ILLINOIS INSTITUTE OF TECHNOLOGY

Feed-forward Neural Networks

CS-585

Natural Language Processing

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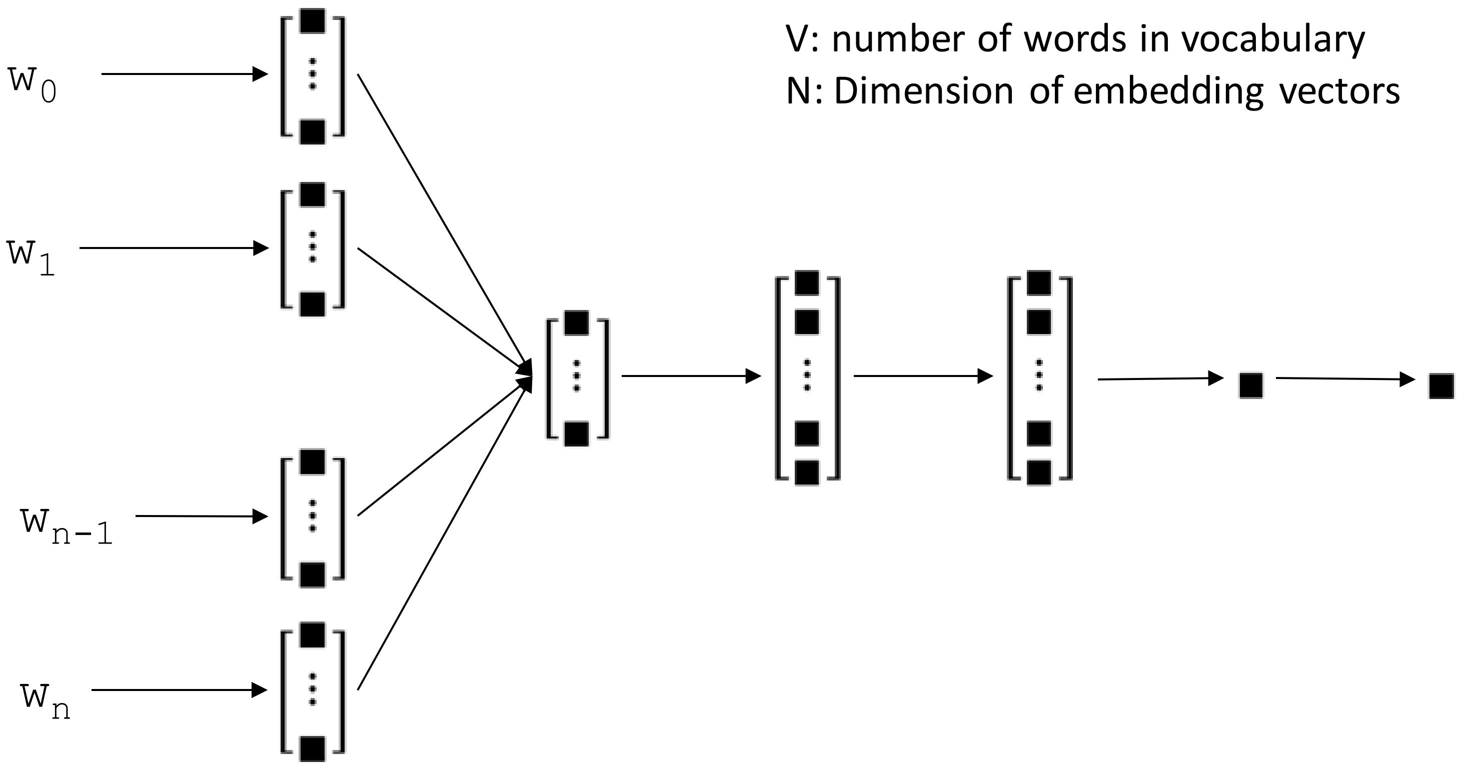
TEXT CATEGORIZATION WITH NEURAL NETWORKS

