(Deep) Neural Networks

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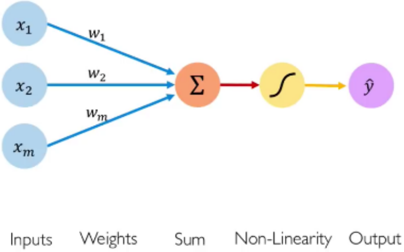
March 22, 2022

Summary of Linear/Logistic Regression



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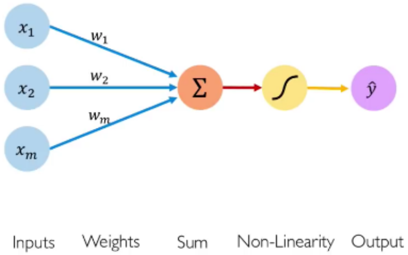

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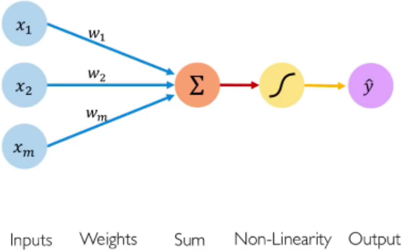

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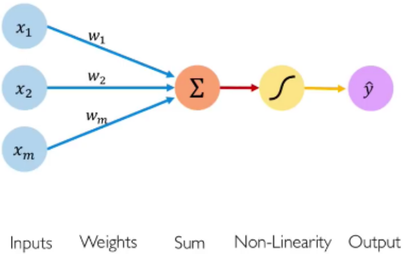

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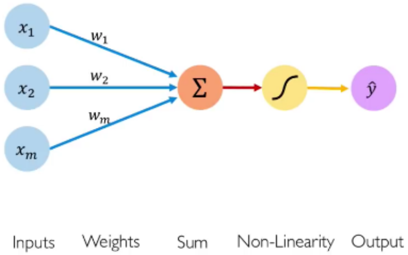

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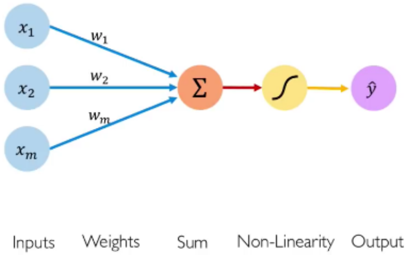

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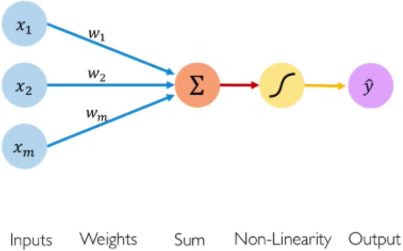

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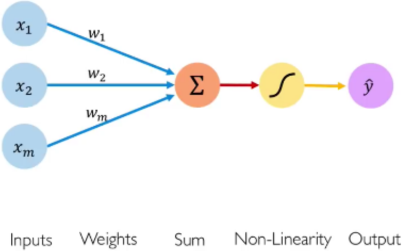

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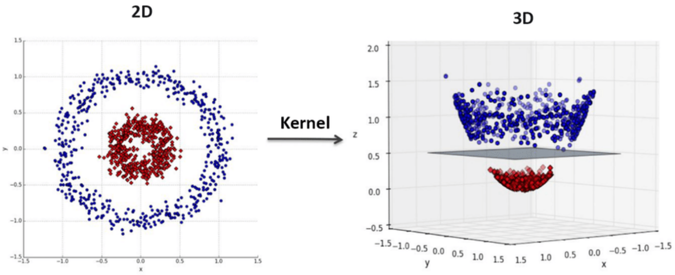
- Models linear ip-op relation or linearly separable boundaries

Cover's Theorem



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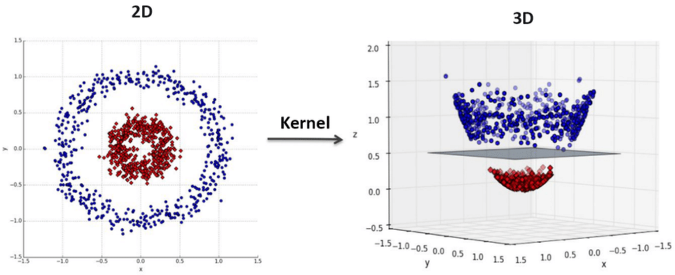

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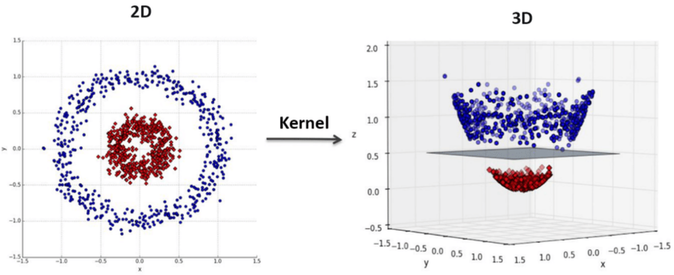

