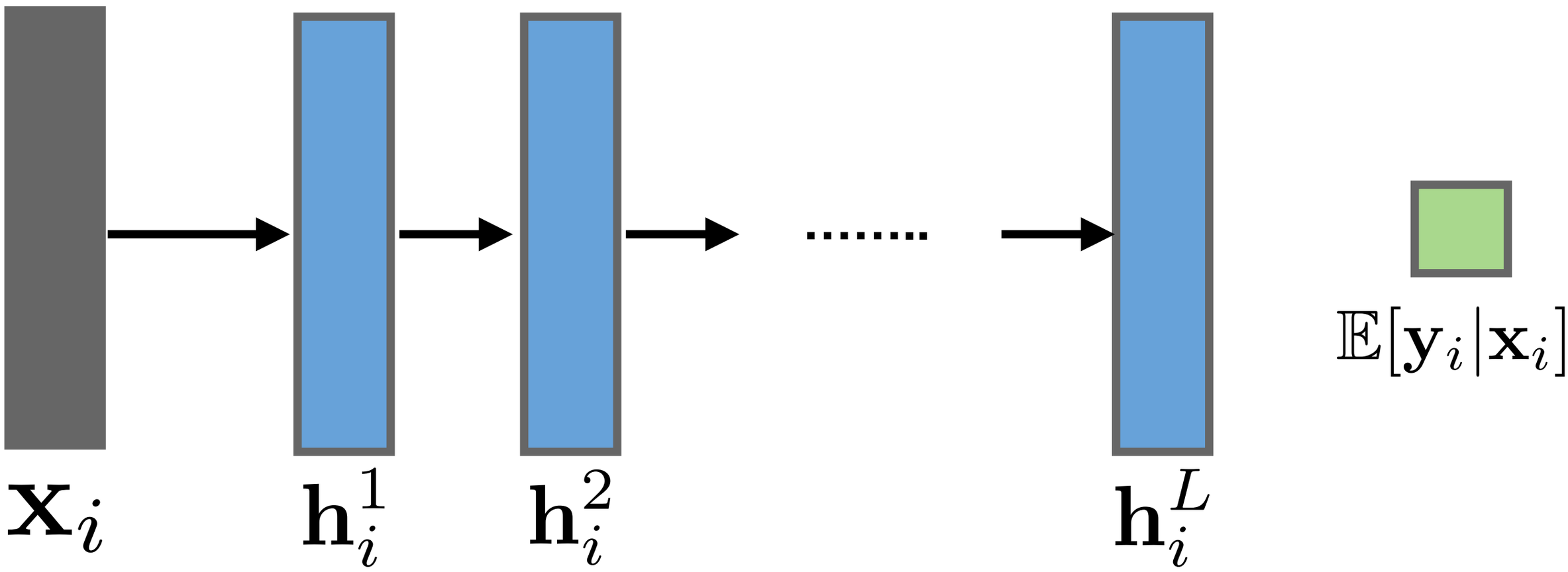
Deep Neural Networks





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

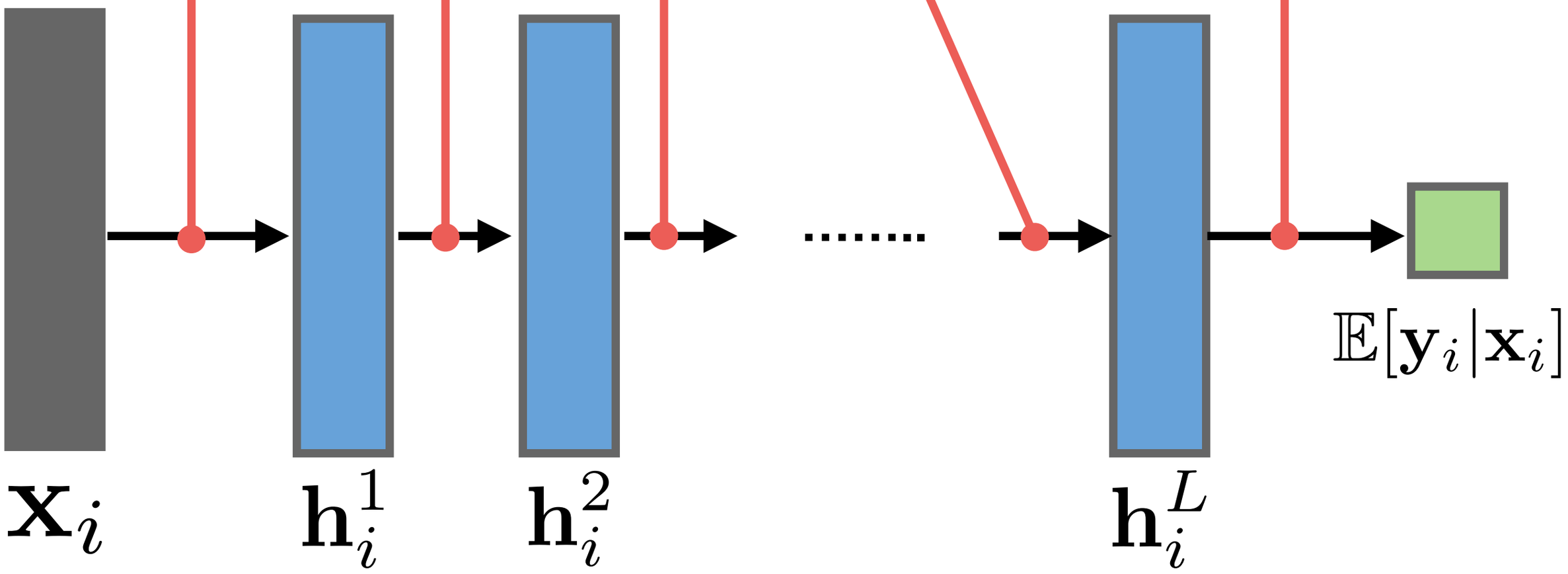
Deep Neural Networks



Deep Neural Networks

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

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

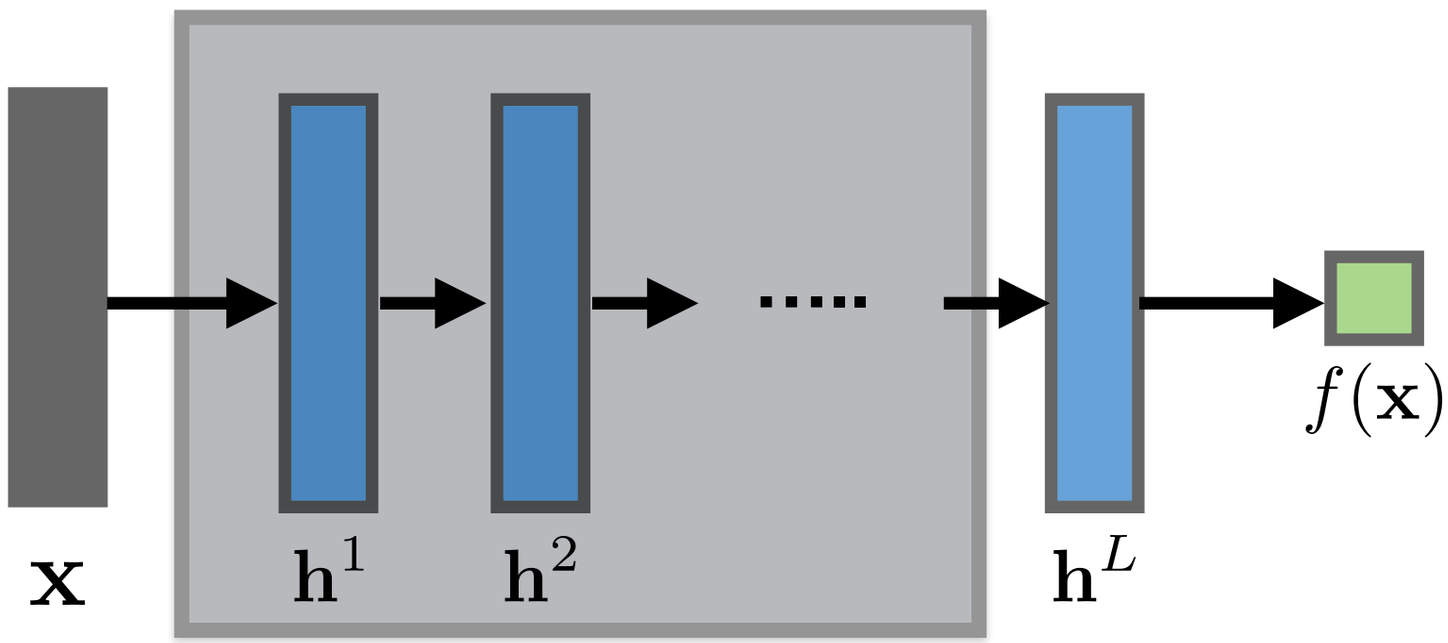


Deep Neural Networks

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

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

NEW REPRESENTATION
OF FEATURES COMPUTED BY NN LAYERS



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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PARAMETER UPDATE

$$\mathbf{W}_l^{t+1} = \mathbf{W}_l^t + \alpha \, \nabla_{\mathbf{W}_l} \mathcal{L}(\mathbf{X}, \mathbf{Y}, \{\mathbf{W}_l\}_1^{L+1}, \{\mathbf{b}_l\}_1^{L+1})$$

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learning rate / step size.

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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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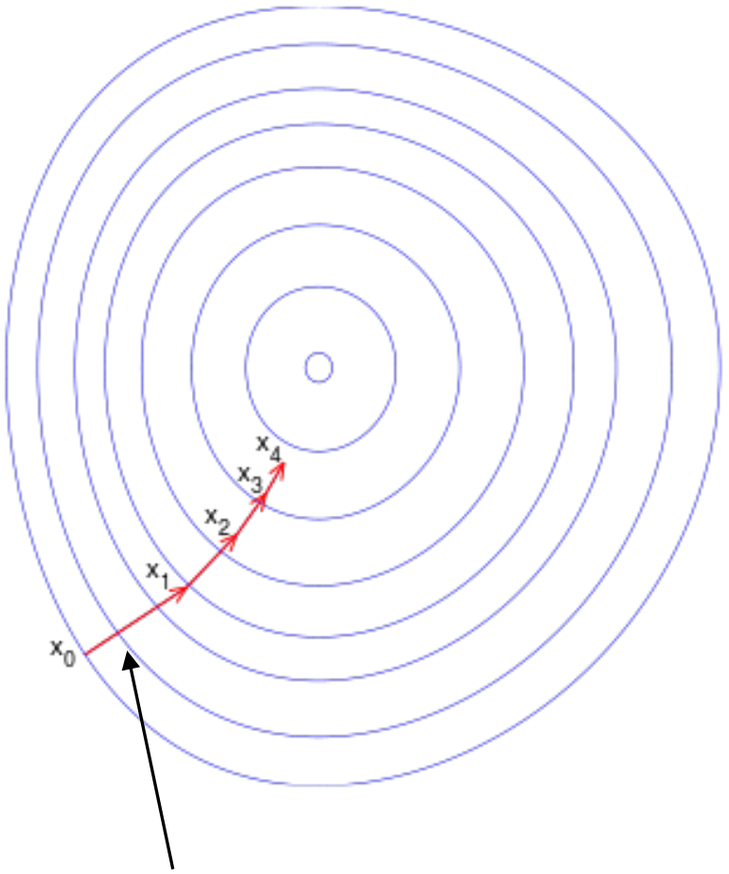

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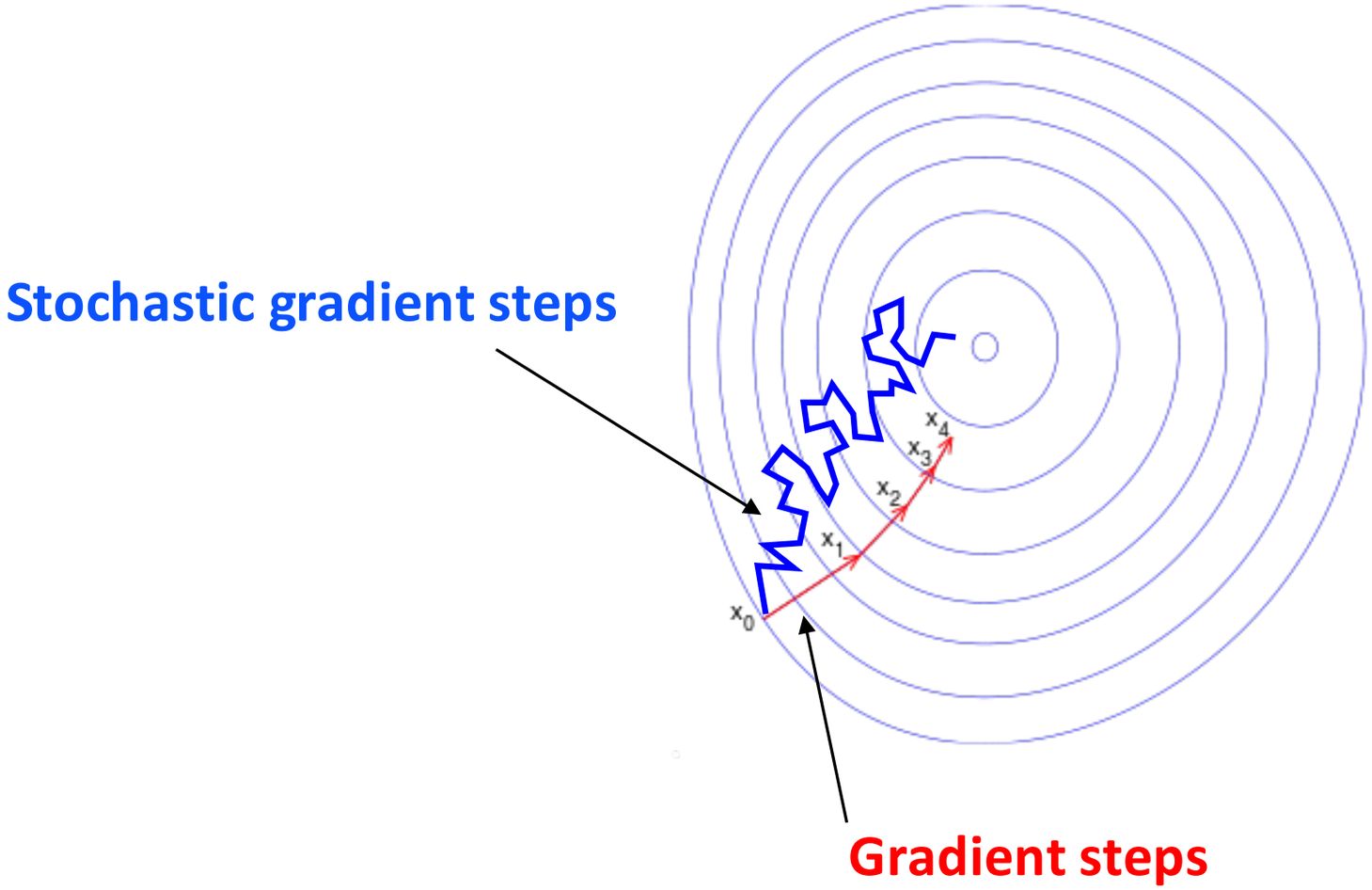

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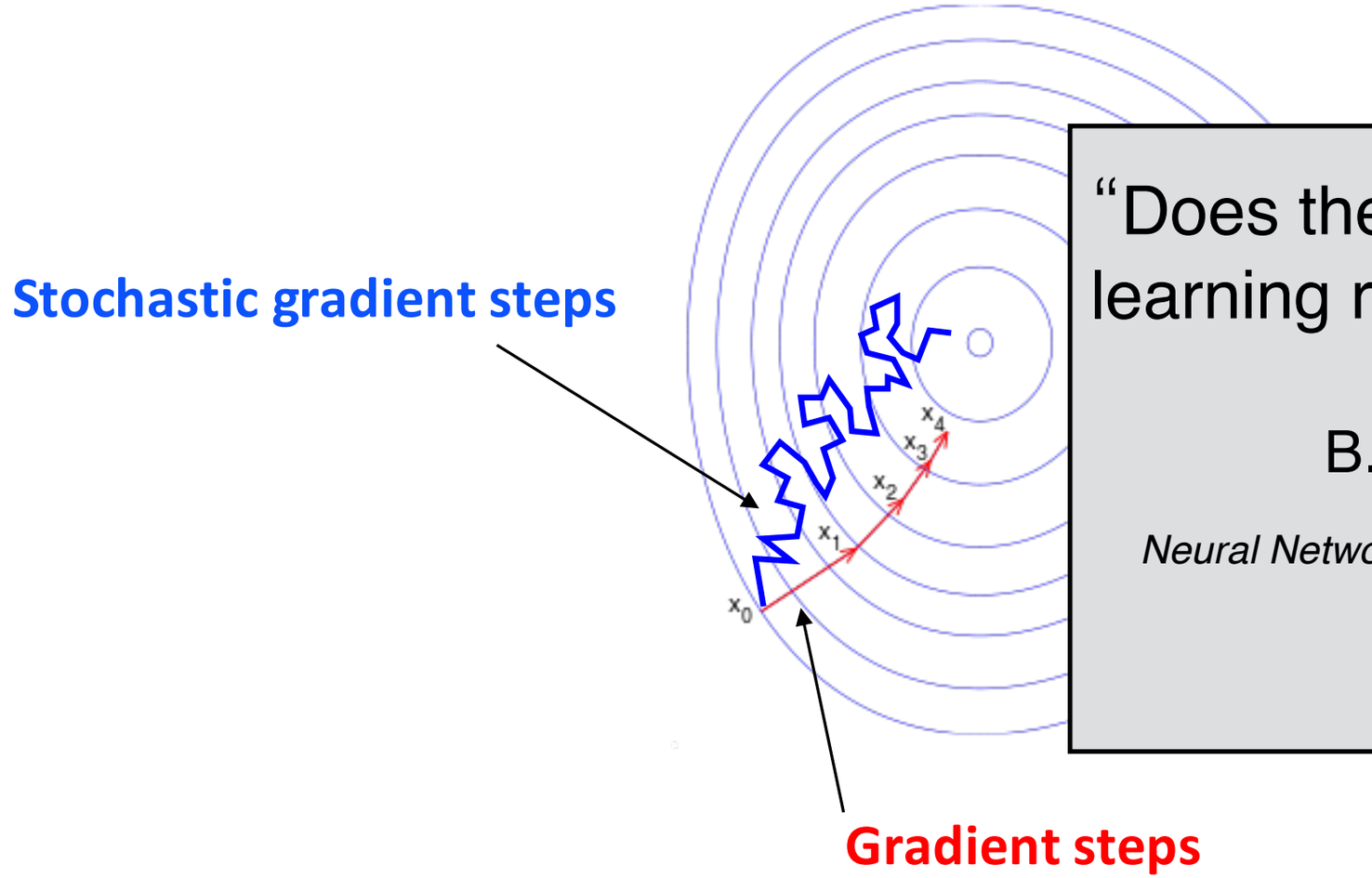


"Does the error-backpropagation learning rule…still have a place?"