Text categorization with neural networks

- Neural networks
  - Use vector/matrix/tensor representations
  - Apply a sequence of algebraic operations (matrix multiplication, etc.)
  - Trained using some variant of gradient descent
- Text categorization architecture
  - Input layer - Bag of words representation, or dense word embeddings (e.g., word2vec)
  - One or more hidden layers ("fully-connected" layers)
  - Probabilistic output layer: logistic sigmoid (binary classification) or softmax (multiclass classification)

Binary text classification model – feed-forward neural network



V: number of words in vocabulary
N: Dimension of embedding vectors

Binary text classification model – feed-forward neural network

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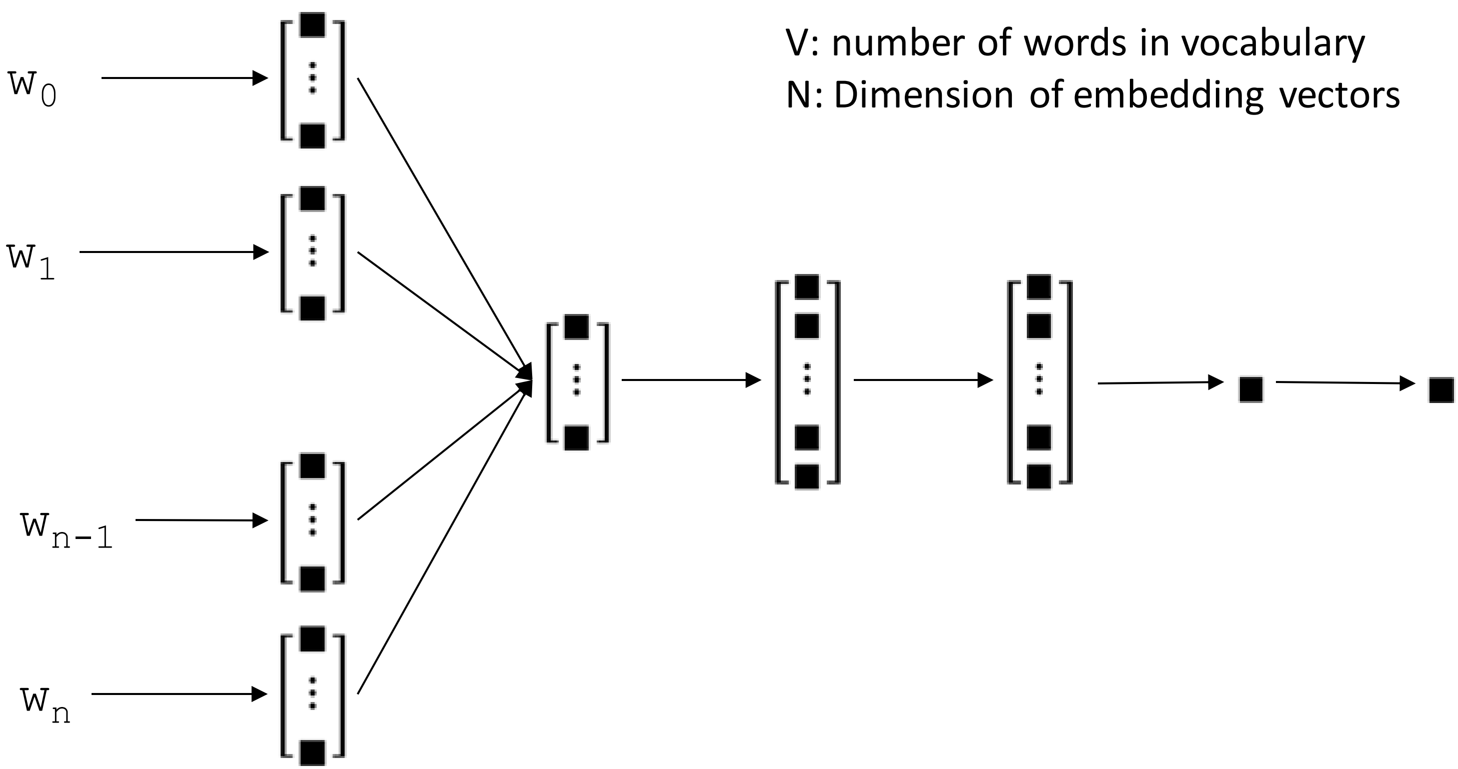
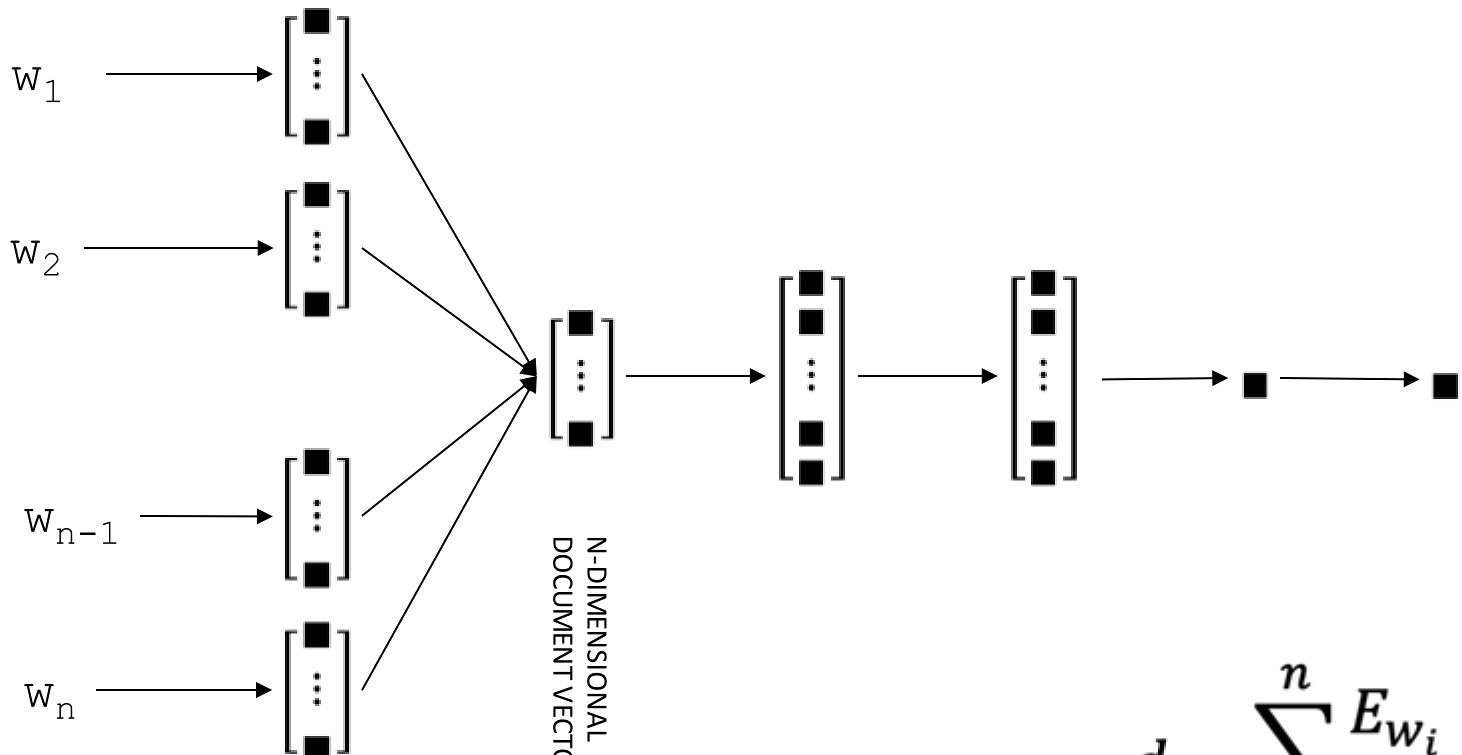