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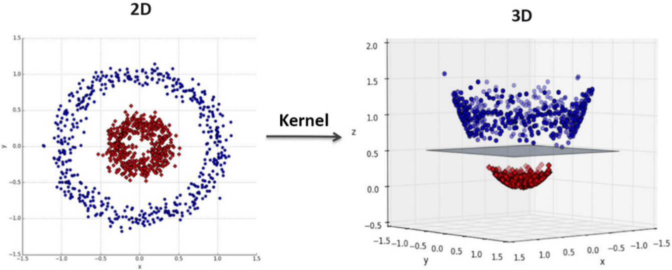

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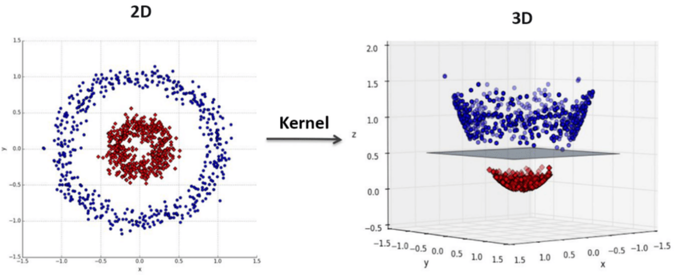

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    - The transformation from input space to feature space is nonlinear
    - The dimensionality of the feature space is high enough
    - $\mathbf{x} = [x_1 \ x_2] \rightarrow \phi(\mathbf{x}) = [x_1^2 \ x_2^2 \ \sqrt{2}x_1x_2]$

Data Independent Transformation

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- Apply linear models in feature space $\phi(\mathbf{x})$:

$$\hat{t} = y(\phi(\mathbf{x}), \mathbf{w}) = h\left(\mathbf{w}^{\mathsf{T}}\phi(\mathbf{x})\right)$$

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- Polynomial kernel of order n: $k(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^\mathsf{T}\mathbf{y} + c)^n$
  - For $\mathbf{x} \in \mathbb{R}^2$, $n = 2$ and $c = 1$: $k(\mathbf{x}, \mathbf{y}) = (x_1 y_1 + x_2 y_2 + 1)^2$
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  - Polynomial kernels are explicit kernels
- Gaussian kernel: $k(\mathbf{x}, \mathbf{y}) = \exp\left(-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{h}\right)$
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  - Feature representation $\phi(\mathbf{x})$ is not available: *Implicit kernel*
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- There is no reason to believe that the same transformation suits well for all domains - image, speech, medical, forensic, financial etc.,

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- Desired output is estimated as linear combination of nonlinear basis functions of the inputs $\mathbf{x} \in \mathbb{R}^D \rightarrow \phi(\mathbf{x}) \in \mathbb{R}^M$

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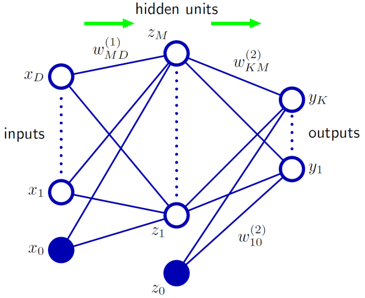
- $h(.)$ can be sigmoid, tanh, relu, softplus etc.,

2-Layer Feed Forward Network



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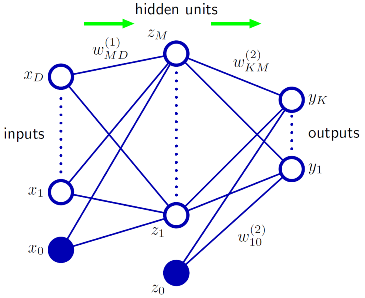

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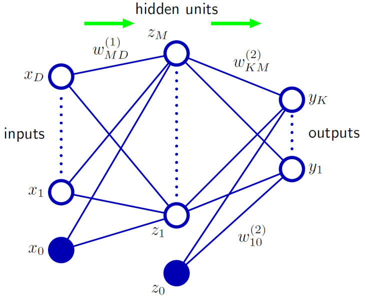

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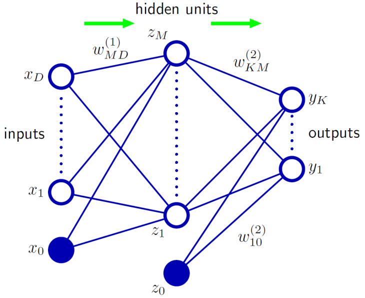