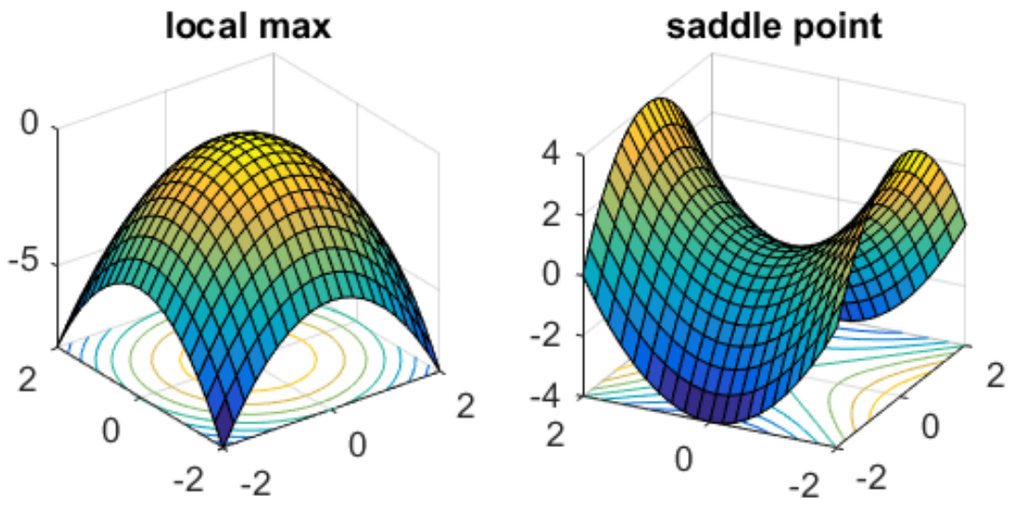
B. Cheng and D. M. Titterington

Neural Networks: A Review from a Statistical Perspective

(1994)

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]



http://www.offconvex.org/2016/03/22/

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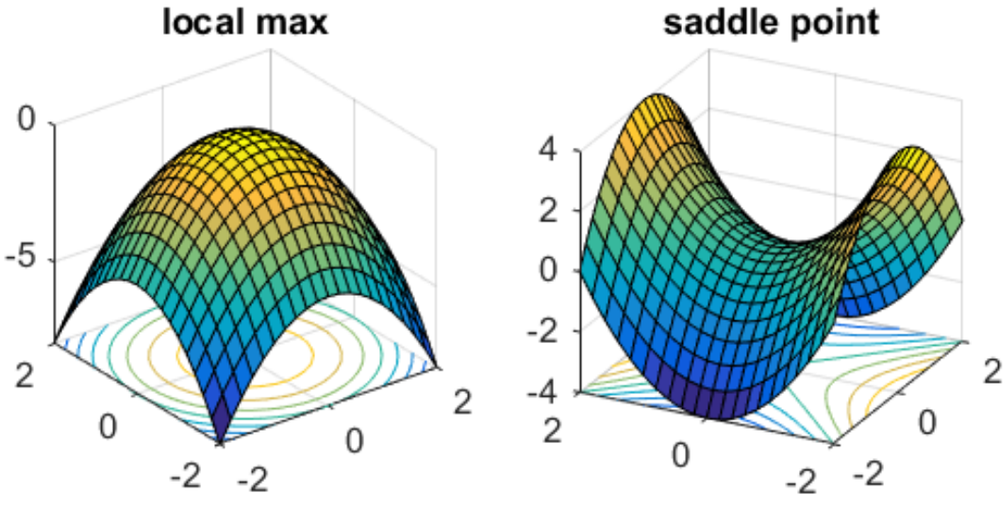

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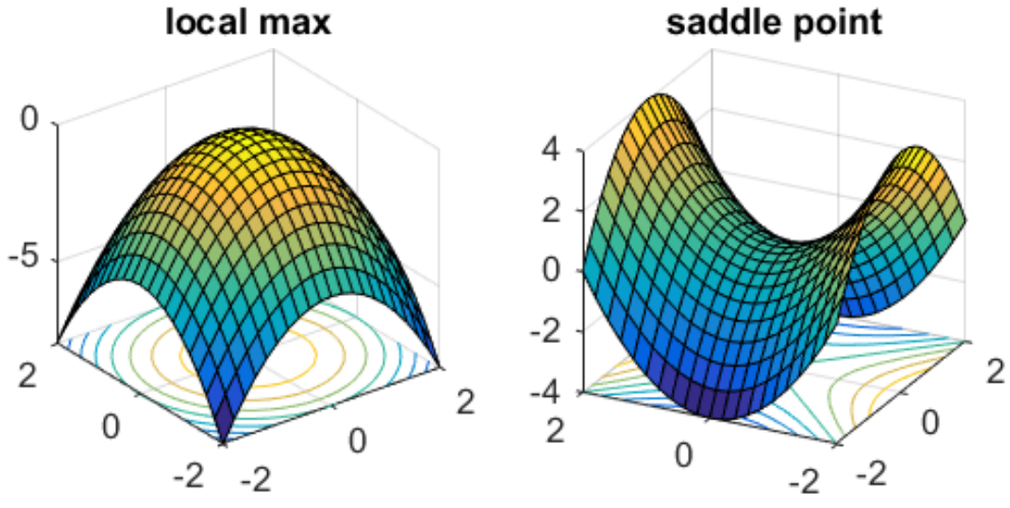
- **Intuition:** It's hard to build a high-dimensional max / min because the surface must be going in the same direction in all dimensions.

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



http://www.offconvex.org/2016/03/22/

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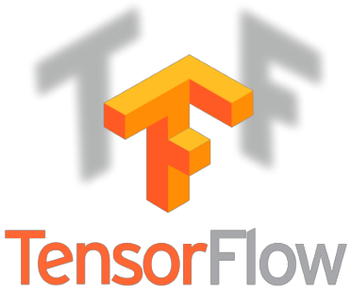
- **Automatic Differentiation**: Various 'autodiff' software libraries can compute these gradients for you, just needing definition of the forward model.

RONAN COLLOBERT (2000)

UNIVERSITY OF MONTREAL (2011)



GOOGLE BRAIN (2009/2015)

FACEBOOK AI (2016)

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MOST POPULAR TODAY

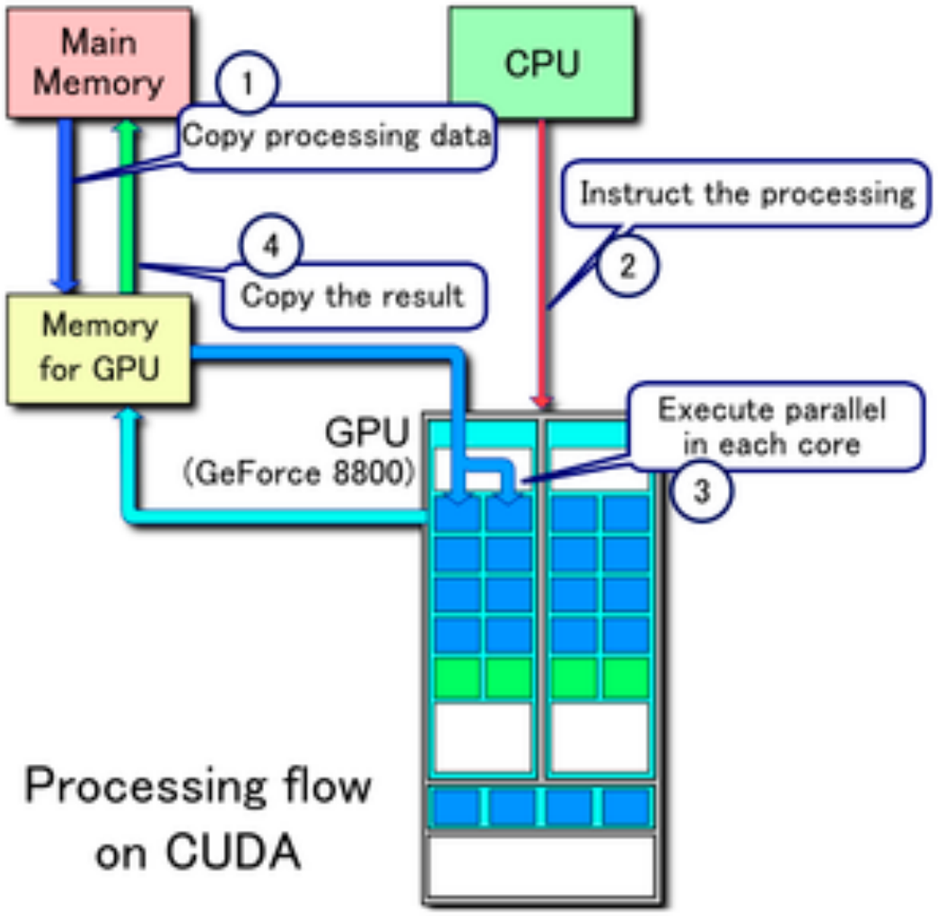
torch — RONAN COLLOBERT (2000)

theano — UNIVERSITY OF MONTREAL (2011)

TensorFlow — GOOGLE BRAIN (2009/2015)

PYTORCH — FACEBOOK AI (2016)

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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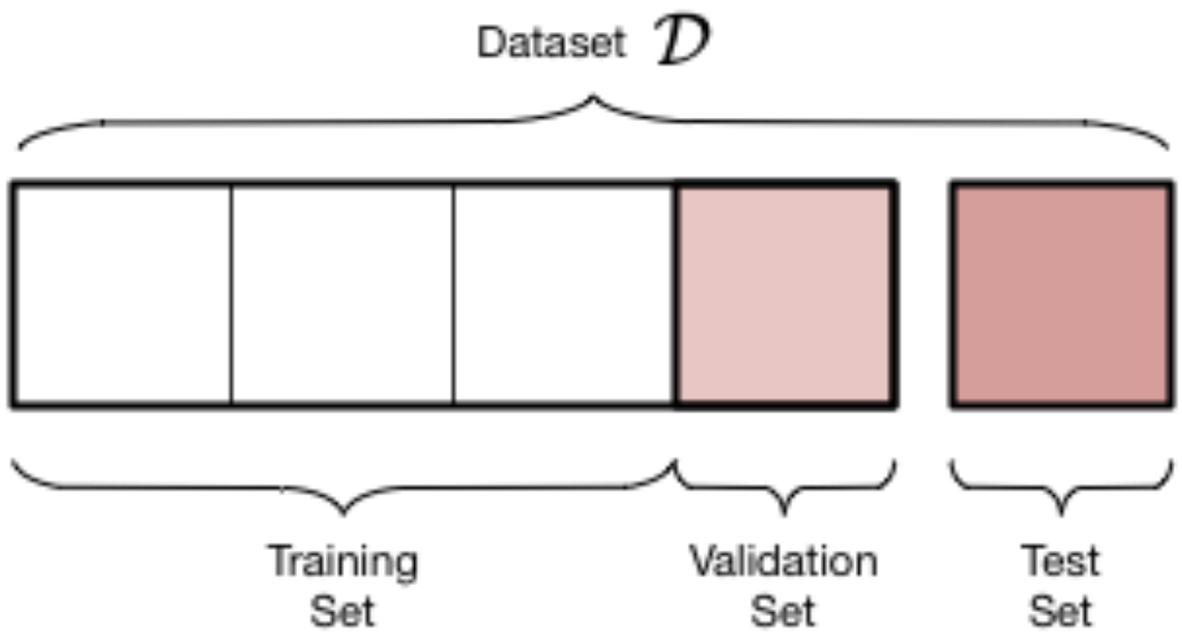

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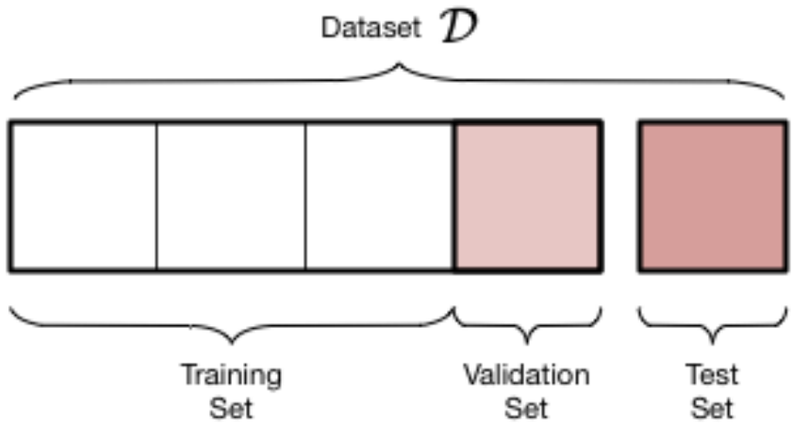
- Usually, a **random or grid search** over hyper parameters is performed, and **performance on a validation set** is used to make the final selection.

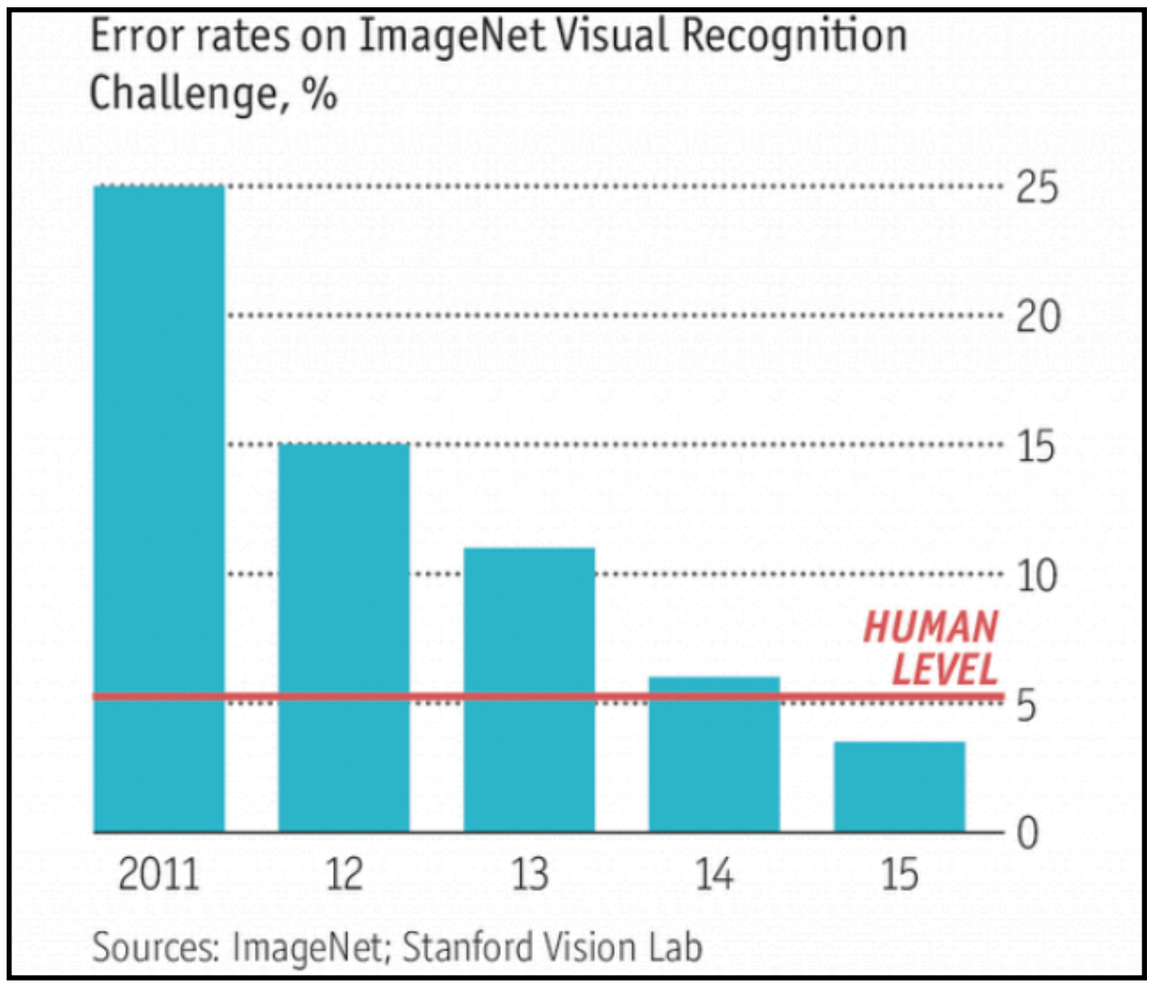
- Improving the model selection process is an on-going area of research. Bayesian optimization, bandit algorithms, and reinforcement learning methods have been proposed.



Dropout Regularization

Deep Learning Results

Computer Vision: Results on ImageNet object classification dataset.



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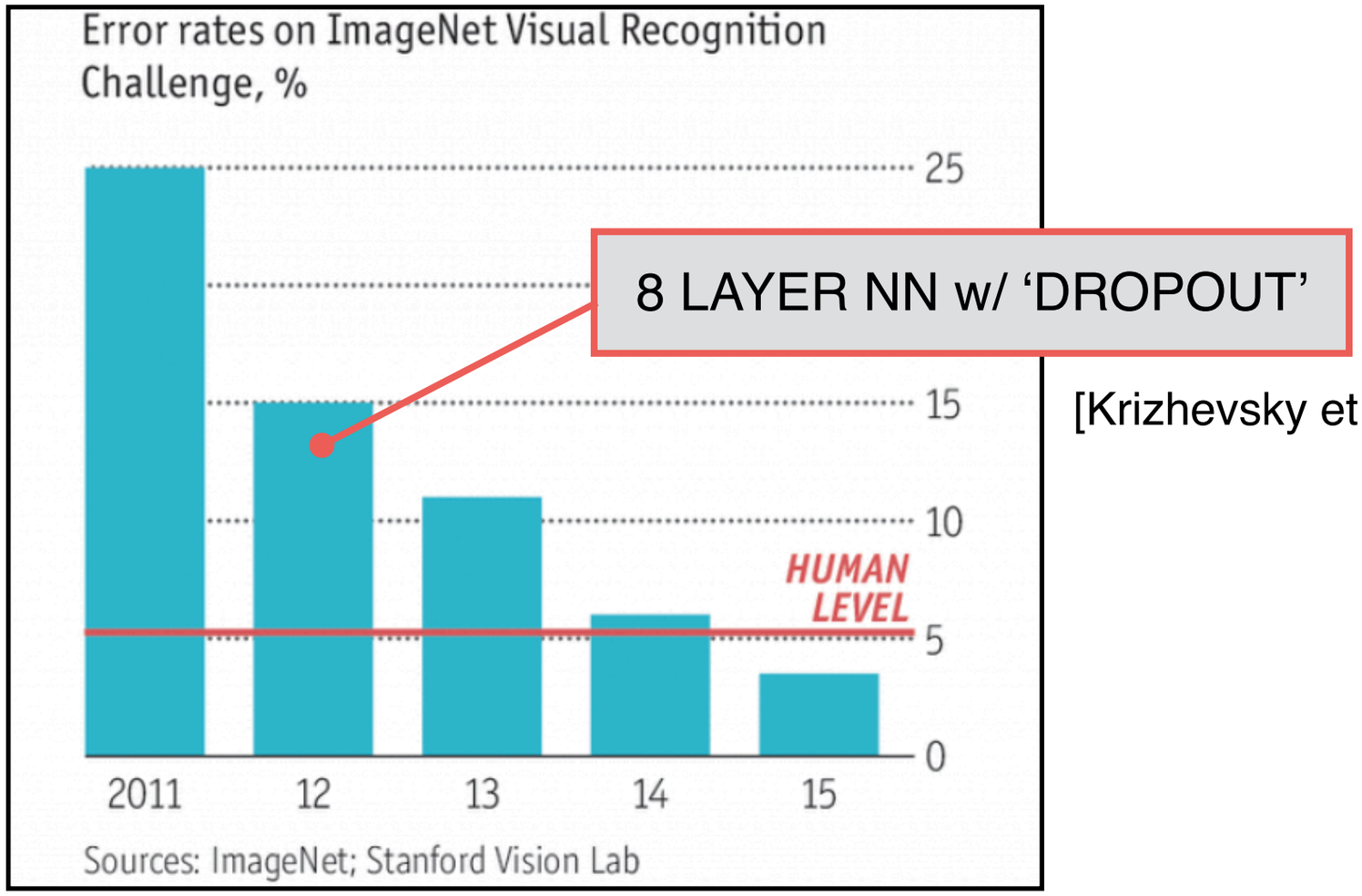

[Krizhevsky et al., 2012]

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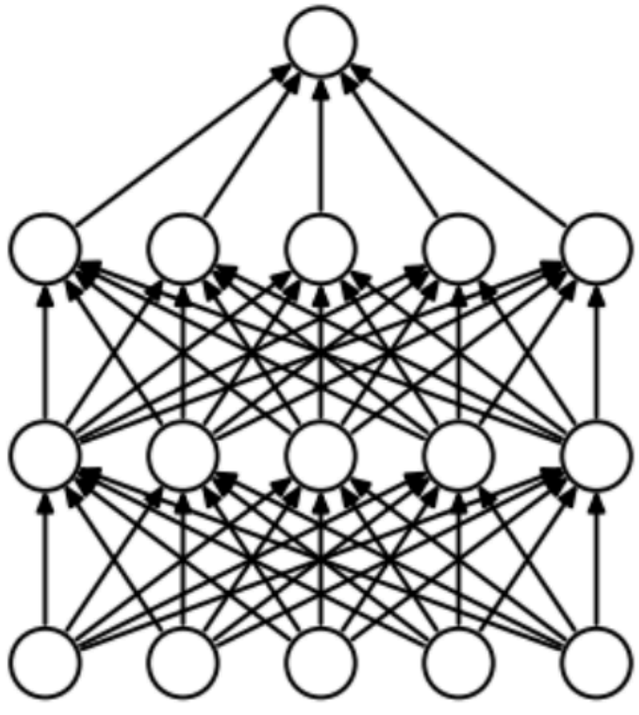

(a) Standard Neural Net

(b) After applying dropout.