Look up words in VxN embedding table

N-DIMENSIONAL WORD VECTORS

Binary text classification model – feed-forward neural network



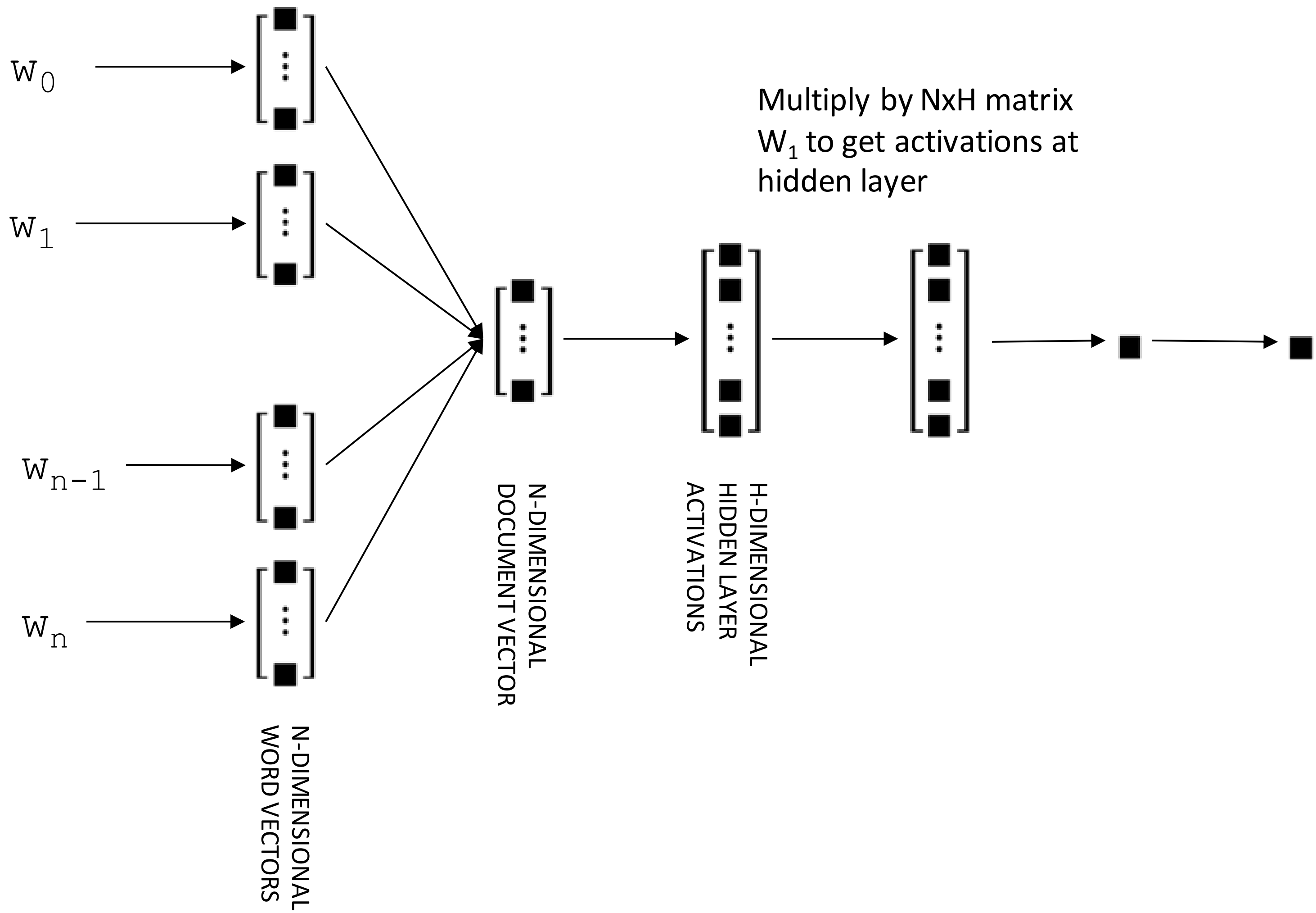