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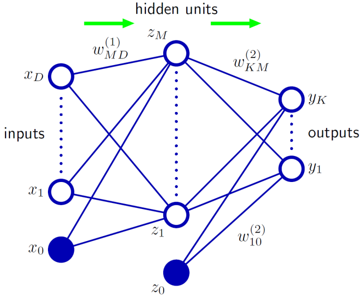

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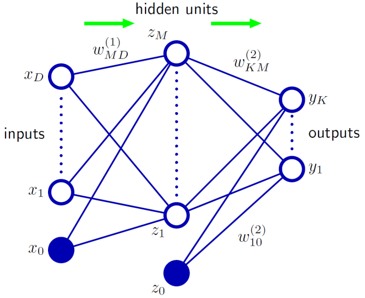

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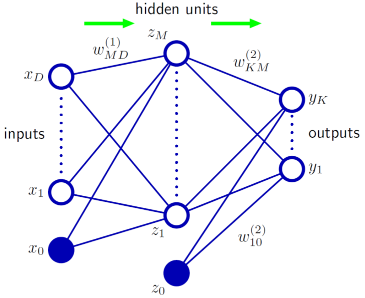

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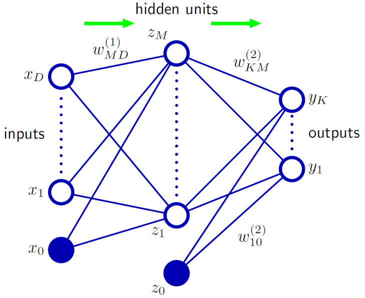

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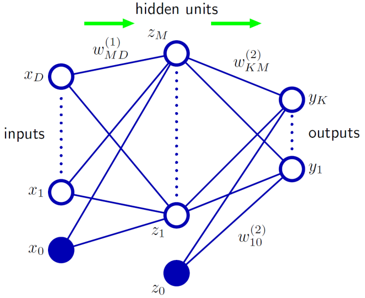

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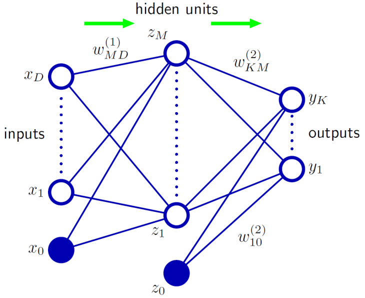

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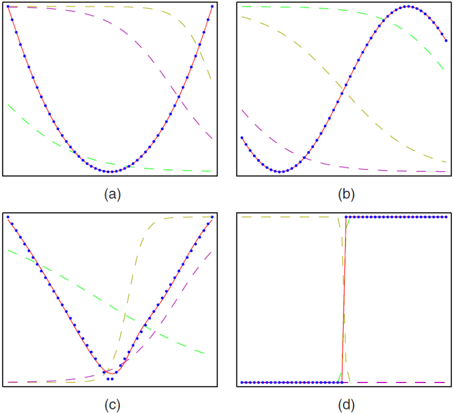
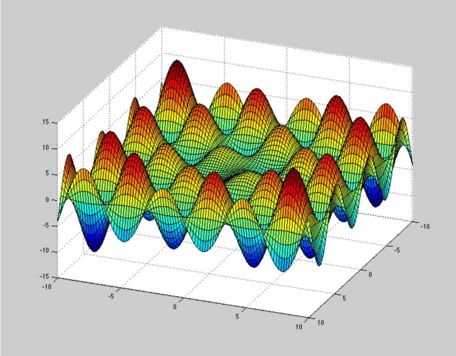
- Choice of $f(.)$ depends on task
  - Linear for Regression
  - Sigmoid for Binary Classification
  - Softmax for Multiclass Classification
- $y_k = f\left(\sum_{i=0}^{M} w_{kj}^{(2)} h\left(\sum_{i=0}^{D} w_{ji}^{(1)} x_i\right)\right)$

Universal Approximator



- (a) $f(x) = x^2$, (b) $f(x) = \sin(x)$ (c) $f(x) = |x|$, (d) $f(x) = sign(x)$
- One hidden layer with 3 tanh(.) units

Weight Space Symmetry



- Error $J(\mathbf{W}) = \mathbb{E}[\|\mathbf{t} - \mathbf{y}\|]$ is nonconvex in $\mathbf{W} = [\mathbf{W}^{(1)}\ \mathbf{W}^{(2)}]$.
- There are $2^M\ M!$ symmetric points with the same error
  - Order of neuronal units in hidden layer does not matter: $M!$
  - Weights leading to and going out of a hidden unit can be negated: 2^M
- Architecture, nonlinearity, loss function and dataset