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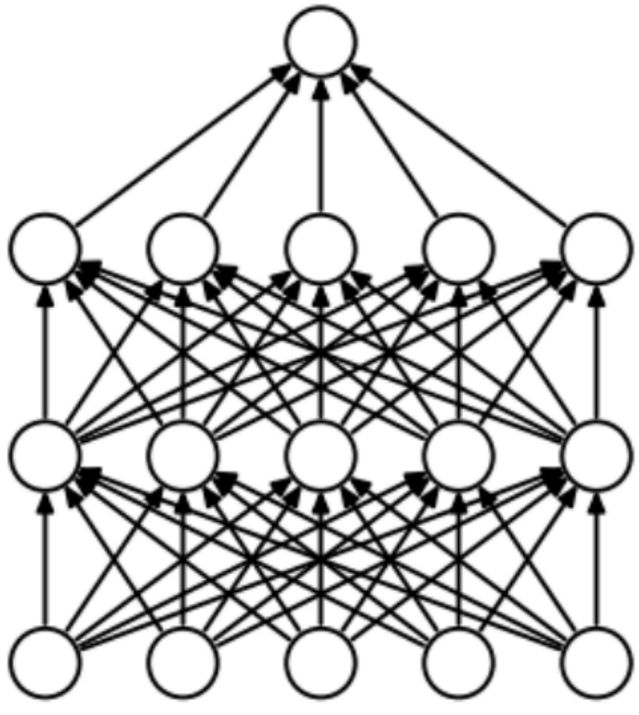

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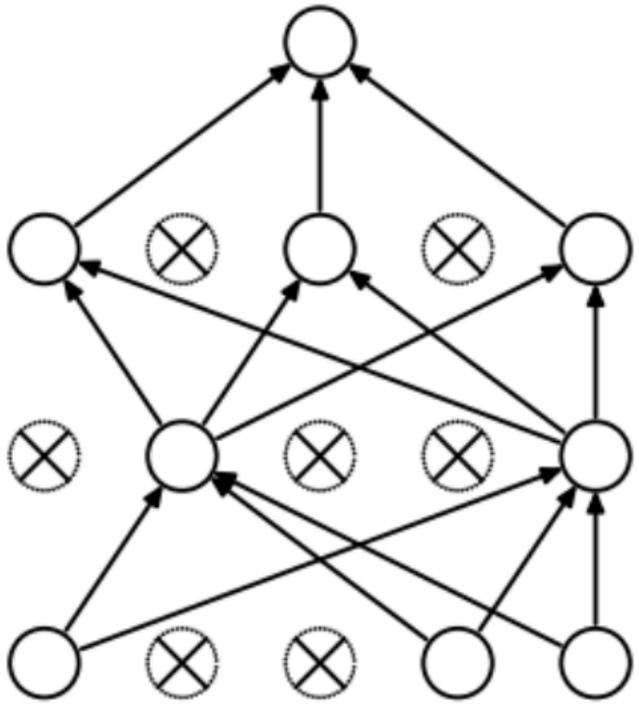

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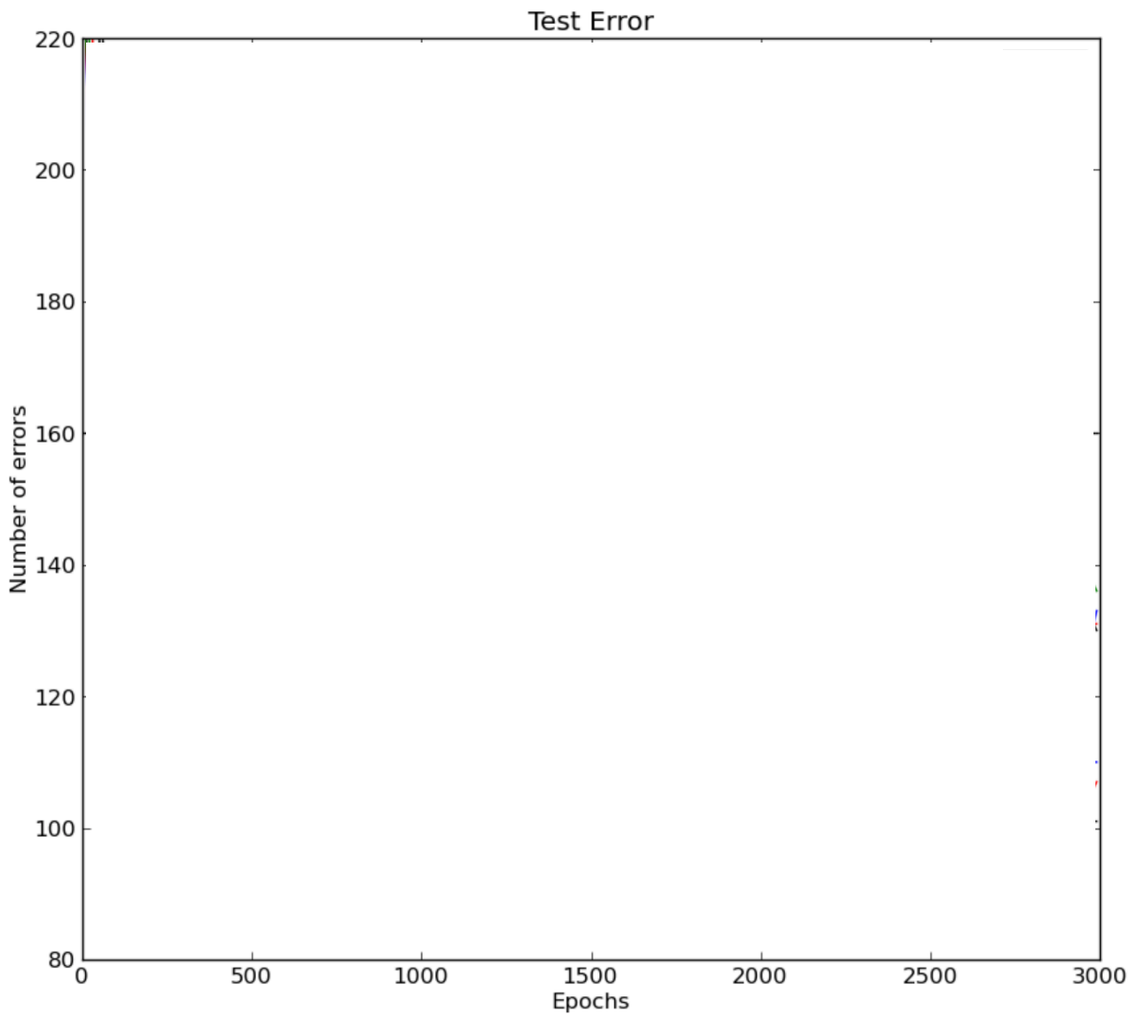

Image Classification (MNIST digits)

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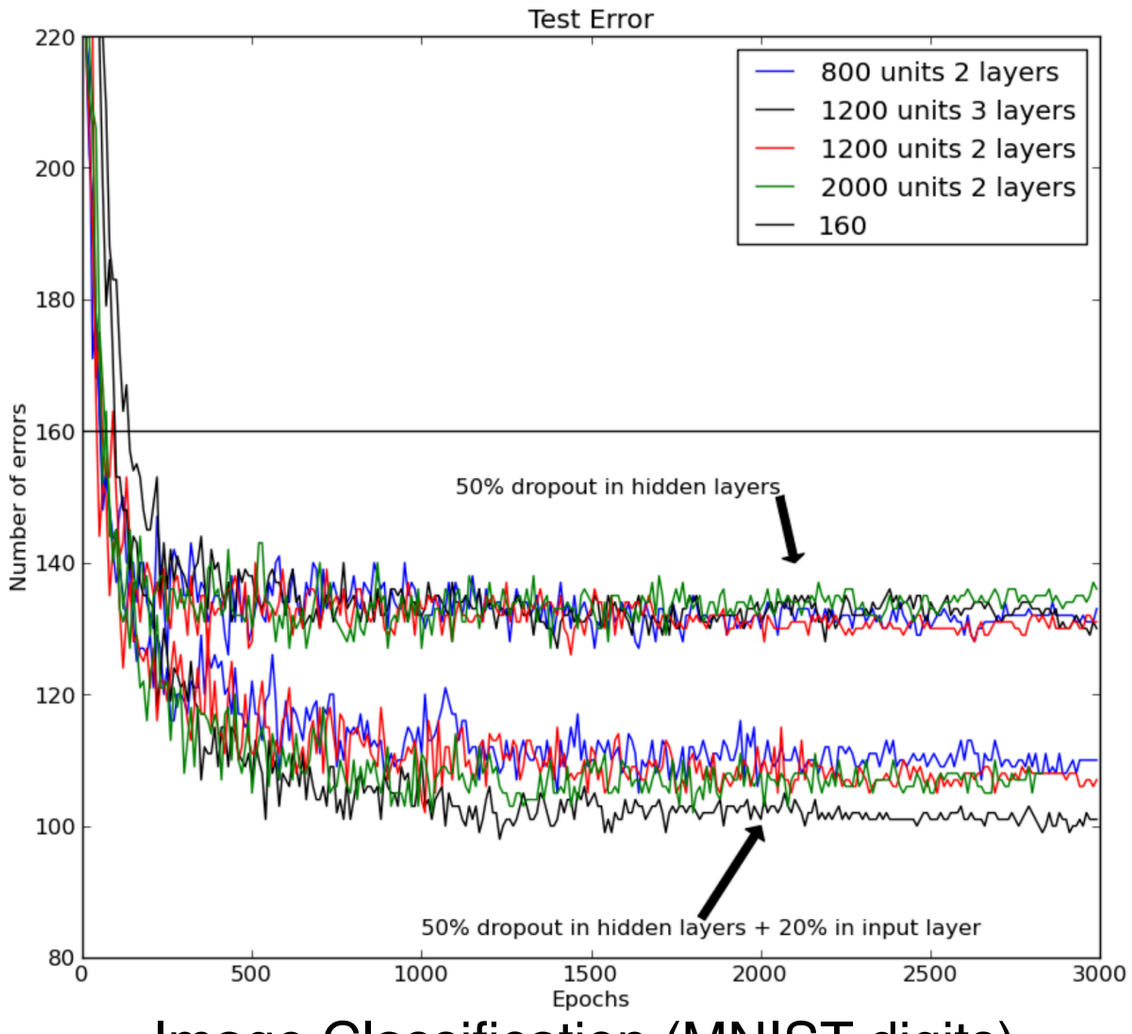

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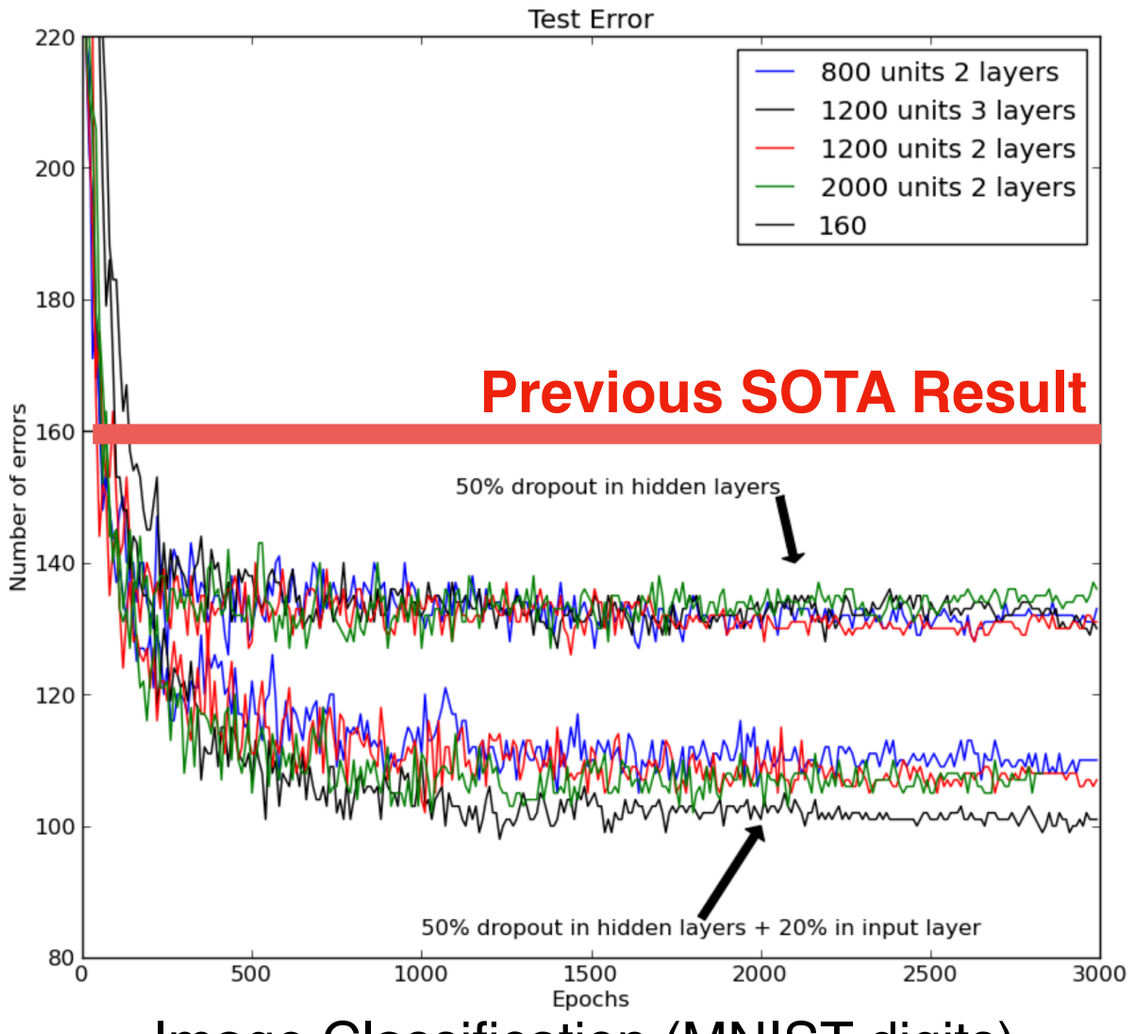

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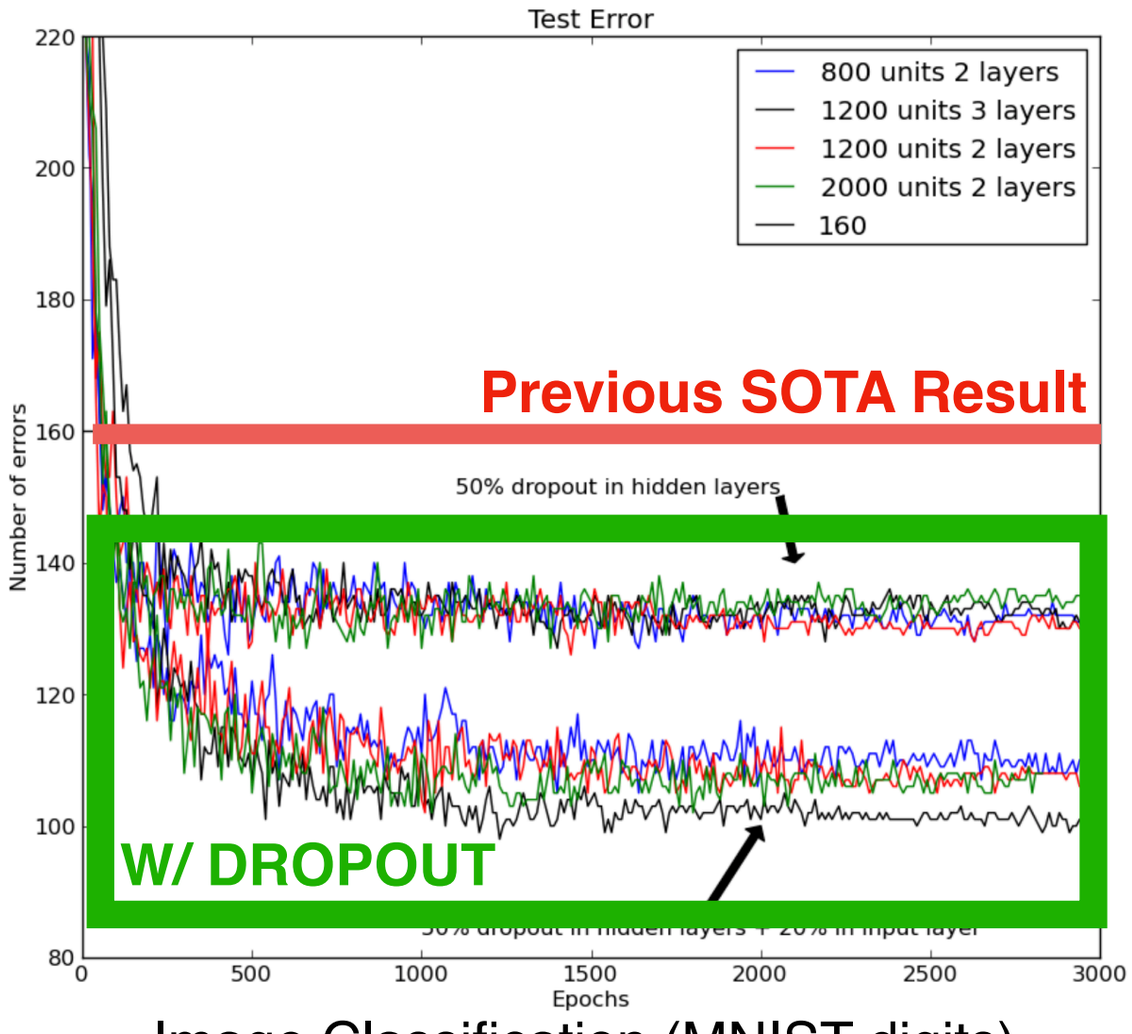

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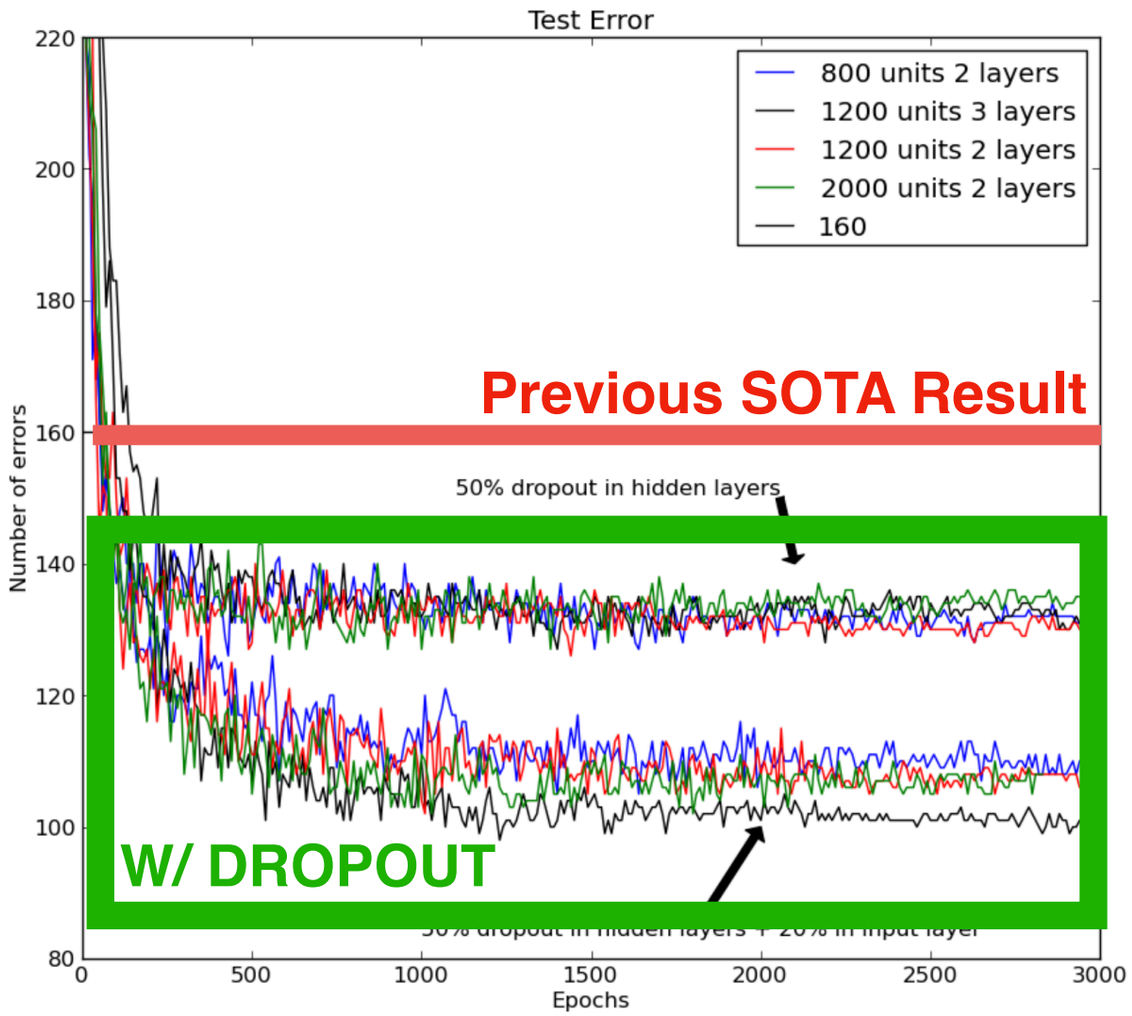