N-DIMENSIONAL
DOCUMENT VECTOR

N-DIMENSIONAL
WORD VECTORS

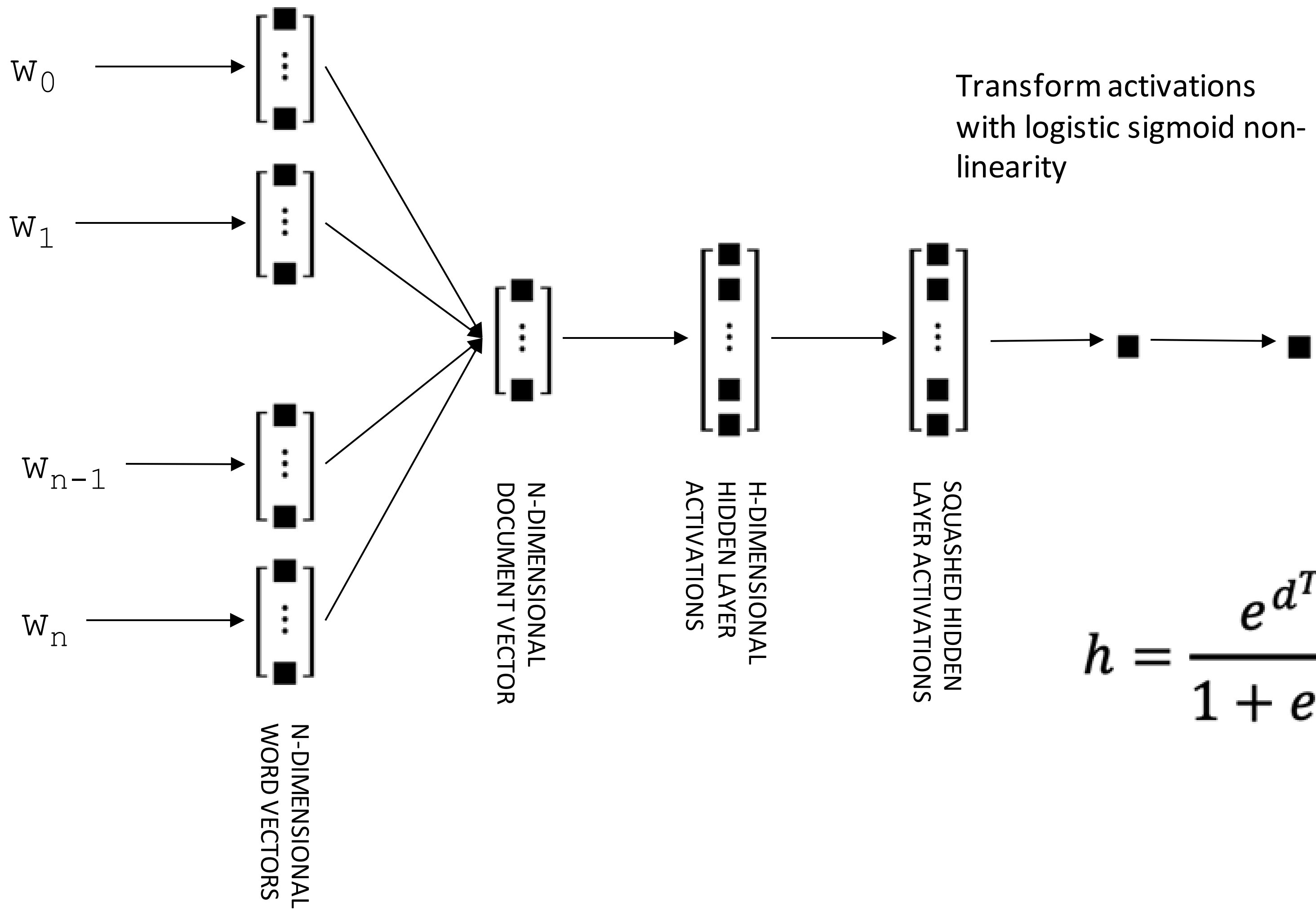
Compute average
of word
embeddings

$$d = \sum_{i=1}^{n} \frac{E_{w_i}}{n}$$