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- Network weights $\mathbf{W} = [\mathbf{W}^{(1)}\ \mathbf{W}^{(2)}]$ have to be adjusted to minimize

$$J(\mathbf{W}) = \sum_{n=1}^{N} J_n(\mathbf{W})$$

$$J_n(\mathbf{W}) = \frac{1}{2}\sum_{k=1}^{K}(y_{nk} - t_{nk})^2$$

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- Gradients $\frac{\partial J(\mathbf{W})}{\partial w_{ji}^{(1)}}$ and $\frac{\partial J(\mathbf{W})}{\partial w_{kj}^{(2)}}$ are computed using error backpropagation

Backpropagation

Forward pass input $\mathbf{x}$

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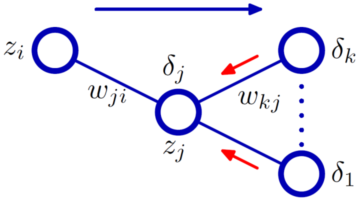
Propagation of Inputs and Errors



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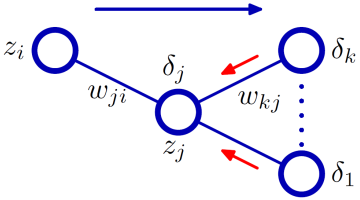

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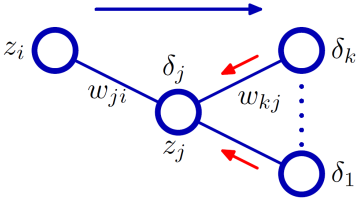

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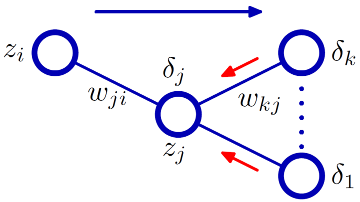

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- $\mathcal{B}$ denotes a random mini-batch of samples drawn from dataset.

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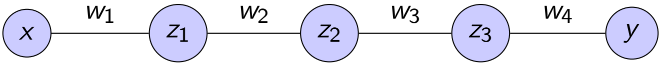
  - Weight space dynamics is influenced by weight initialization, batch size, order of presentation, learning rate schedule.

Vanishing Gradients



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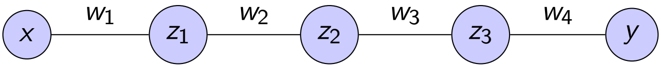

$$a_1 = w_1 x$$

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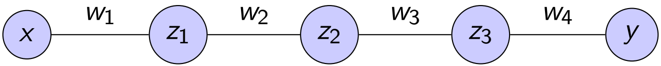

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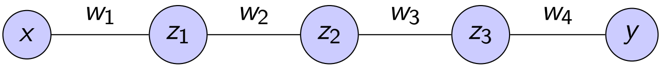

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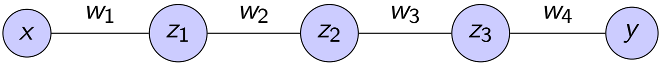

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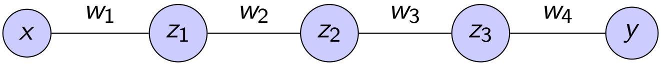

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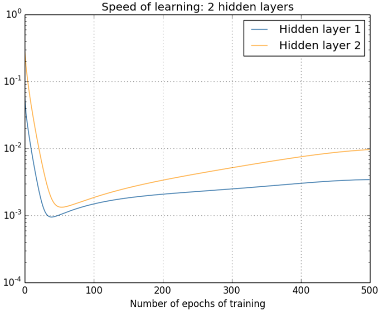
$$= (y - t)\, w_4\, h'(a_3)\, w_3\, h'(a_2)\, w_2\, h'(a_1)\, x$$

- Initial layer gradients are much smaller

Training Speed



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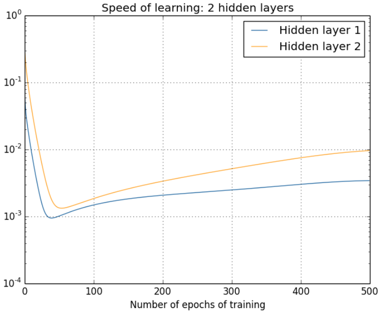

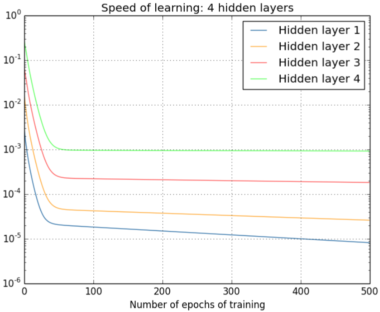

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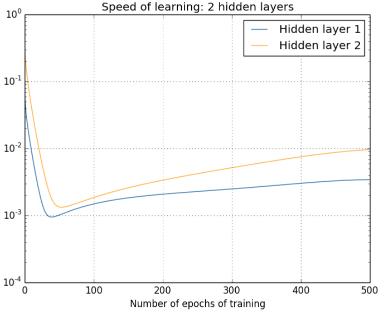