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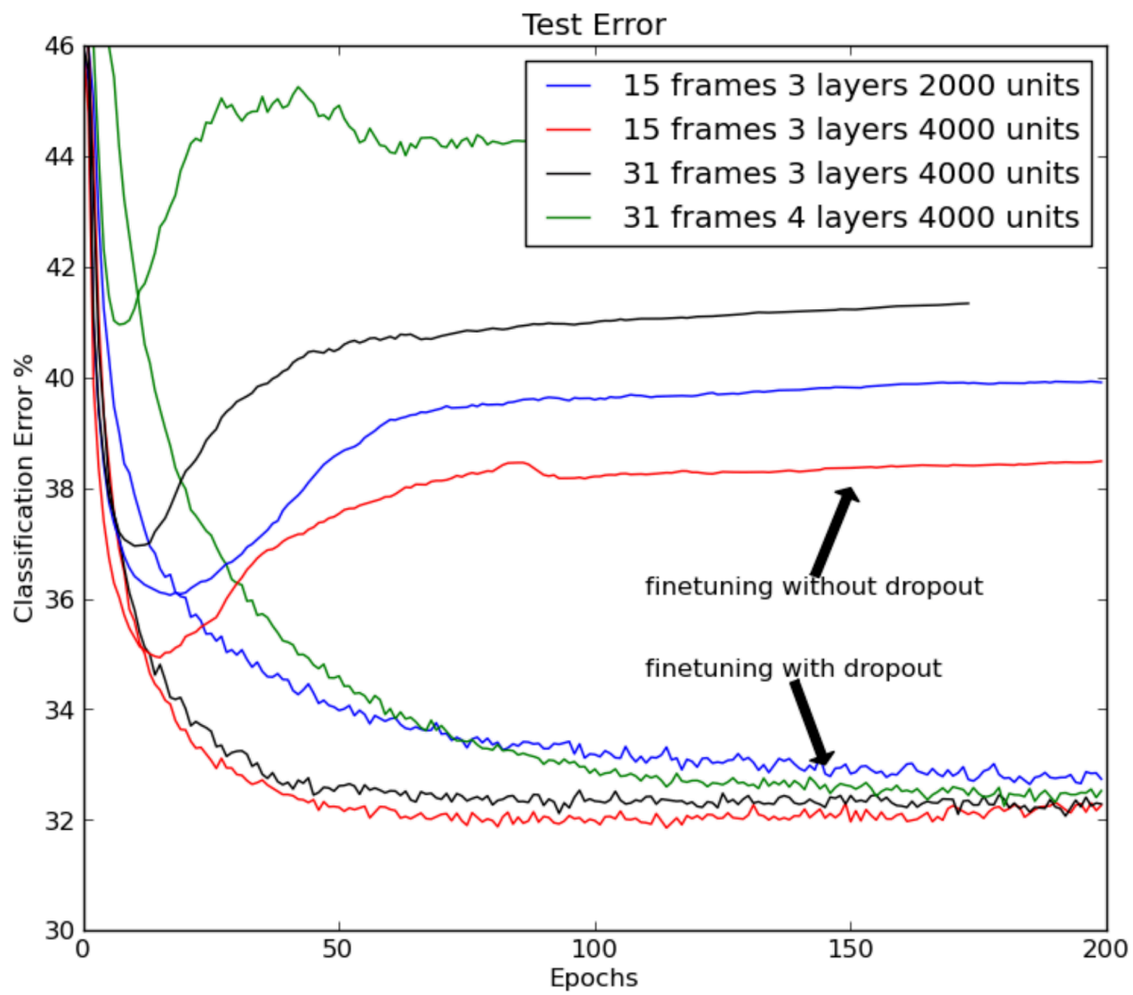

Phoneme Classification (TIMIT speeches)

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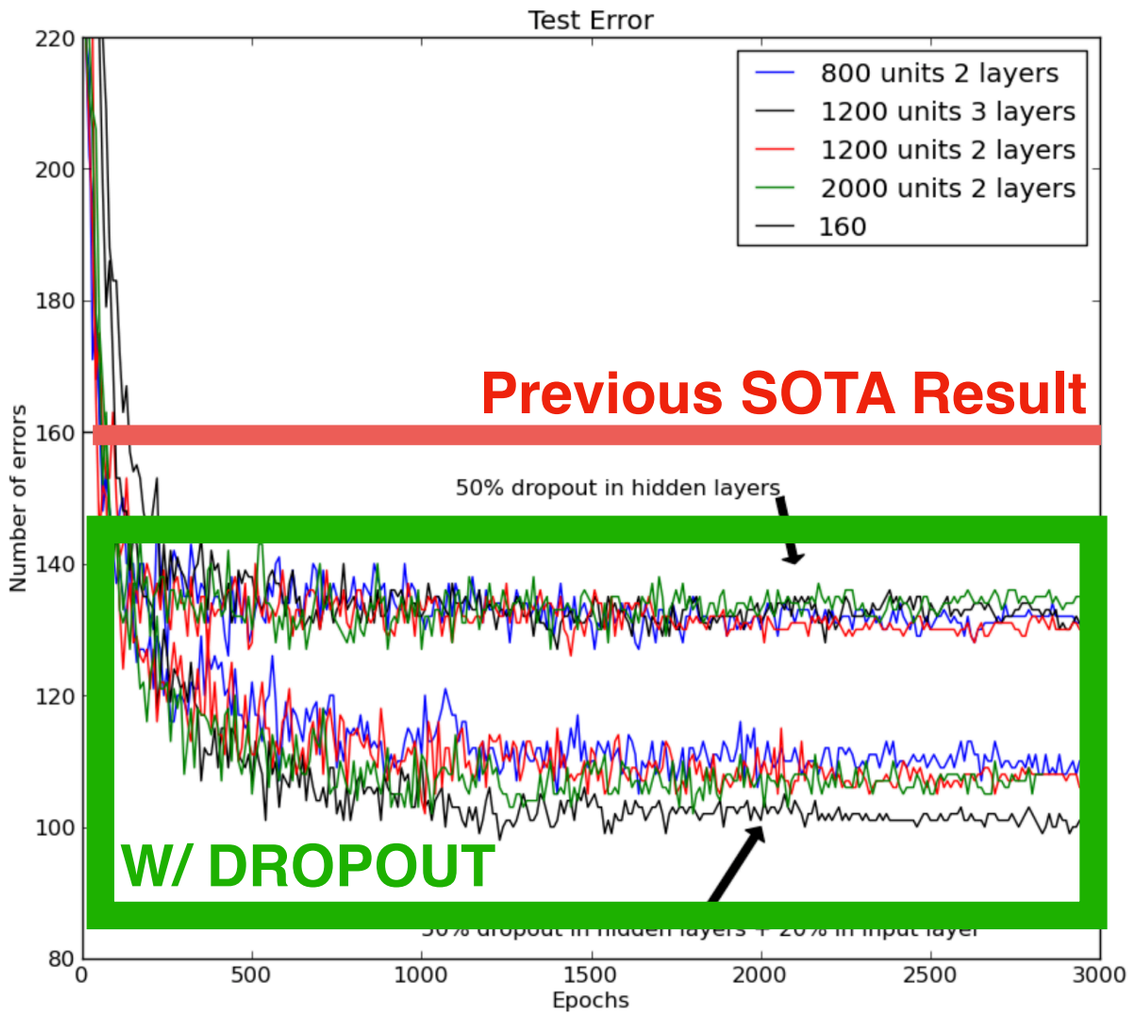

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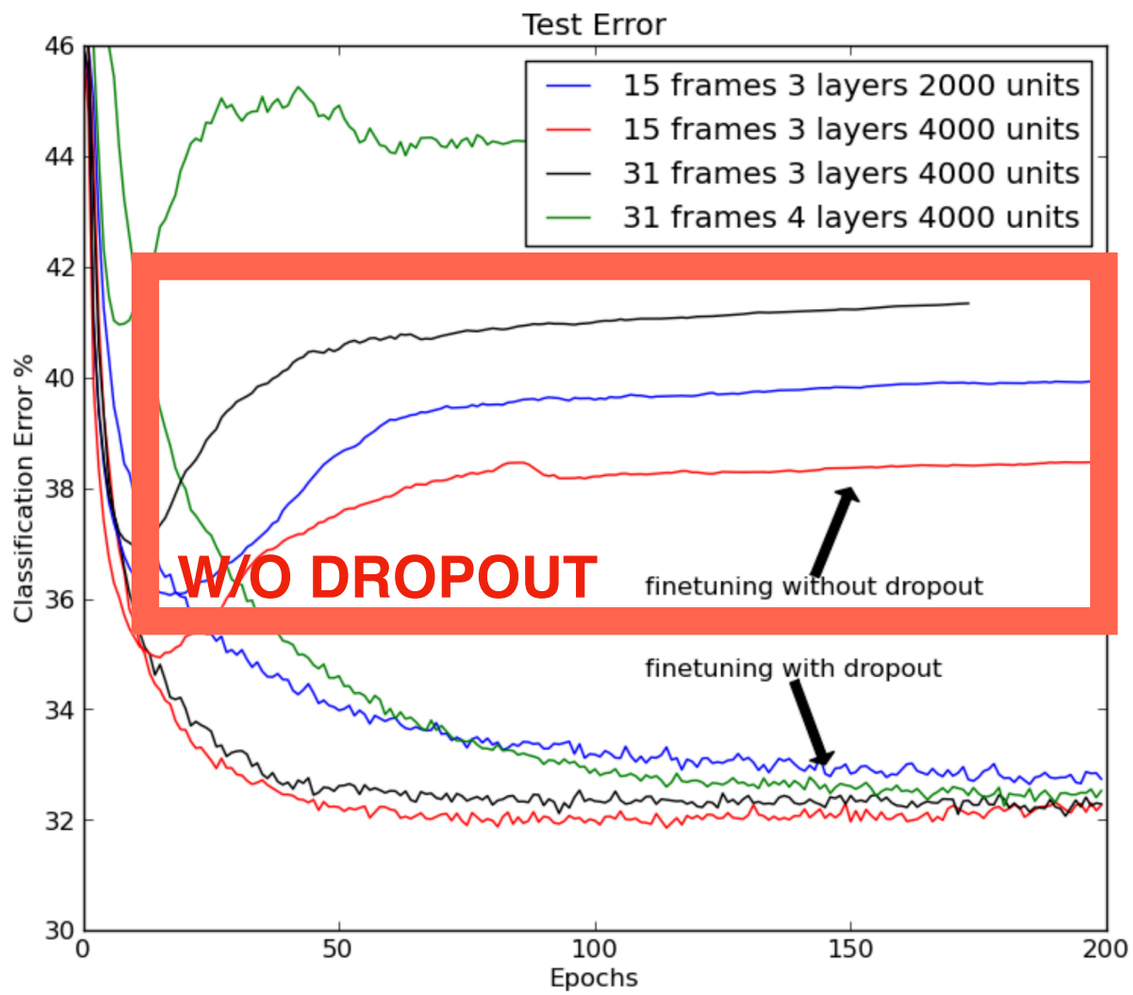

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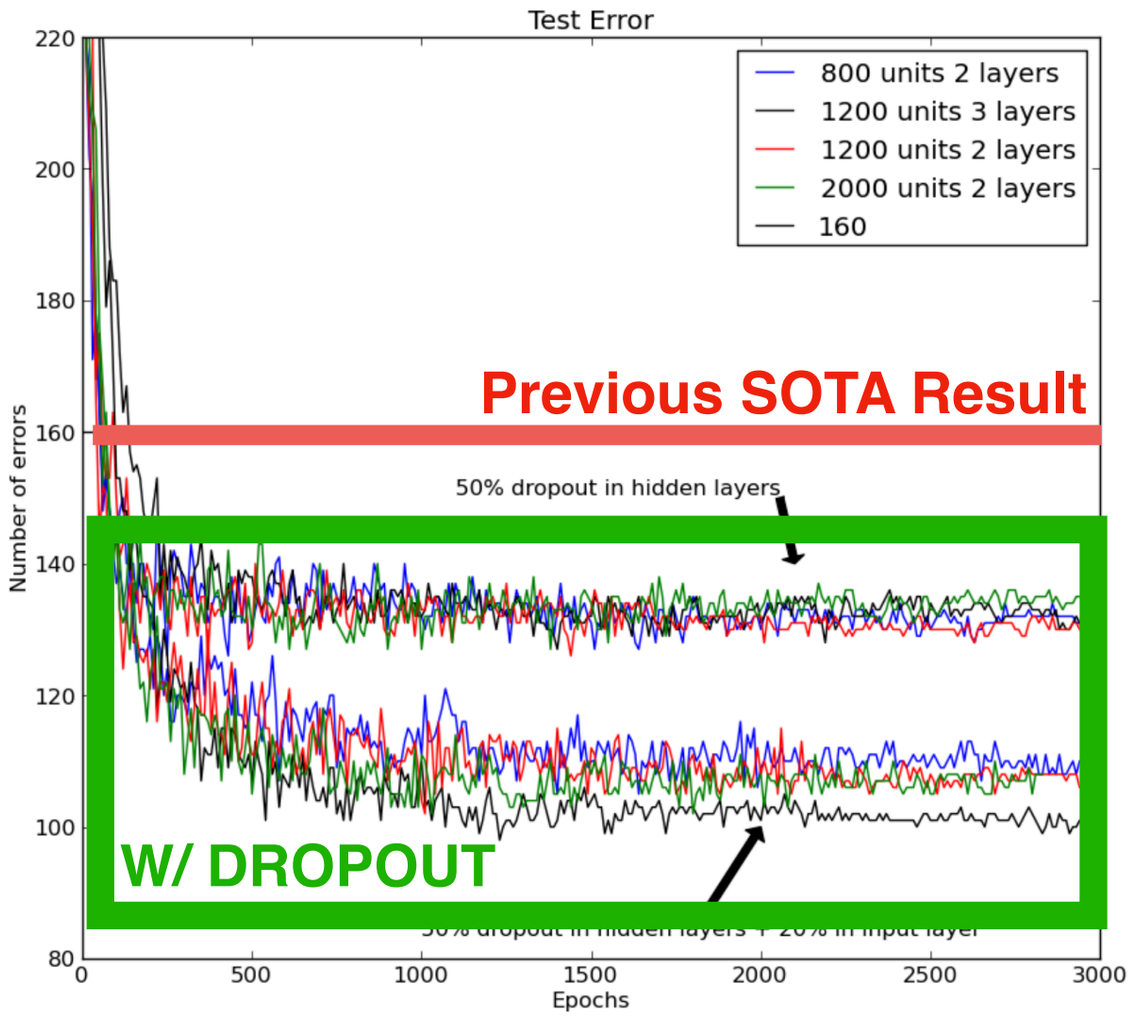

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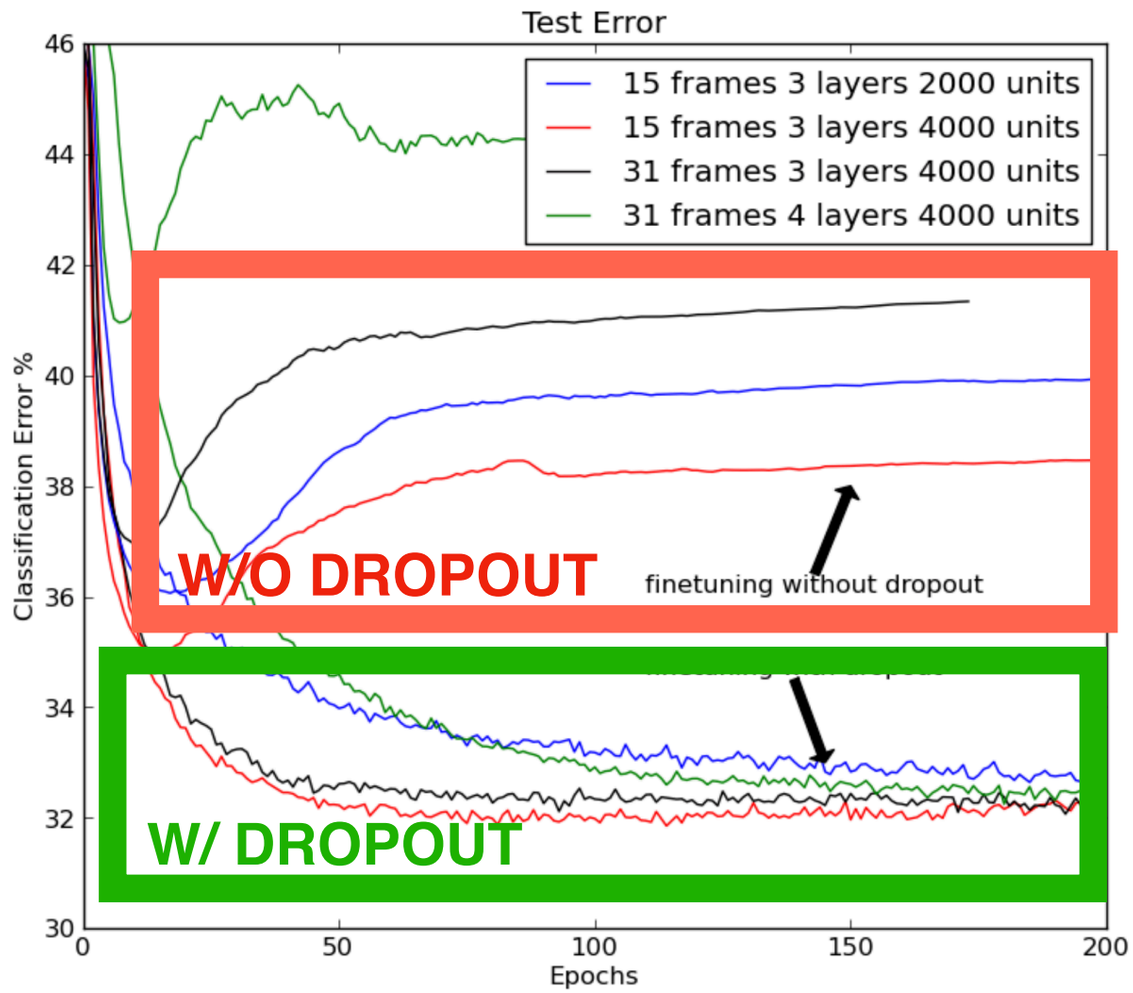