Binary text classification model – feed-forward neural network



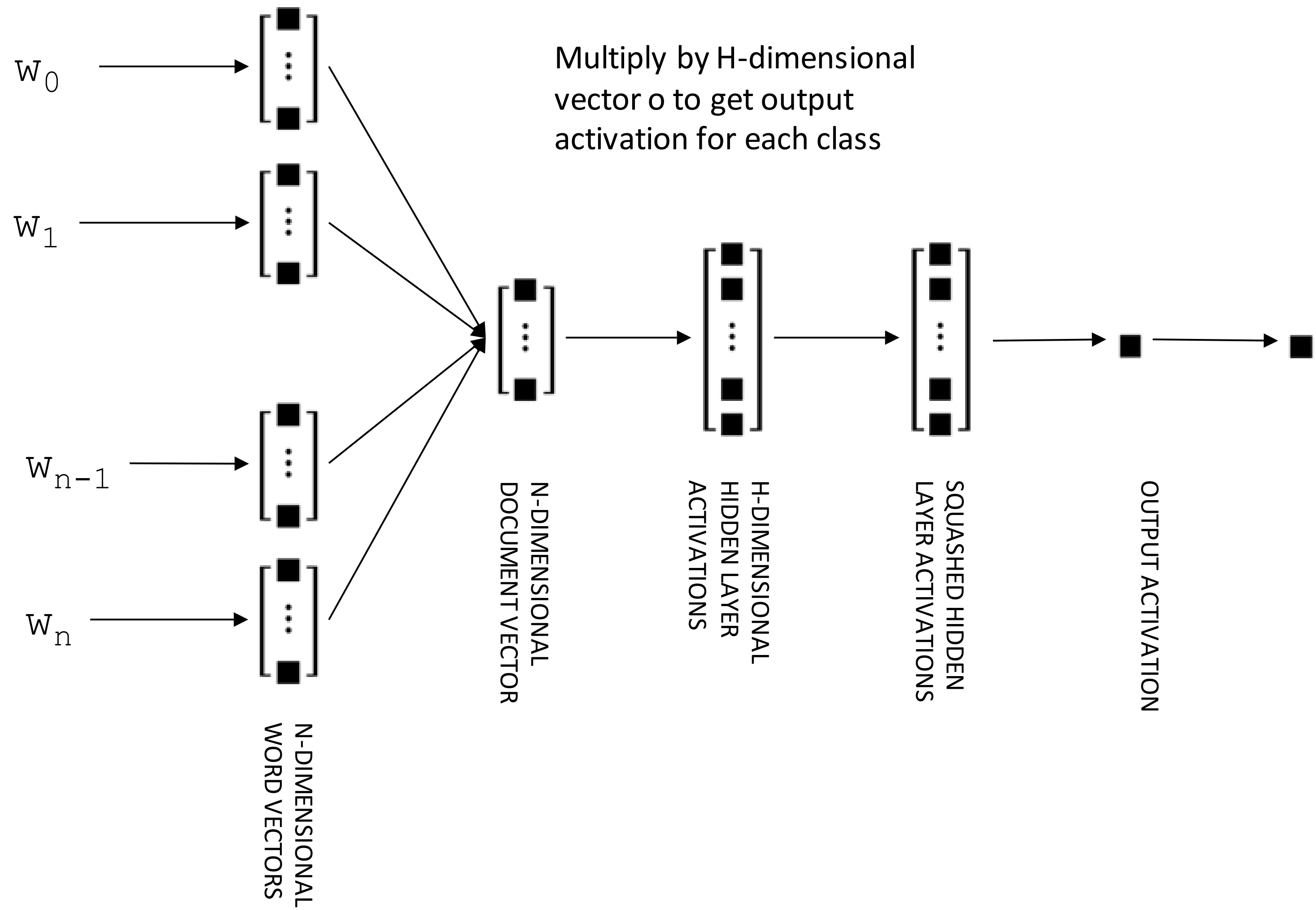
Binary text classification model – feed-forward neural network