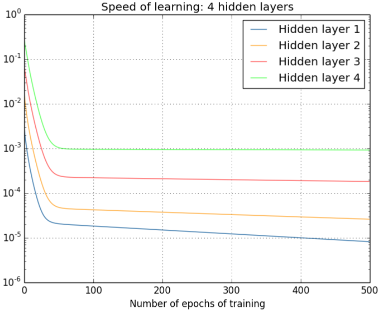

- Training speed is quantified using the norm of the weight update ΔW
- The updates are much smaller for initial layers - hence not trained
- The representations supplied to the deeper layers are not reliable

Derivatives of Activation Functions

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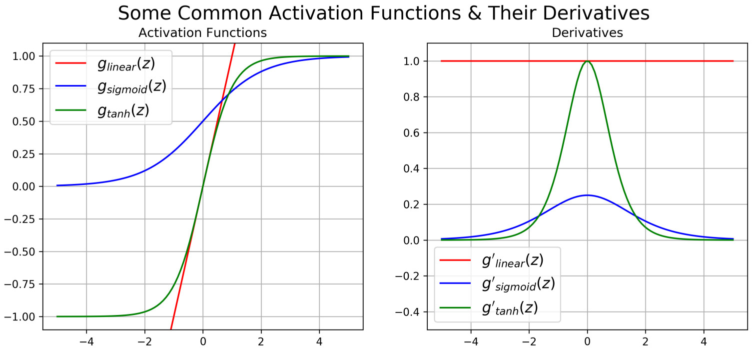

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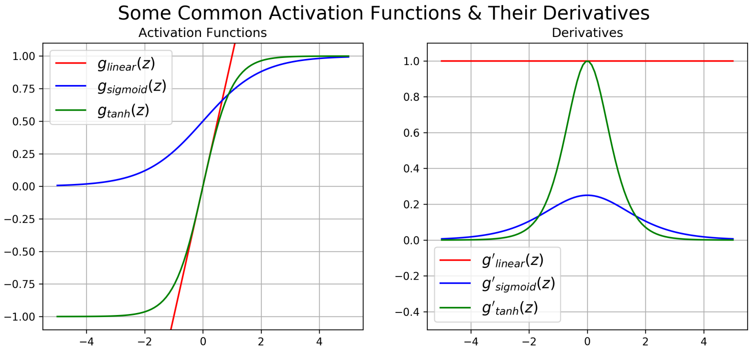
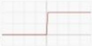
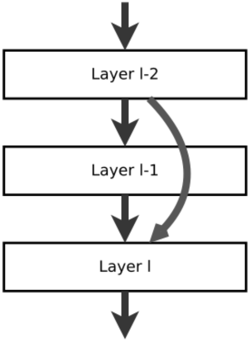


- The magnitude of derivatives of tanh(.) and $\sigma(.)$ are less than 1
- Deep cascade of such activation layers lead to vanishing gradients
- ReLU address this issue as it offers unity gradient for $+$ve values

Choice of Nonlinearity

Name	Plot	Equation	Derivative
Identity		$f(x) = x$	$f'(x) = 1$
Binary step		$f(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ 1 & \text{for} \quad x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for} \quad x \neq 0 \\ ? & \text{for} \quad x = 0 \end{cases}$
Logistic (a.k.a Soft step)		$f(x) = \frac{1}{1 + e^{-x}}$	$f'(x) = f(x)(1 - f(x))$
TanH		$f(x) = \tanh(x) = \frac{2}{1 + e^{-2x}} - 1$	$f'(x) = 1 - f(x)^2$
ArcTan		$f(x) = \tan^{-1}(x)$	$f'(x) = \frac{1}{x^2 + 1}$
Rectified Linear Unit (ReLU)		$f(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ x & \text{for} \quad x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ 1 & \text{for} \quad x \geq 0 \end{cases}$
Parameteric Rectified Linear Unit (PReLU) [2]		$f(x) = \begin{cases} \alpha x & \text{for} \quad x < 0 \\ x & \text{for} \quad x \geq 0 \end{cases}$	$f'(x) = \begin{cases} \alpha & \text{for} \quad x < 0 \\ 1 & \text{for} \quad x \geq 0 \end{cases}$
Exponential Linear Unit (ELU) [3]		$f(x) = \begin{cases} \alpha(e^x - 1) & \text{for} \quad x < 0 \\ x & \text{for} \quad x \geq 0 \end{cases}$	$f'(x) = \begin{cases} f(x) + \alpha & \text{for} \quad x < 0 \\ 1 & \text{for} \quad x \geq 0 \end{cases}$
SoftPlus		$f(x) = \log_e(1 + e^x)$	$f'(x) = \frac{1}{1 + e^{-x}}$