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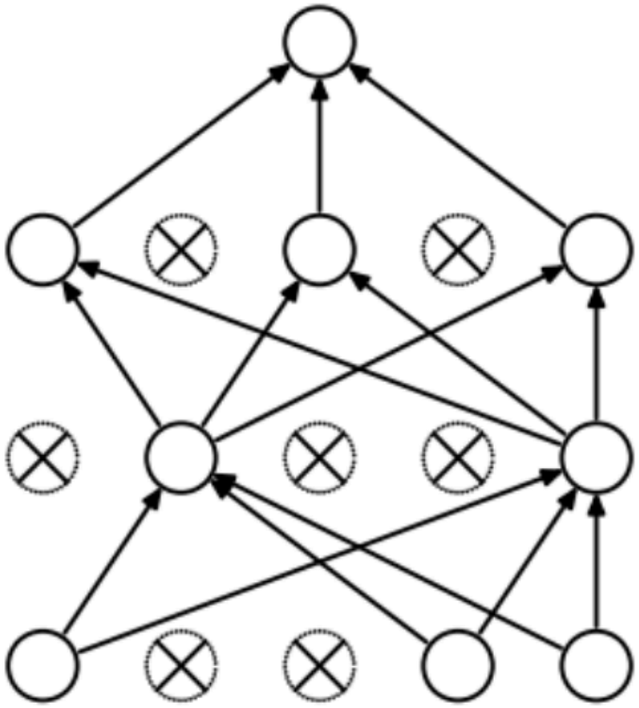

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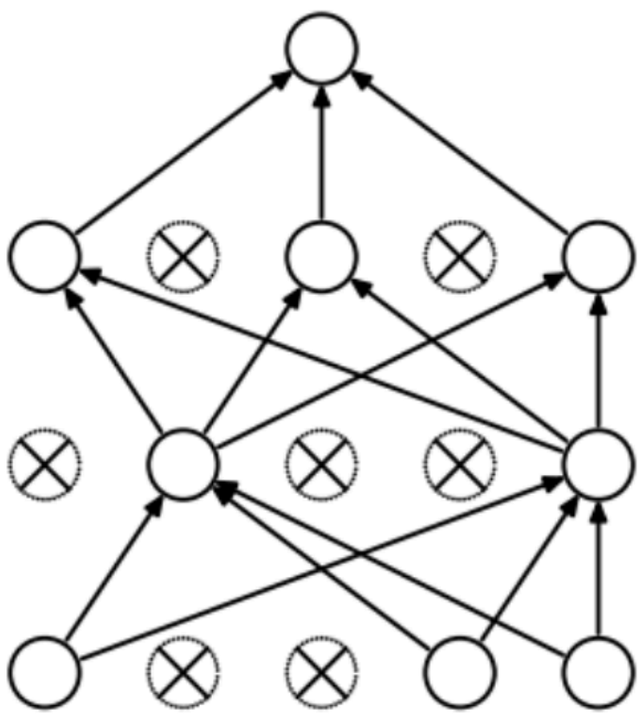

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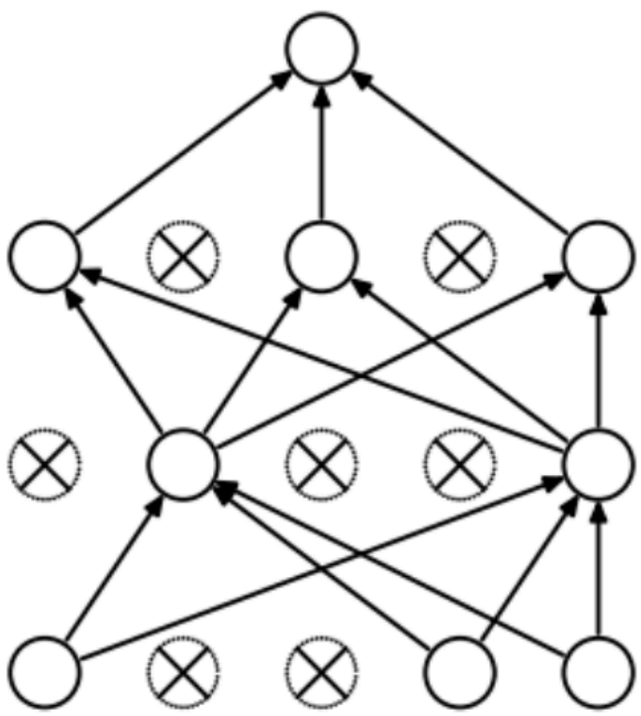

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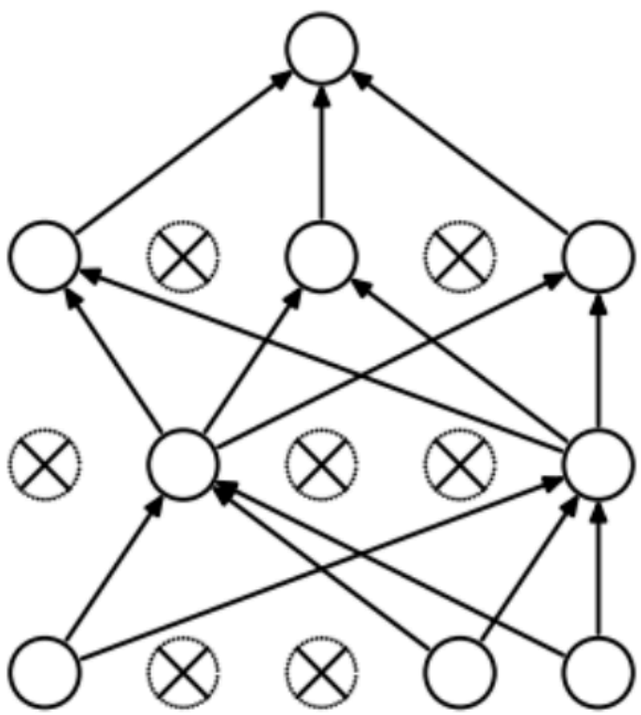

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$$\begin{aligned}
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&\quad = \mathbb{E}_{p(\lambda)}[\log p(\mathbf{y}|\mathbf{X}, \{\mathbf{W}_l\}_{l=1}^{L+1}, \{\mathbf{\Lambda}_l\}_{l=1}^{L})] \\
&\quad \approx \frac{1}{S}\sum_{s=1}^{S} \log p(\mathbf{y}|\mathbf{X}, \{\mathbf{W}_l\}_{l=1}^{L+1}, \{\hat{\mathbf{\Lambda}}_{l,s}\}_{l=1}^{L})
\end{aligned}$$

Understanding Dropout

- **How should we interpret dropout?**
  How does it work?

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"I went to my bank. The tellers kept changing and…this made me realize that ***randomly removing a different subset of neurons on each example would prevent conspiracies and thus reduce overfitting****."*

~ Geoffrey Hinton

Understanding Dropout

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Dropout Training as Adaptive Regularization

Stefan Wager*, **Sida Wang**†, and **Percy Liang**†
Departments of Statistics* and Computer Science†
Stanford University, Stanford, CA-94305
swager@stanford.edu, {sidaw, pliang}@cs.stanford.edu

(2013)

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$$\approx \log p(\mathbf{y}|\mathbf{X}, \{\mathbf{W}_l\}_{l=1}^{L+1}, \{\boldsymbol{\mu}_l^{\Lambda}\}_{l=1}^{L}) + \frac{1}{2}\text{Var}[\lambda]\text{Tr}\left\{\nabla^2_{\boldsymbol{\mu}^{\Lambda}} \log p(\mathbf{y}|\mathbf{X}, \{\mathbf{W}_l\}_{l=1}^{L+1}, \{\boldsymbol{\mu}_l^{\Lambda}\}_{l=1}^{L})\right\}$$

Log-Likelihood

Regularization Penalty

Understanding Dropout

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For logistic regression:

$$\frac{1}{2}\mathrm{Var}[\lambda]\mathrm{Tr}\left\{\nabla^2_{\boldsymbol{\mu}^\Lambda}\log p(\mathbf{y}|\mathbf{X},\{\mathbf{W}_l\}_{l=1}^{L+1},\{\boldsymbol{\mu}_l^\Lambda\}_{l=1}^{L})\right\} =$$

$$-\frac{1}{2}\pi(1-\pi)\sum_{n=1}^{N}\sum_{d=1}^{D} f(\boldsymbol{\beta}^T\mathbf{x}_n)(1-f(\boldsymbol{\beta}^T\mathbf{x}_n))x_{n,d}^2\beta_d^2$$

Understanding Dropout

- **General case of deep neural networks thought to be hopeless due to intractability of expectation.**

$$\mathbb{E}_{p(\lambda)}[\log p(\mathbf{y}|\mathbf{X}, \{\mathbf{W}_l\}_{l=1}^{L+1}, \{\mathbf{\Lambda}_l\}_{l=1}^{L})]$$

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- **Open Questions**
  - **Why Bernoulli noise?**: Other noise distributions shown to work just as well (e.g. Gaussian). What does the choice of distribution mean?

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- **Open Questions**
  - **Why Bernoulli noise?**: Other noise distributions shown to work just as well (e.g. Gaussian). What does the choice of distribution mean?
  - **Why drop hidden units?**: Dropping hidden units (instead of weights) results in best performance—why?

Understanding Dropout

- **General case of deep neural networks thought to be hopeless due to intractability of expectation.**

$$\mathbb{E}_{p(\lambda)}[\log p(\mathbf{y}|\mathbf{X}, \{\mathbf{W}_l\}_{l=1}^{L+1}, \{\mathbf{\Lambda}_l\}_{l=1}^{L})]$$

- **Open Questions**
  - **Why Bernoulli noise?**: Other noise distributions shown to work just as well (e.g. Gaussian). What does the choice of distribution mean?
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Dropout as Structured Bayesian Shrinkage

A Bayesian Interpretation

Idea: Don't go through the expectation, go around it.

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$$w \sim \mathrm{N}(0, \sigma_0^2)$$

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Assume a Gaussian prior on a weight:

$$w \sim \mathrm{N}(0, \sigma_0^2)$$

Consider the product of the weight and noise:

$$\lambda \cdot w, \quad \lambda \sim p(\lambda)$$

What's the distribution of this product?

A Bayesian Interpretation

Scale Mixtures! [Beale & Mallows, 1959; Andrews & Mallows, 1974]:

$$\lambda \cdot w, \quad \lambda \sim p(\lambda), \quad w \sim \mathrm{N}(0, \sigma_0^2)$$

Definition of a Gaussian scale mixture

A Bayesian Interpretation

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$$\lambda \cdot w, \quad \lambda \sim p(\lambda), \quad w \sim \mathrm{N}(0, \sigma_0^2)$$

Definition of a Gaussian scale mixture

- **Can switch to a hierarchical parametrization:**

$$w \sim \mathrm{N}(0, \lambda^2 \sigma_0^2), \;\; \lambda \sim p(\lambda)$$

Reparametrizing Deep Networks

Can apply the trick inside the deep network:

$$\mathbf{h}_{n,l} = f_l(\mathbf{h}_{n,l-1}\mathbf{\Lambda}_l\mathbf{W}_l)$$

Induced scale mixture

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Reparametrize

Noise moves from likelihood to prior

$$\mathbf{h}_{n,l} = f_l(\mathbf{h}_{n,l-1}\mathbf{W}_l), \quad w_{i,j} \sim \mathrm{N}(0, \lambda_i^2\sigma_0^2)$$

Works no matter how deep the NN or the type of non-linearity!

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Structure?

Works no matter how deep the NN or the type of non-linearity!

Reparametrizing Deep Networks

Sampling the noise on the hidden units induces structure:

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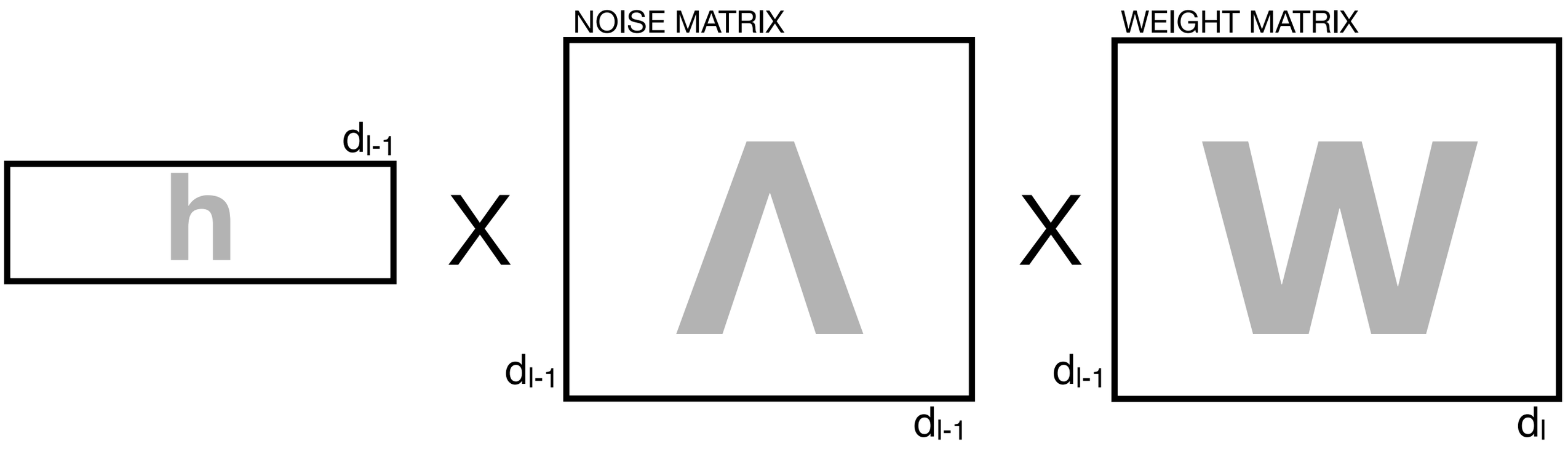

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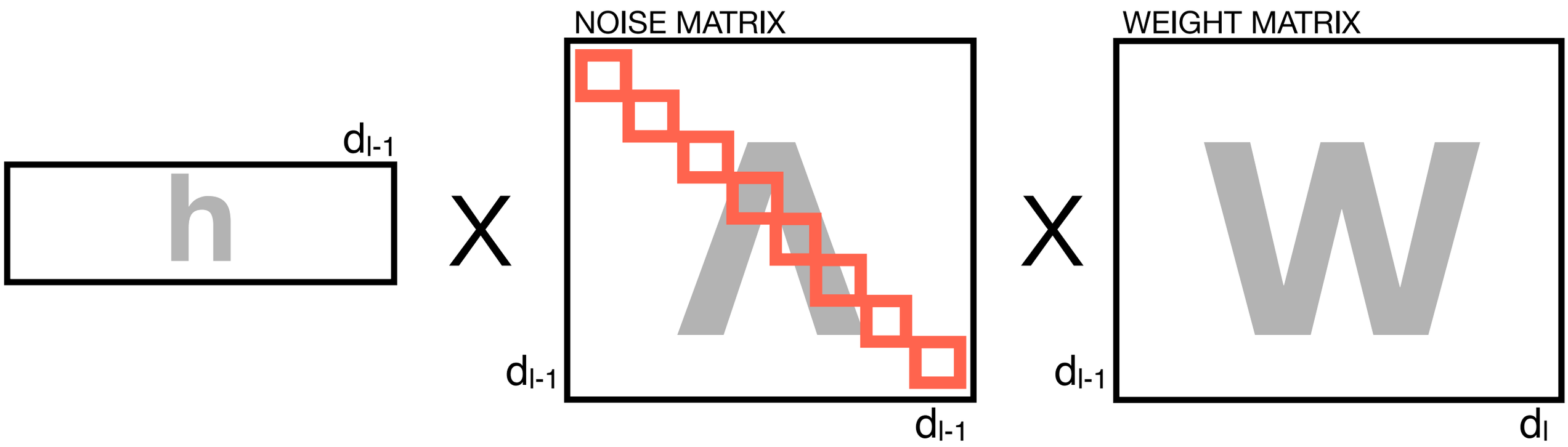

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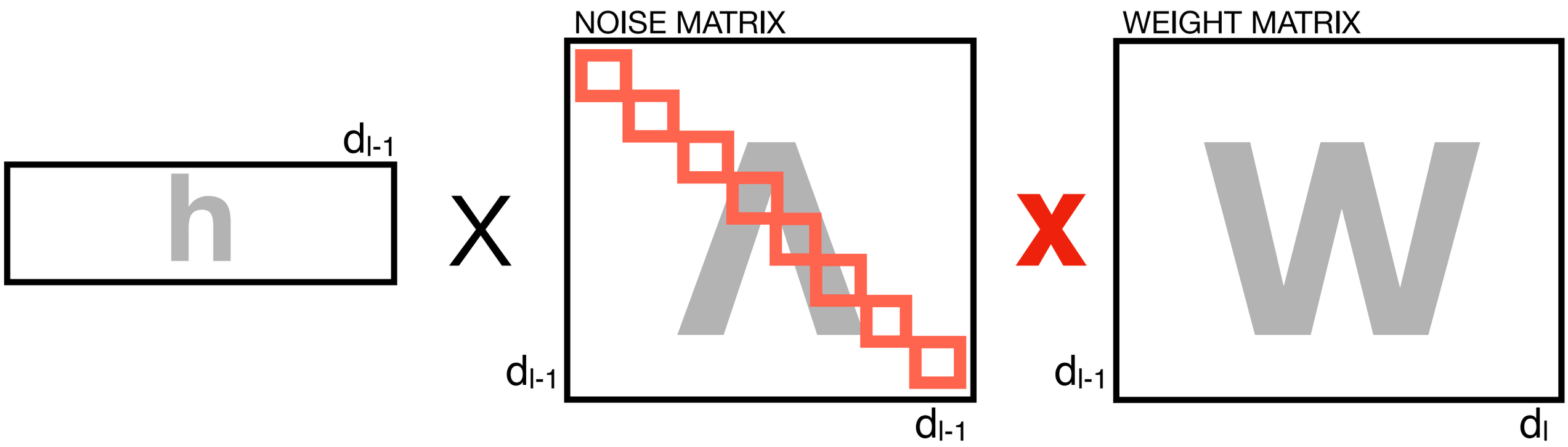

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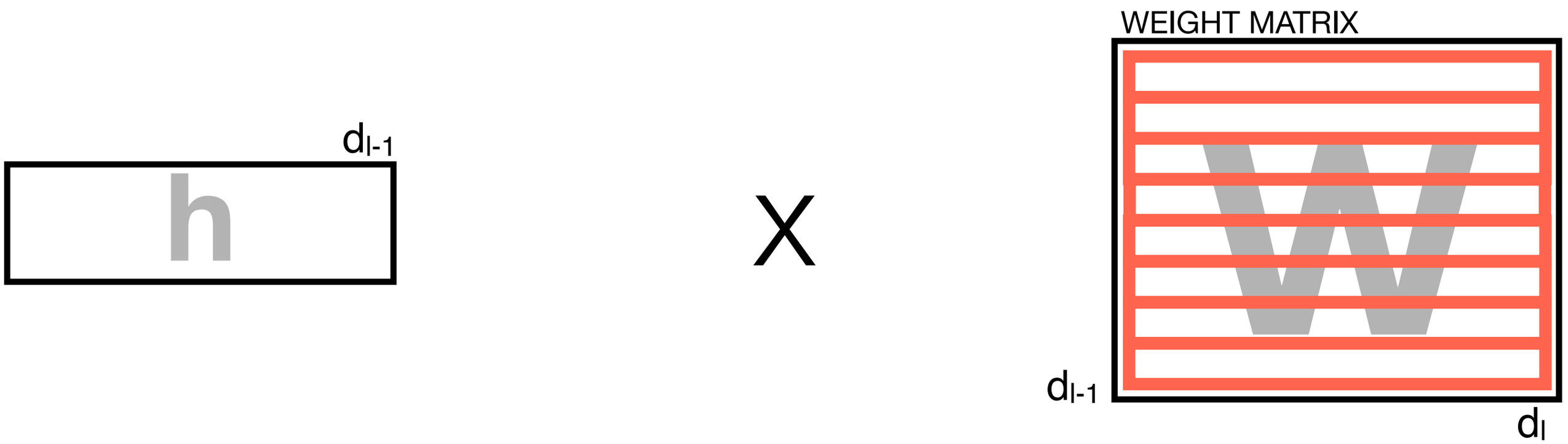

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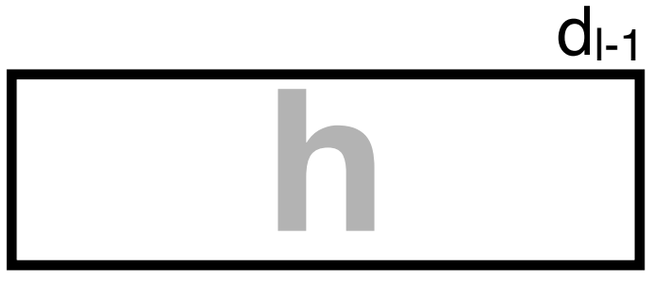
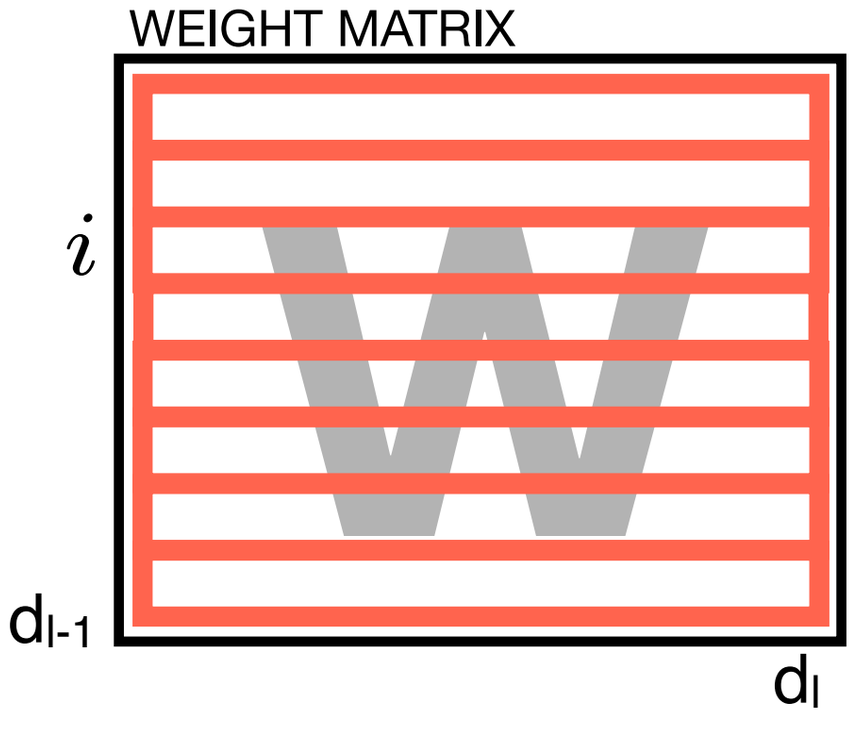
$$\lambda_i \sim p(\lambda_i)$$

Selects for **number of hidden units** (i.e. layer width).