Residual Networks (ResNet)



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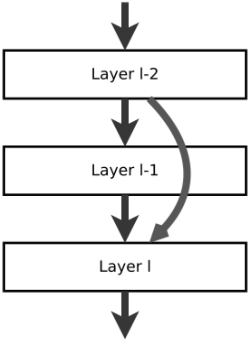

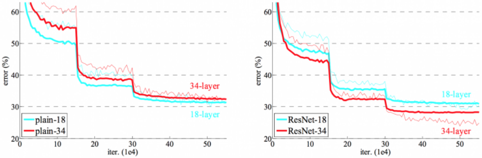

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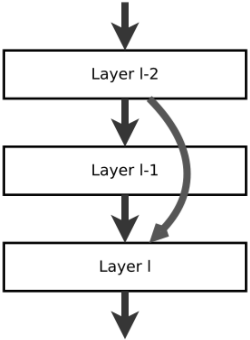

- 18 layer net has lower error than 34 layer net!
- Skip-connections to overcome vanishing grd.

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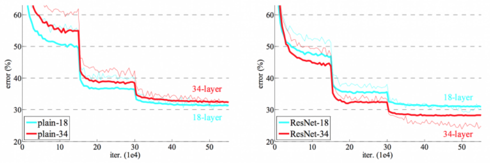

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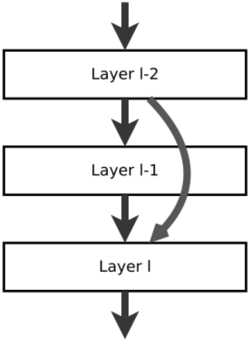

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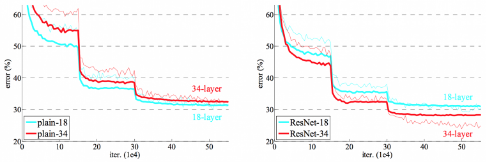

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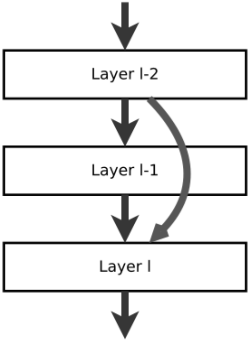

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- Backpropagation

$$\Delta\mathbf{W}^{(l-1,l)} = -\eta\, \mathbf{z}^{(l-1)}\, \boldsymbol{\delta}_l$$

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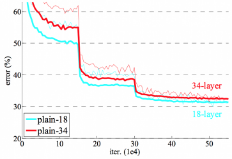
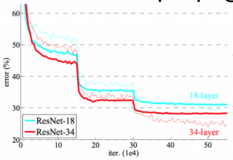
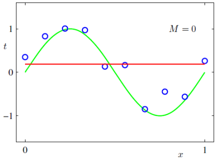
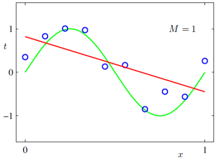




Overfitting





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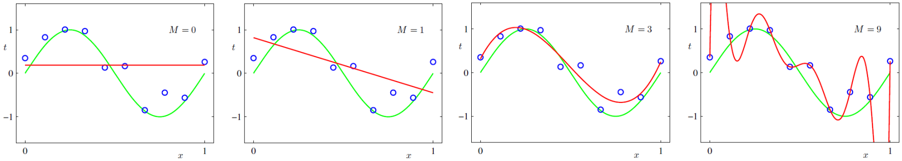

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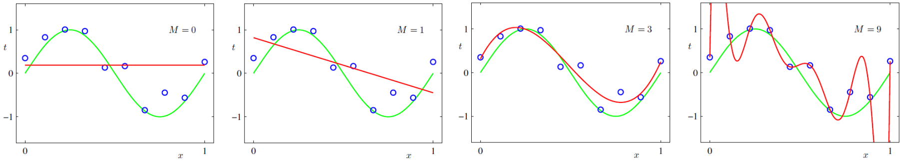

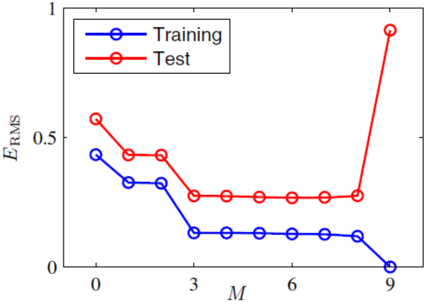

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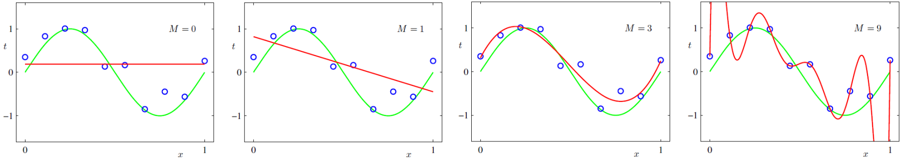