X



Reparametrizing Deep Networks

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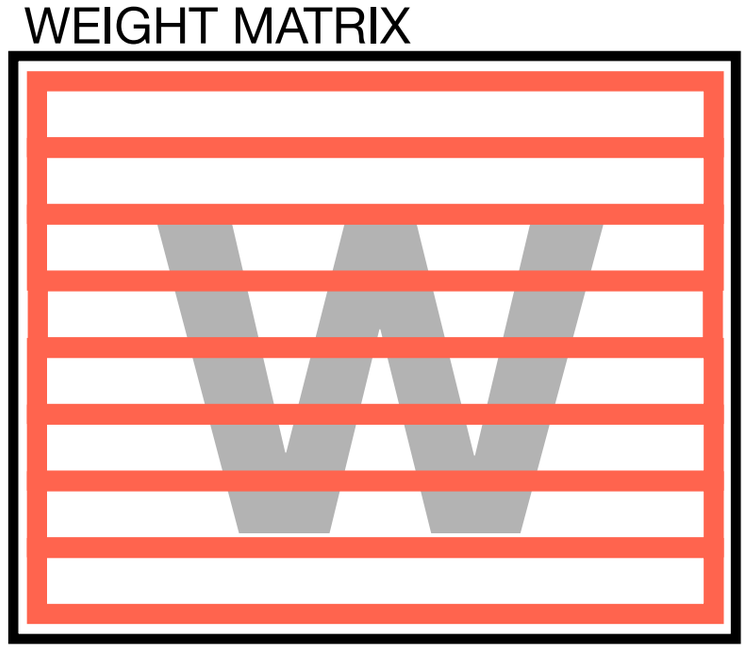
i indexes rows

Exactly the *automatic relevance determination* (ARD) prior proposed by D. MacKay and R. Neal (1994)

MacKay

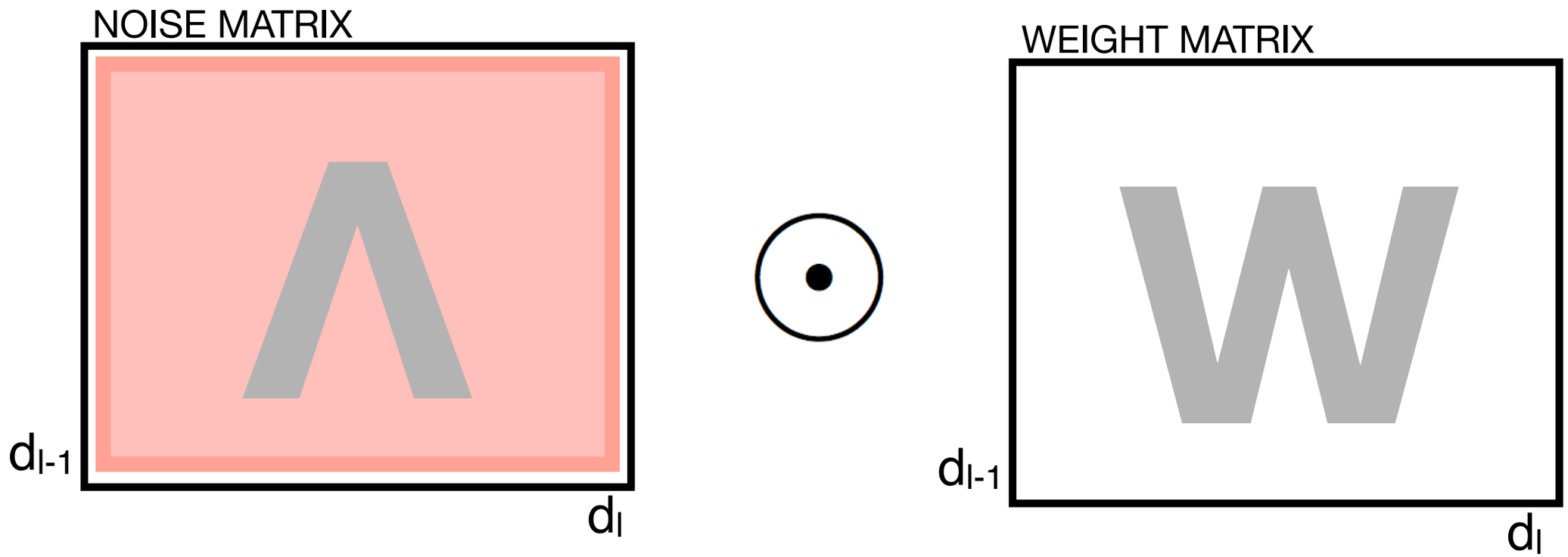
Neal



Shared scale

DropConnect

Previous work by Wan et al. (2013) proposed ***dropconnect***, which drops weights independently.



Has **not** gained wide adoption—likely because **ARD structure is broken.**

Understanding Dropout

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Pushing through to the hierarchical parametrization,
we can see dropout's corresponding **marginal prior**:

$$
\begin{aligned}
p(w) &= \sum_{\lambda \in \{0,1\}} \texttt{Bernoulli}(\lambda; \pi)\ \mathrm{N}(0, \lambda^2 \sigma_0^2) \\
&= \pi\ \mathrm{N}(w; 0, \sigma_0^2) + (1 - \pi)\ \delta[w]
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Spike and slab prior commonly used for Bayesian variable selection. The **expanded parametrization** (i.e. likelihood noise) was used at least as early as Kuo and Mallick (1998).

Noise Priors

Other scale mixture priors as noise:

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

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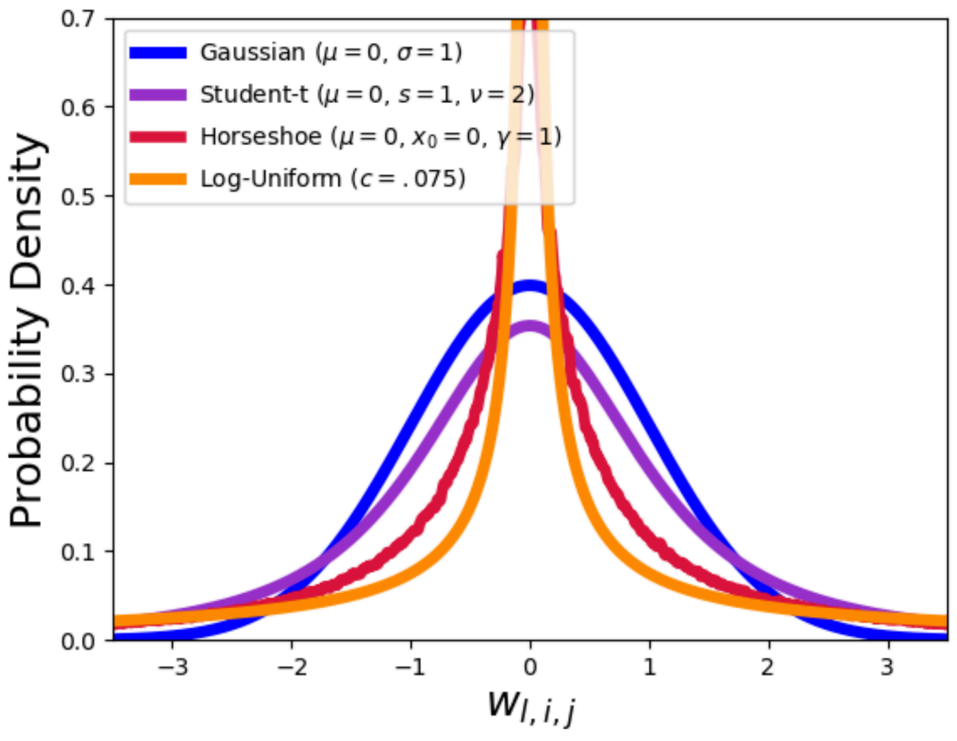
Bernoulli noise is not essential and lots of other noise models / marginal priors work well, e.g. Horseshoe [Ghosh et al., 2018].



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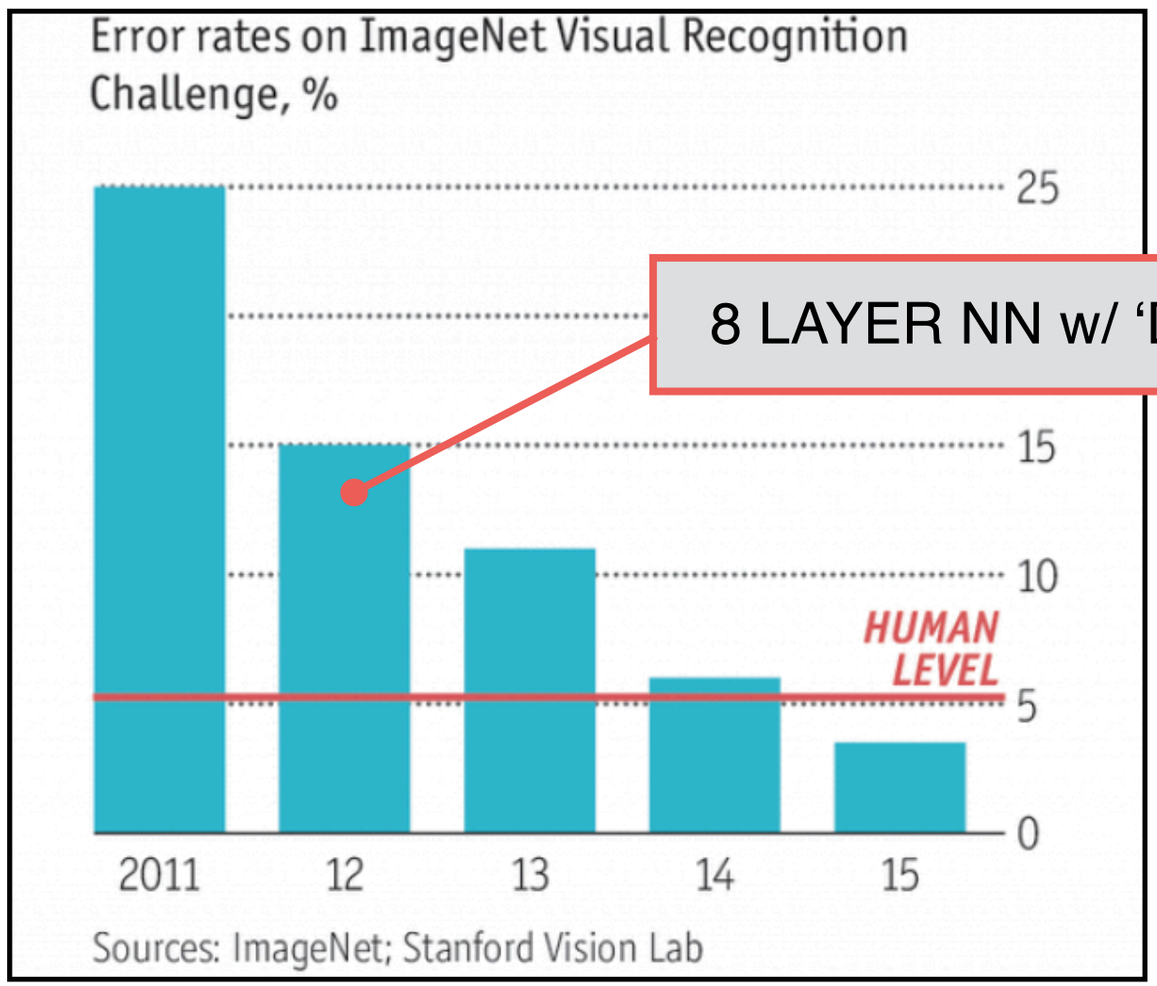
Residual Networks and Skip Connections

Computer Vision: Results on ImageNet object classification dataset.



[Krizhevsky et al., 2012]

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

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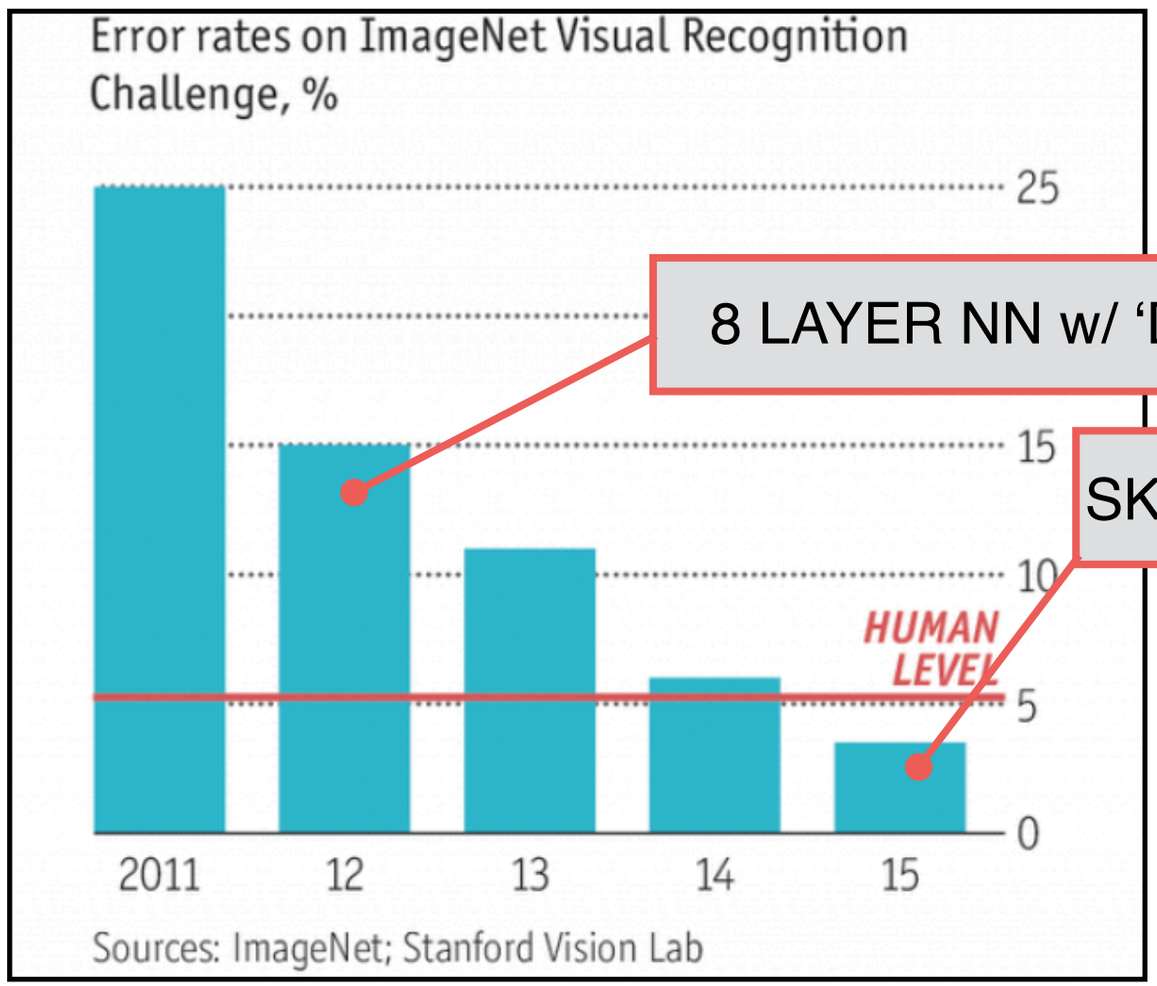

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Residual Networks and Skip Connections

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

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

NONLINEAR TRANSFORM — SKIP CONNECTION

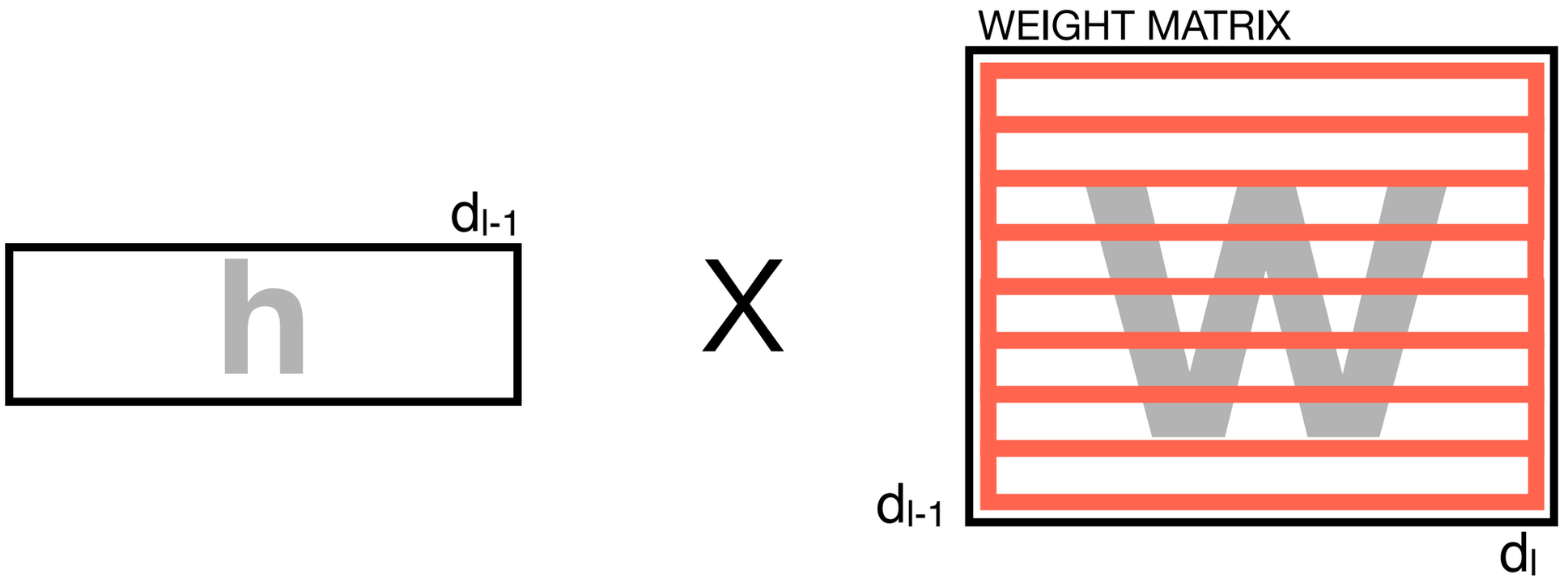
OLD — NEW

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

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

Residual Networks and Skip Connections

How should we implement dropout / multiplicative noise with skip connections?



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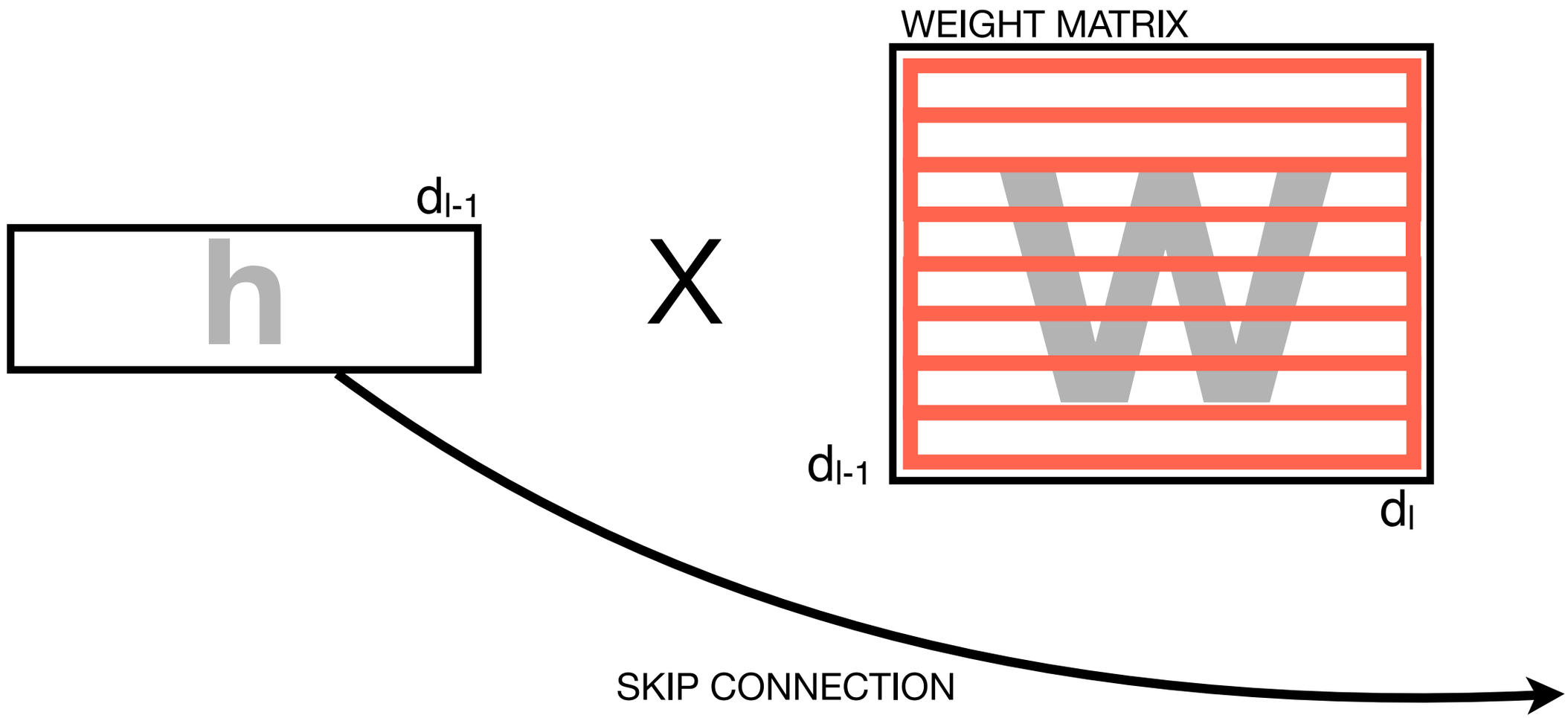

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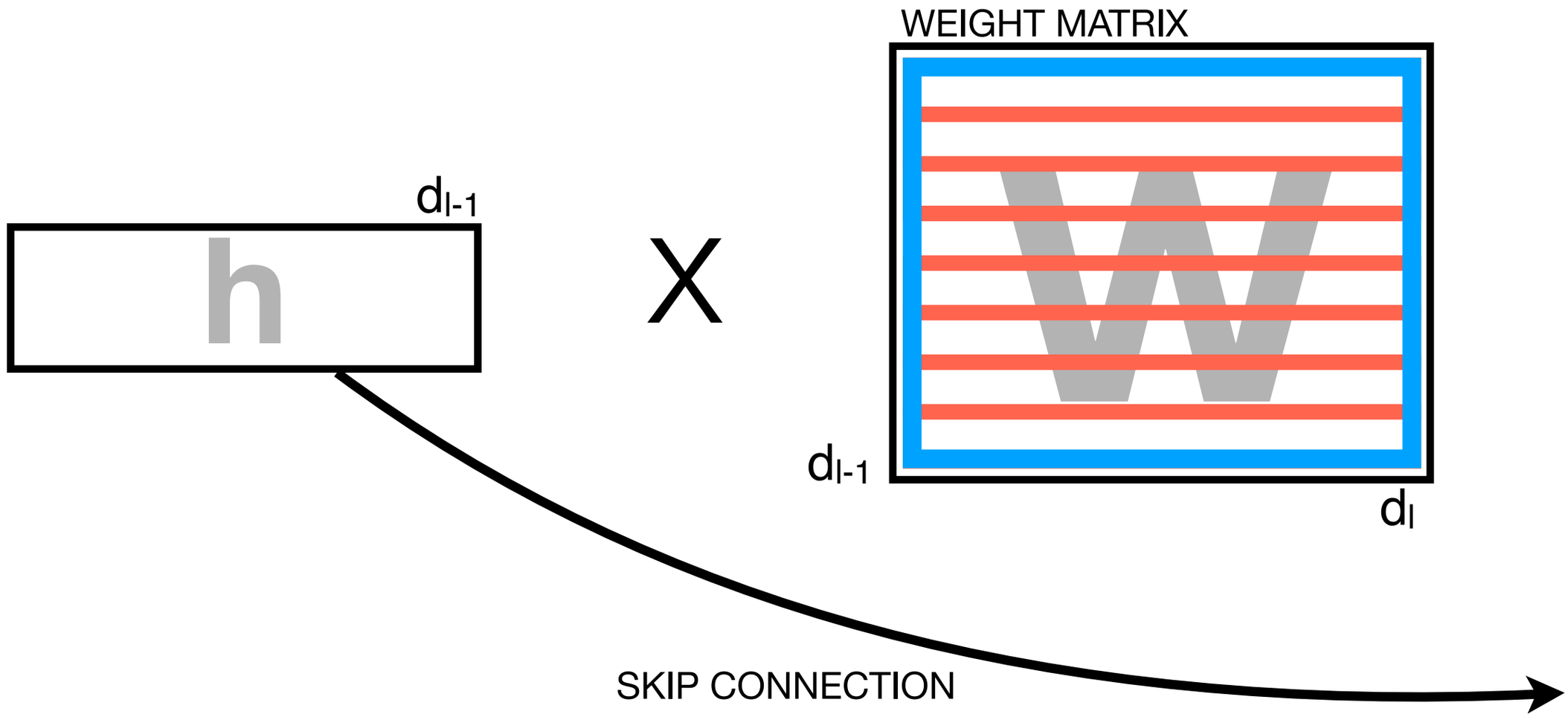

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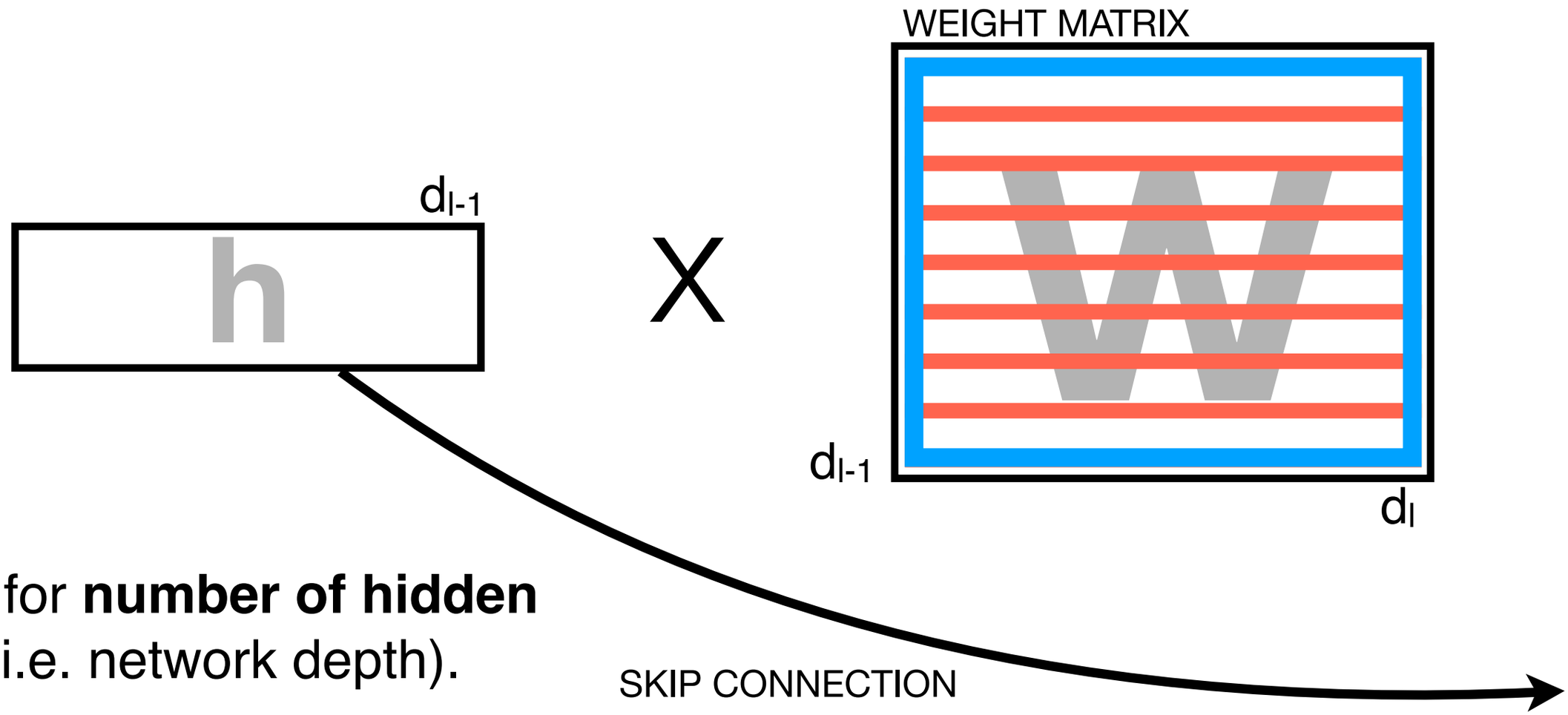

Selects for **number of hidden layers** (i.e. network depth).

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

Automatic Depth Determination

We can extend ARD to layer with the following prior, which we call **automatic depth determination** (ADD).

$$w_{l,i,j} \sim \mathbf{N}(w_{l,i,j}; 0, \sigma_0^2 \tau_{l,.,.}), \quad \tau_{l,.,.} \sim p(\tau_l)$$

Can reparametrize to interpret as multiplicative noise:

$$\mathbf{h}_{n,l} = f_l(\mathbf{h}_{n,l-1}\mathbf{W}_l) + \mathbf{h}_{n,l-1}$$

$$\xrightarrow{\text{reparametrization}} \quad f_l(\tau_l \mathbf{h}_{n,l-1}\mathbf{W}_l) + \mathbf{h}_{n,l-1}$$

Structured Priors

(a) Unstructured (DropConnect)

(b) ARD (Dropout)

(c) ADD (Stochastic Depth)

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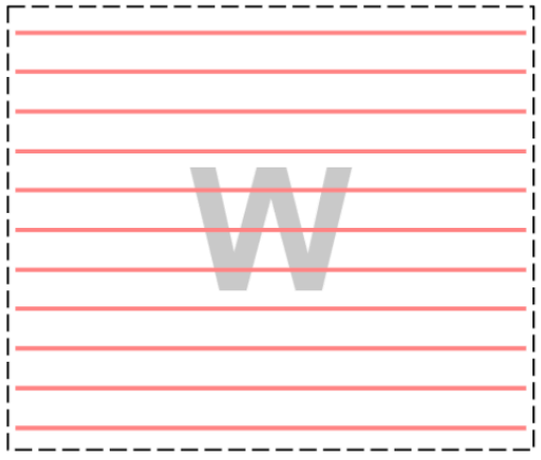

(b) ARD (Dropout)

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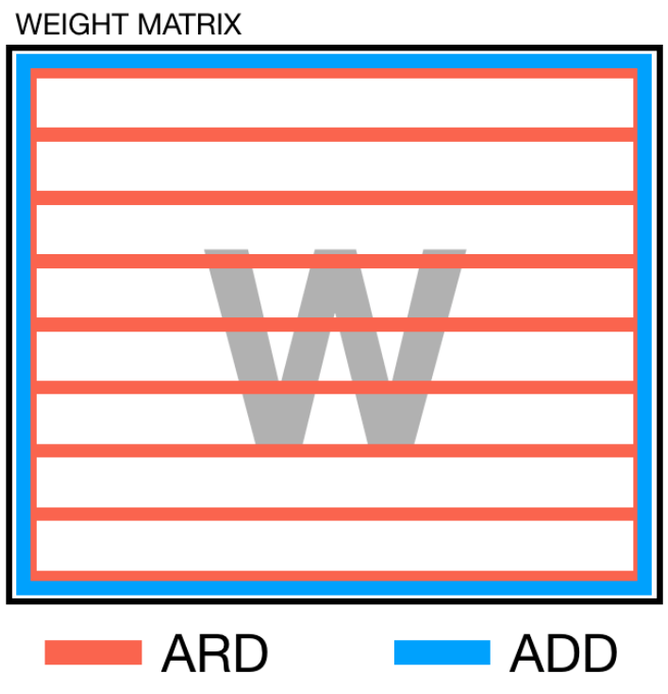

Combine

$$w_{l,i,j} \sim \mathbf{N}(w_{l,i,j}; 0, \sigma_0^2 \lambda_{l,i,.} \tau_{l,.,.}),$$

$$\lambda_{l,i,.} \sim p(\lambda_{l,i}), \quad \tau_{l,.,.} \sim p(\tau_l)$$

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    Think about params that should share scales (and be pruned together)

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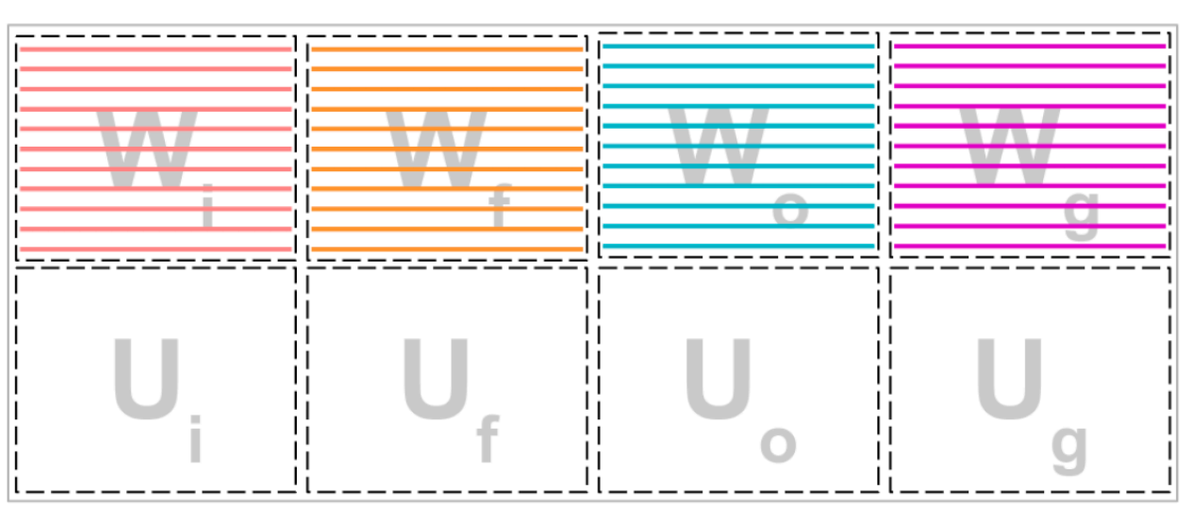
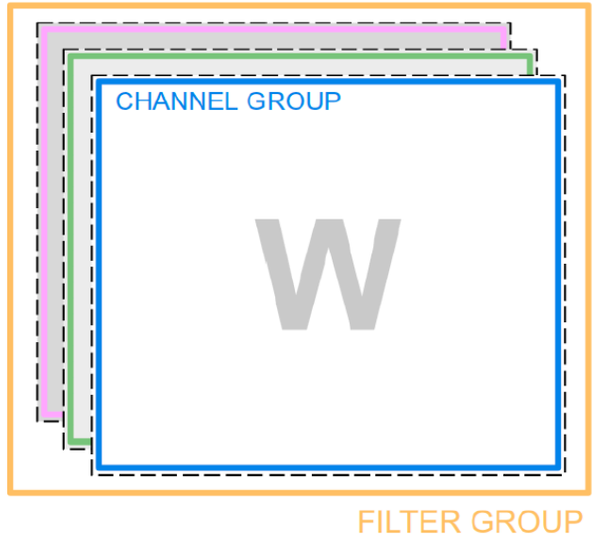


(d) LSTM ARD



(e) CNN ARD (SpatialDropout)

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Hold on: Aren't we sweeping all of this under the rug that is posterior inference?

Posterior Inference for Neural Networks

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$$p(\{\mathbf{W}\}_{l=1}^{L+1}, \{\mathbf{\Lambda}_l\}_{l=1}^{L+1}, \{\tau_l\}_{l=1}^{L+1} | \mathbf{y}, \mathbf{X}) =$$

$$\frac{p(\mathbf{y}|\mathbf{X}, \{\mathbf{W}\}_{l=1}^{L+1}) p(\{\mathbf{W}\}_{l=1}^{L+1} | \{\mathbf{\Lambda}_l\}_{l=1}^{L+1}, \{\tau_l\}_{l=1}^{L+1})\ p(\{\mathbf{\Lambda}_l\}_{l=1}^{L+1})\ p(\{\tau_l\}_{l=1}^{L+1})}{p(\mathbf{y}|\mathbf{X})}$$

where *L* can be 150+?!

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Posterior inference is an open problem. Especially with heavy-tailed priors. Previous work has needed truncated approximations [Ghosh et al., 2018], alternate parametrizations [Ingraham & Marks, 2017], and quasi-divergences [Hron et al., 2018] in addition to variational methods.

Light-Weight EM Algorithm

[Nalisnick & Hernández-Lobato, 2018]

Variational Inference for W: Perform backprop-style gradient updates for a Normal approx. of the weights.

$$\frac{\partial}{\partial \boldsymbol{\phi}} \mathcal{J}_{\text{ELBO}}(\boldsymbol{\phi}, \bar{\lambda}_i^*, \bar{\tau}_l^*) = \frac{\partial}{\partial \boldsymbol{\phi}} \mathbb{E}_{\text{N}(\boldsymbol{W};\boldsymbol{\phi})} \left[\log p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{W})\right] - \frac{\partial}{\partial \boldsymbol{\phi}} \text{KL}\left[\text{N}(\boldsymbol{W};\boldsymbol{\phi})||\text{N}(\boldsymbol{W}|\bar{\lambda}_i^*, \bar{\tau}_l^*)\right]$$

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Closed-Form Updates for λ and τ: Update based on current estimates of **W**'s posterior parameters.