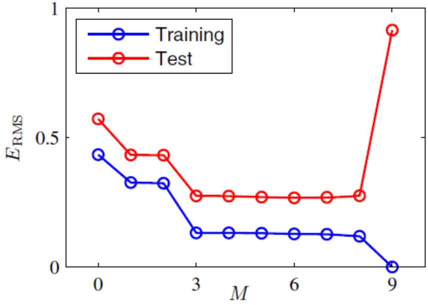

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$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
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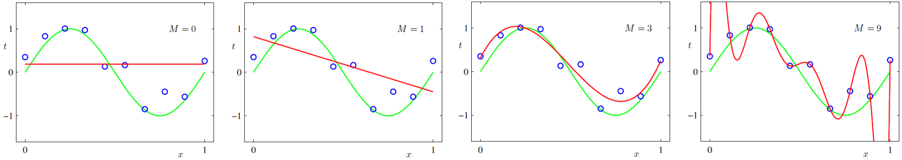

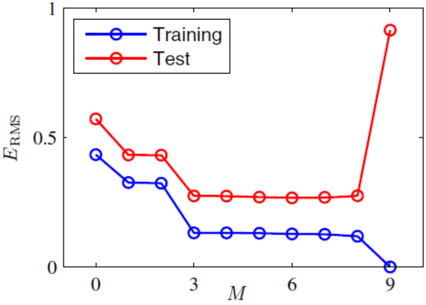

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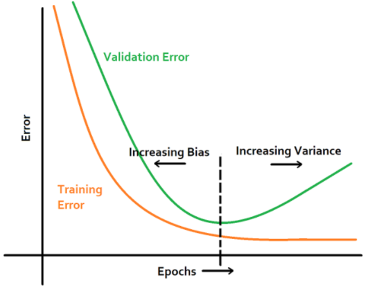
Regularization Techniques

- DNNs with large number of parameters tend to overfit
  - Error on training data reduces, but not on validation/test data
  - Performance on test data could be worse than smaller models (paradox)
  - With larger parameters, the model gets tuned to noise in training data
  - Weights blow up to capture the noisy fluctuations
- Arrest the growth of the weights to avoid overfitting to training data
- Finding the right balance between bias and variance trade-off.
- Common regularization techniques for DNNs include:
  - Early Stopping, explicit weight regularization, activity regularization/constraints, dropout, input corruption with noise

Early Stopping

- Initialize the weights with small random values
  - Glorot Normal - $w_{ji} \in \mathcal{N}\left(0, \frac{\sqrt{2}}{f_{in}+f_{out}}\right)$
  - Update the weights using backpropagation algorithm
- Monitor training and validation errors after every epoch.
- Stop the training when validation error starts to increase

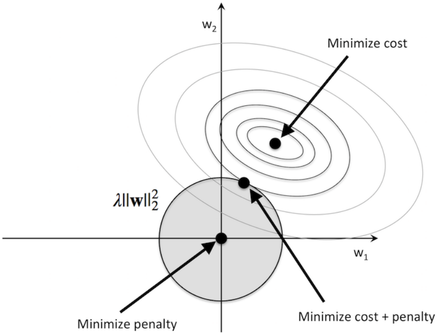


Weight Regularization

- Add a penalty term to the error function to discourage weight growth

$$J(\mathbf{W}) = \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K}(y_{nk} - d_{nk})^2 + \lambda\|\mathbf{W}\|_p$$

- λ controls the trade-off between bias and variance



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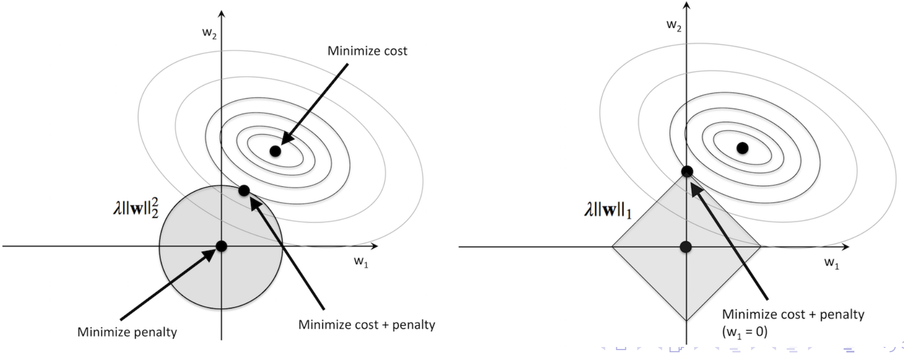
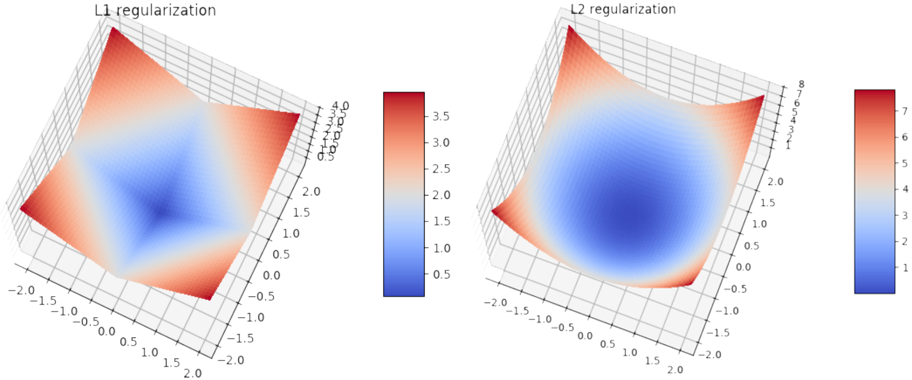


L_1 vs L_2



- L_1 regularization promotes sparser solutions
- L_1 regularization $\implies$ Laplacian priors
- L_2 regularization $\implies$ Gaussian priors

Dropout

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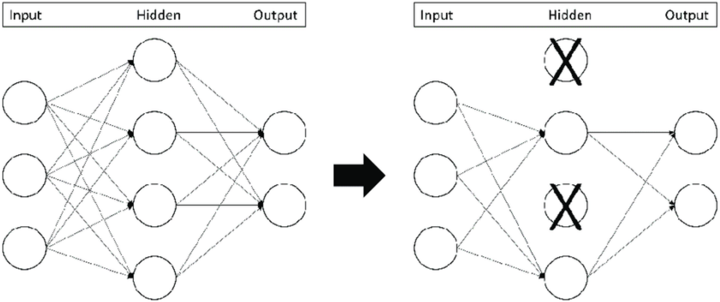

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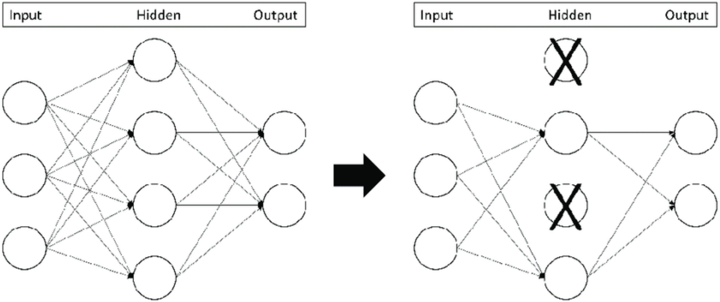

- Some nodes may tend to be too critical in network operation
- Avoid such situation by sharing the responsibility across the nodes
- Drop nodes in the hidden layers with a probability $p{=}(0.5)$
- With M hidden units, it can create 2^M different network architectures

Dropout Implementation

- Network training
  - Forwardpass the input to evaluate neuronal outputs in the hidden layer
    $$a_j = \sum_{i=0}^{D} w_{ji}^{(1)} x_i \qquad z_j = h(a_j)\, m_j$$
  - m_j is the mask drawn from a Bernoulli distribution with parameter p
  - Backpropagate the error to evaluate the share of the hidden neuron
    $$\delta_j = m_j\, h'(a_j) \textstyle\sum_{k=1}^{K} w_{kj} \delta_k$$

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- Interpretation of Dropout
  - Dropout can be interpreted as mixture of experts (novel combination)
  - A node is expected to perform in different configurations: Regularization

Limitations for Fully Connected (Dense) Networks

- FFNN offers data-dependent nonlinear transformation

$$\mathbf{z}[n] = \phi(\mathbf{x}[\boldsymbol{n}]) = g(\mathbf{W}^{(1)}\mathbf{x}[n]) \qquad \mathbf{y}[n] = f(\mathbf{W}^{(2)}\mathbf{z}[n])$$

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    - Need to explore nonlinear sequential models for signal processing
- Incorporate sequential information in the transformed representation
    - Finite memory: $\mathbf{z}[n] = \phi(\mathbf{x}[n-k] : \mathbf{x}[n+k])$ CNNs
    - Infinite memory: $\mathbf{z}[n] = \phi(\mathbf{x}[-\infty] : \mathbf{x}[\infty])$ RNNs