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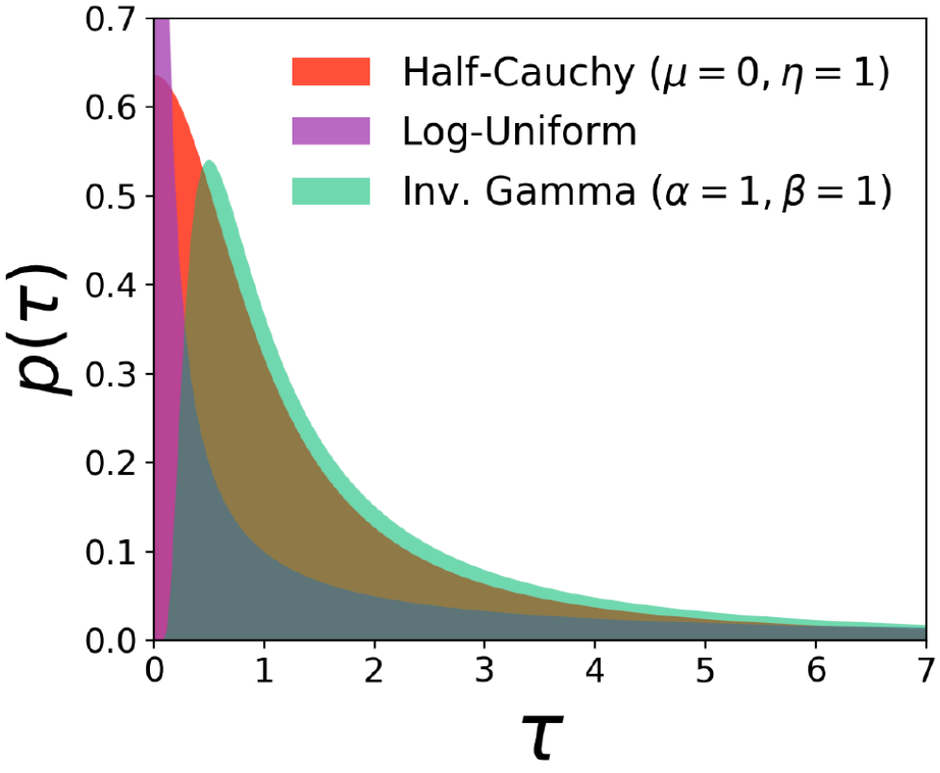
Closed-Form Updates for λ and τ: Update based on current estimates of **W**'s posterior parameters.

Example, Inv. Gamma:

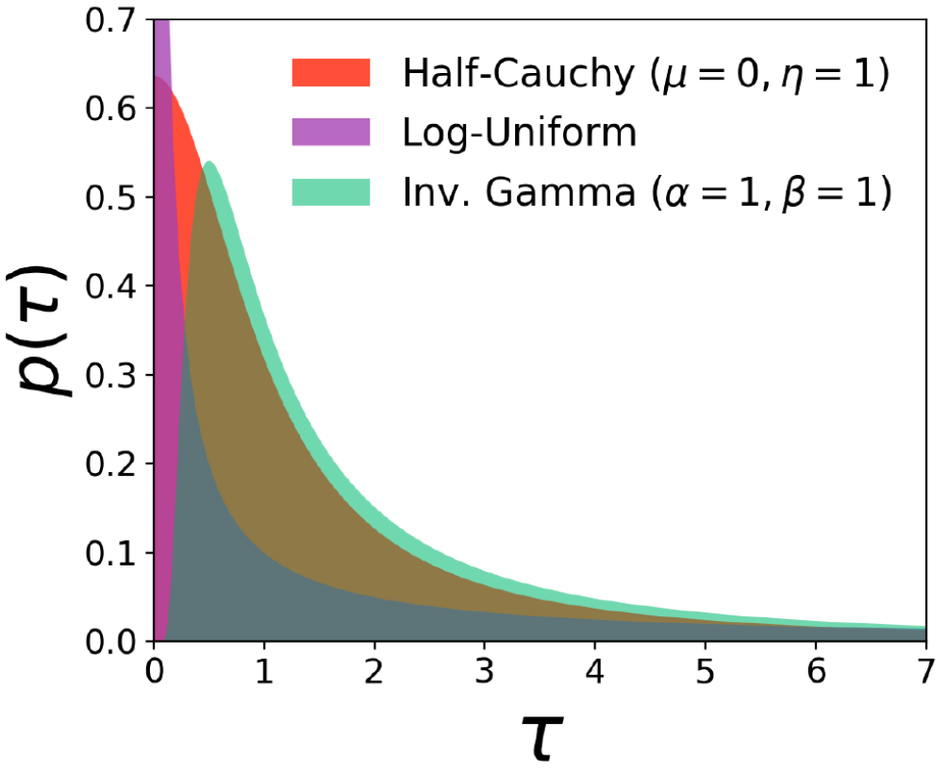
$$\bar{\lambda}_i^* = \frac{2\beta\bar{\tau}_l + \sum_j \sigma_{i,j}^2 + \mu_{i,j}^2}{\bar{\tau}_l(D_i + 2\alpha + 2)} \qquad \bar{\tau}_l^* = \frac{2\beta + \sum_i \bar{\lambda}_i^{-1} \sum_j \sigma_{i,j}^2 + \mu_{i,j}^2}{D + 2\alpha + 2}$$

EM Updates

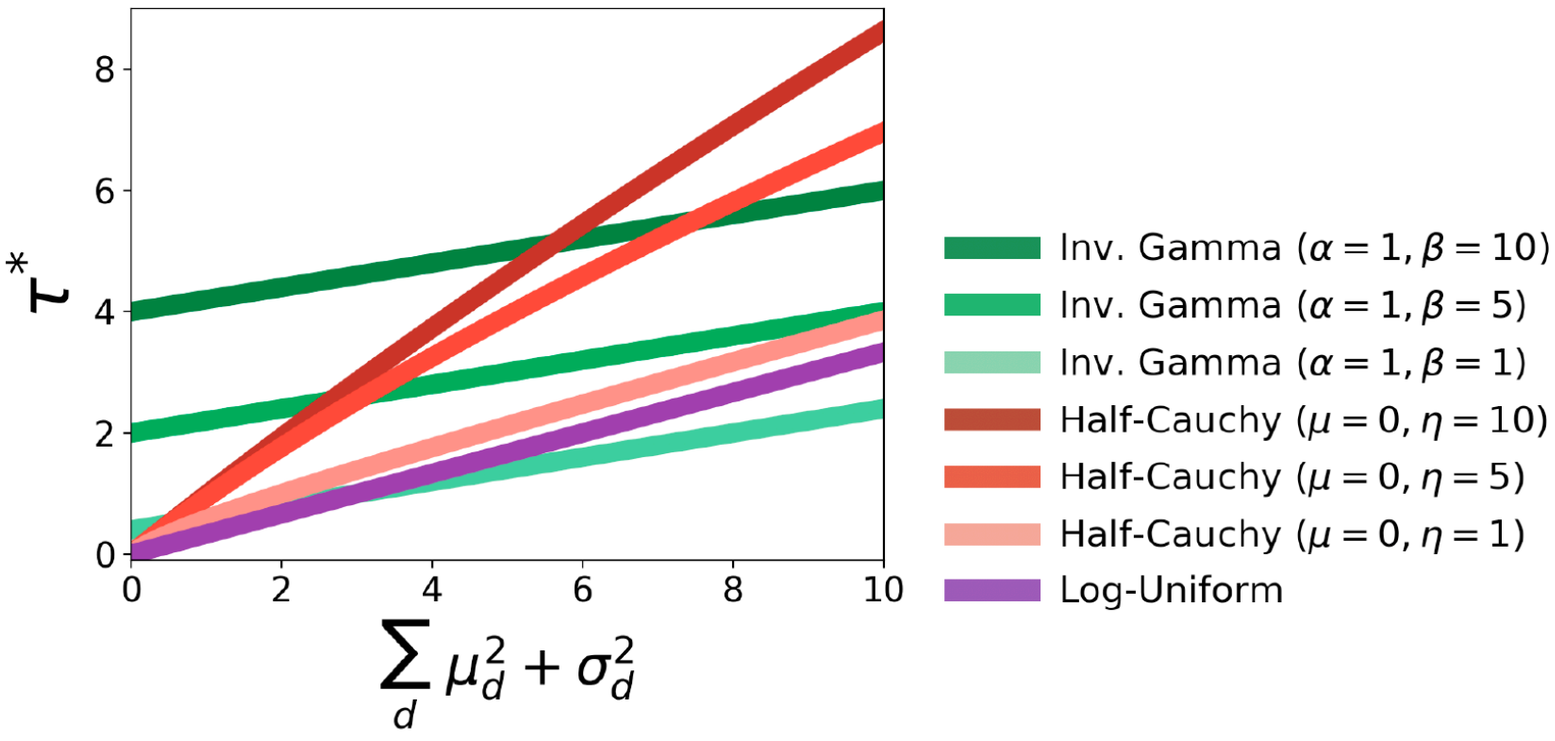


(a) Hyper-Priors

EM Updates



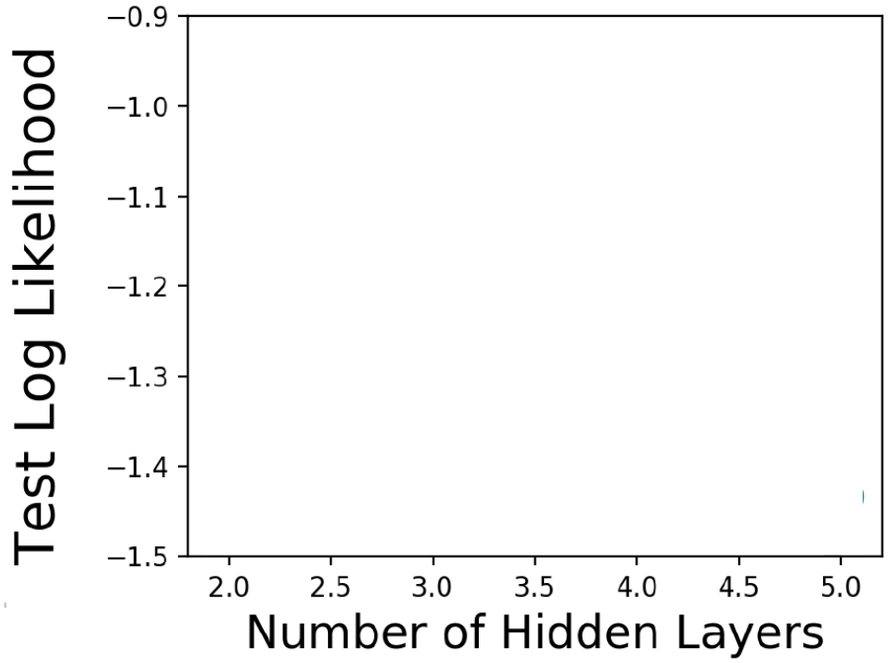
(a) Hyper-Priors



(b) EM Updates for Variance

Regression Results

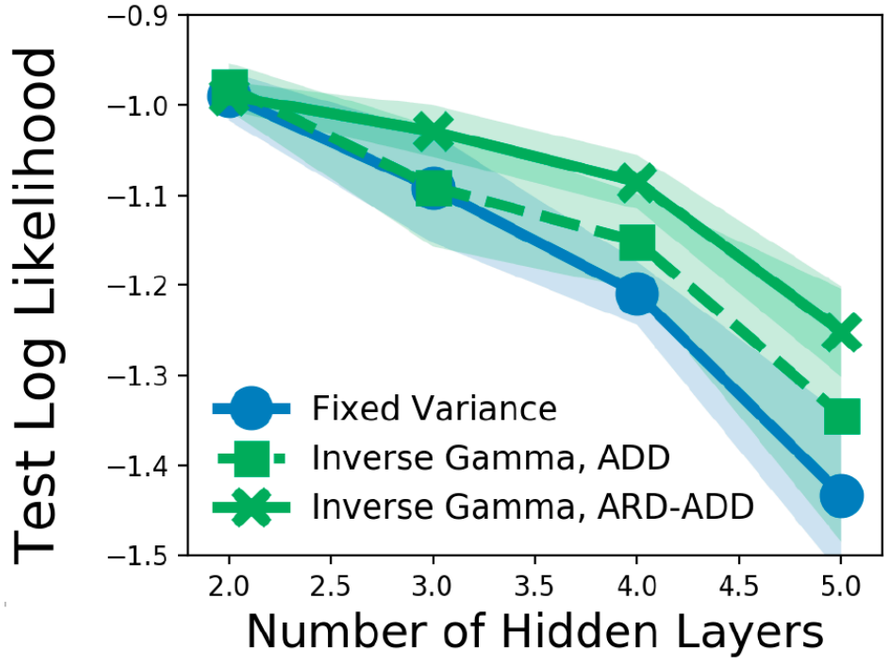
Regression: Test set performance on Yacht data set.



(a) Inverse Gamma $(\alpha = 1, \beta = 1)$

Regression Results

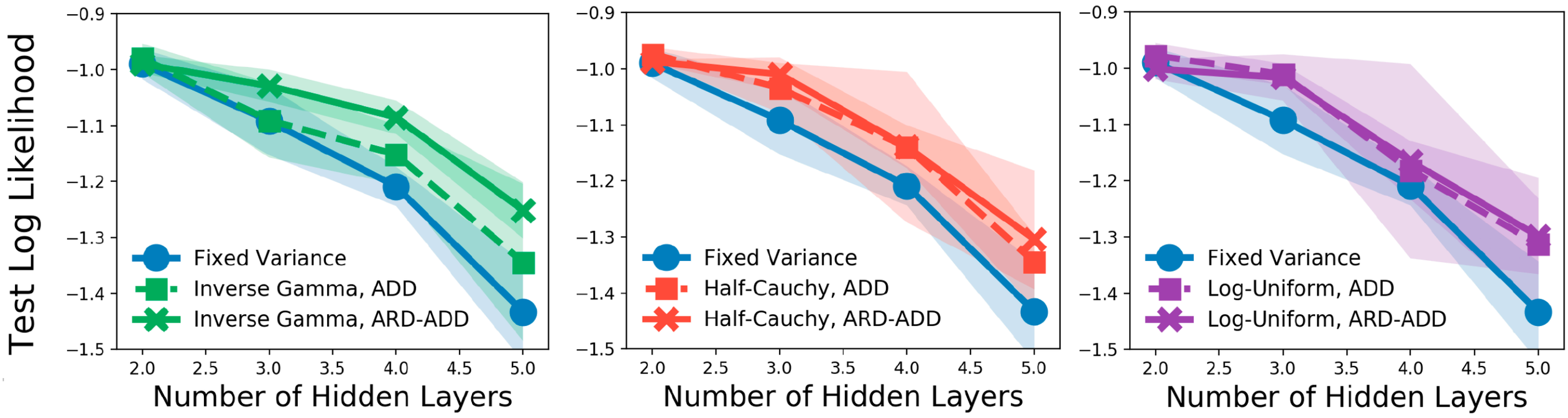
Regression: Test set performance on Yacht data set.



(a) Inverse Gamma $(\alpha = 1, \beta = 1)$

Regression Results

Regression: Test set performance on Yacht data set.



(a) Inverse Gamma $(\alpha = 1, \beta = 1)$ (b) Half-Cauchy $(\mu = 0, \eta = 2)$ (c) Log-Uniform

DISCUSSION

Statistics and Deep Learning

https://xkcd.com/1838/

We need principled approaches…

https://xkcd.com/1838/

Further Reading from a Statistical Perspective

- [ ] B. Cheng and D. M. Titterington
Neural Networks: A Review from a Statistical Perspective
Statistical Science, 1994

- [ ] 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, P. Smyth, and Y. W. Teh
Deep Learning: A Synthesis from Probabilistic Foundations
coming soon…

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Further Reading from a Statistical Perspective

B. Cheng and D. M. Titterington
Neural Networks: A Review from a Statistical Perspective
Statistical Science, 1994

The commentary is better yet…

Brian Ripley referring to some early NN experiments:
"…inadequately designed propaganda studies."

Further Reading from a Statistical Perspective

- [ ] B. Cheng and D. M. Titterington
Neural Networks: A Review from a Statistical Perspective
Statistical Science, 1994

Two lists from R. Tibshirani:

WHAT THE STATISTICIAN CAN LEARN FROM NEURAL NETWORK RESEARCHERS

1. We should worry less about statistical optimality and more about finding methods that work, especially with large data sets.
2. We should tackle difficult real data problems like some of those addressed by neural network researchers, like character and speech recognition and DNA structure prediction. As John Tukey has said, it is often better to get an approximate solution to a real problem than an exact solution to an oversimplified one.
3. Models with very large numbers of parameters can be useful for prediction, especially for large data sets and problems exhibiting high signal-to-noise ratios.
4. Modelling linear combinations of input variables can be a very effective approach because it provides both feature extraction and dimension reduction.
5. Iterative, nongreedy fitting algorithms (like steepest descent with a learning rate) can help to avoid overfitting in models with large numbers of parameters.
6. We (statisticians) should sell ourselves better.

WHAT THE NEURAL NETWORK RESEARCHER CAN LEARN FROM STATISTICIANS

1. They should worry more about statistical optimality or at least about the statistical properties of methods.
2. They should spend more effort comparing their methods to simpler statistical approaches. They will be surprised how often linear regression performs as well as a multilayered perceptron. They should not use a complicated model where a simple one will do.

Thank you. Questions?

In collaboration with…

Padhraic Smyth

José Miguel Hernández-Lobato

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Nitish Srivastava, Geoffrey E Hinton, Alex Krizhevsky, Ilya Sutskever, and Ruslan Salakhutdinov. Dropout: a simple way to prevent neural networks from overfitting. *Journal of machine learning research*, 15(1):1929–1958, 2014.

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Appendix

Dropout Objective as Marginal MAP

$$p(\{\mathbf{W}_l\}_{l=1}^{L+1}|\mathbf{y},\mathbf{X}) \propto p(\{\mathbf{W}_l\}_{l=1}^{L+1})\ \mathbb{E}_{p(\xi)}\left[p(\mathbf{y}|\mathbf{X},\{\mathbf{W}_l\}_{l=1}^{L+1},\{\mathbf{\Xi}_l\}_{l=1}^{L})\right]. \tag{9}$$

The marginal MAP estimate of the weights is then found by maximizing the logarithm of this expression:

$$\begin{aligned}
&\log p(\{\mathbf{W}_l\}_{l=1}^{L+1}|\mathbf{y},\mathbf{X}) \\
&\propto \log \mathbb{E}_{p(\xi)}\left[p(\mathbf{y}|\mathbf{X},\{\mathbf{W}_l\}_{l=1}^{L+1},\{\mathbf{\Xi}_l\}_{l=1}^{L})\right] \\
&\qquad + \frac{-1}{2\sigma_0^2}\sum_{l=1}^{L+1}\sum_{r=1}^{D_{l-1}}\sum_{j=1}^{D_l} w_{l,r,j}^2 \\
&= \mathcal{L}_{\text{MAP}}(\{\mathbf{W}_l\}_{l=1}^{L+1}).
\end{aligned} \tag{10}$$

Lastly, we perform the final two steps in the derivation: *(i)* use Jensen's inequality to lower-bound the first term, and *(ii)* assume the variance of the prior on the weights goes to infinity.

$$\begin{aligned}
&\mathcal{L}_{\text{MAP}}(\{\mathbf{W}_l\}_{l=1}^{L+1}) \\
&\geq \mathbb{E}_{p(\xi)}\left[\log p(\mathbf{y}|\mathbf{X},\{\mathbf{W}_l\}_{l=1}^{L+1},\{\mathbf{\Xi}_l\}_{l=1}^{L})\right] \\
&\qquad + \frac{-1}{2\sigma_0^2}\sum_{l=1}^{L+1}\sum_{r=1}^{D_{l-1}}\sum_{j=1}^{D_l} w_{l,r,j}^2 \\
&\to \mathbb{E}_{p(\xi)}\left[\log p(\mathbf{y}|\mathbf{X},\{\mathbf{W}_l\}_{l=1}^{L+1},\{\mathbf{\Xi}_l\}_{l=1}^{L})\right] \\
&= \mathcal{L}_{\text{MN}}(\{\mathbf{W}_l\}_{l=1}^{L+1}) \\
&\approx \frac{1}{S}\sum_{s=1}^{S}\log p(\mathbf{y}|\mathbf{X},\{\mathbf{W}_l\}_{l=1}^{L+1},\{\hat{\mathbf{\Xi}}_{l,s}\}_{l=1}^{L})
\end{aligned} \tag{11}$$