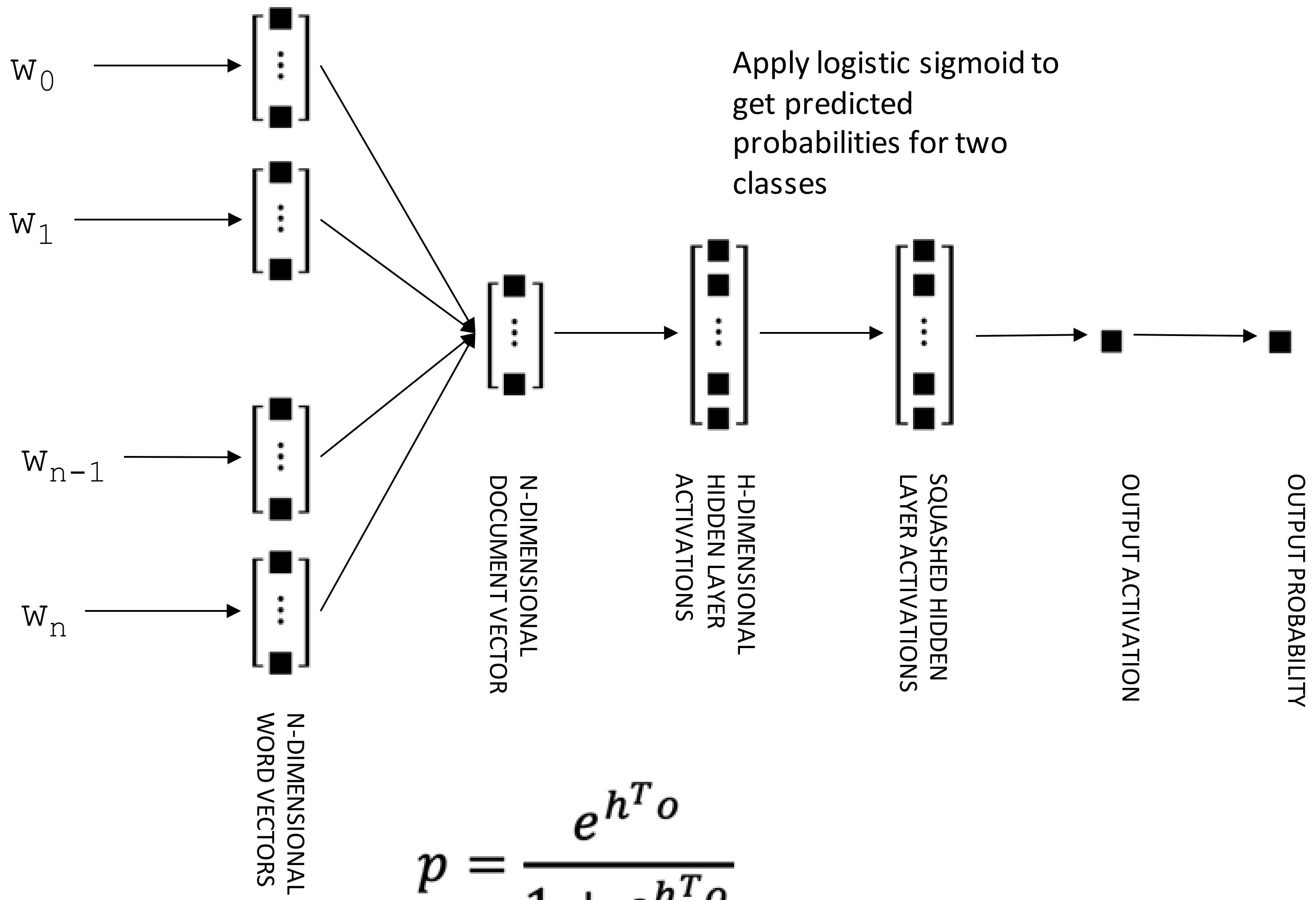
Transform activations with logistic sigmoid non-linearity

$$h = \frac{e^{d^T W_1}}{1 + e^{d^T W_1}}$$

Binary text classification model – feed-forward neural network



Binary text classification model – feed-forward neural network



$$p = \frac{e^{h^T o}}{1 + e^{h^T o}}$$

Feed-forward text categorization network: summary

Words → document representation

$$d = \sum_{i=1}^{n} \frac{E_{w_i}}{n}$$

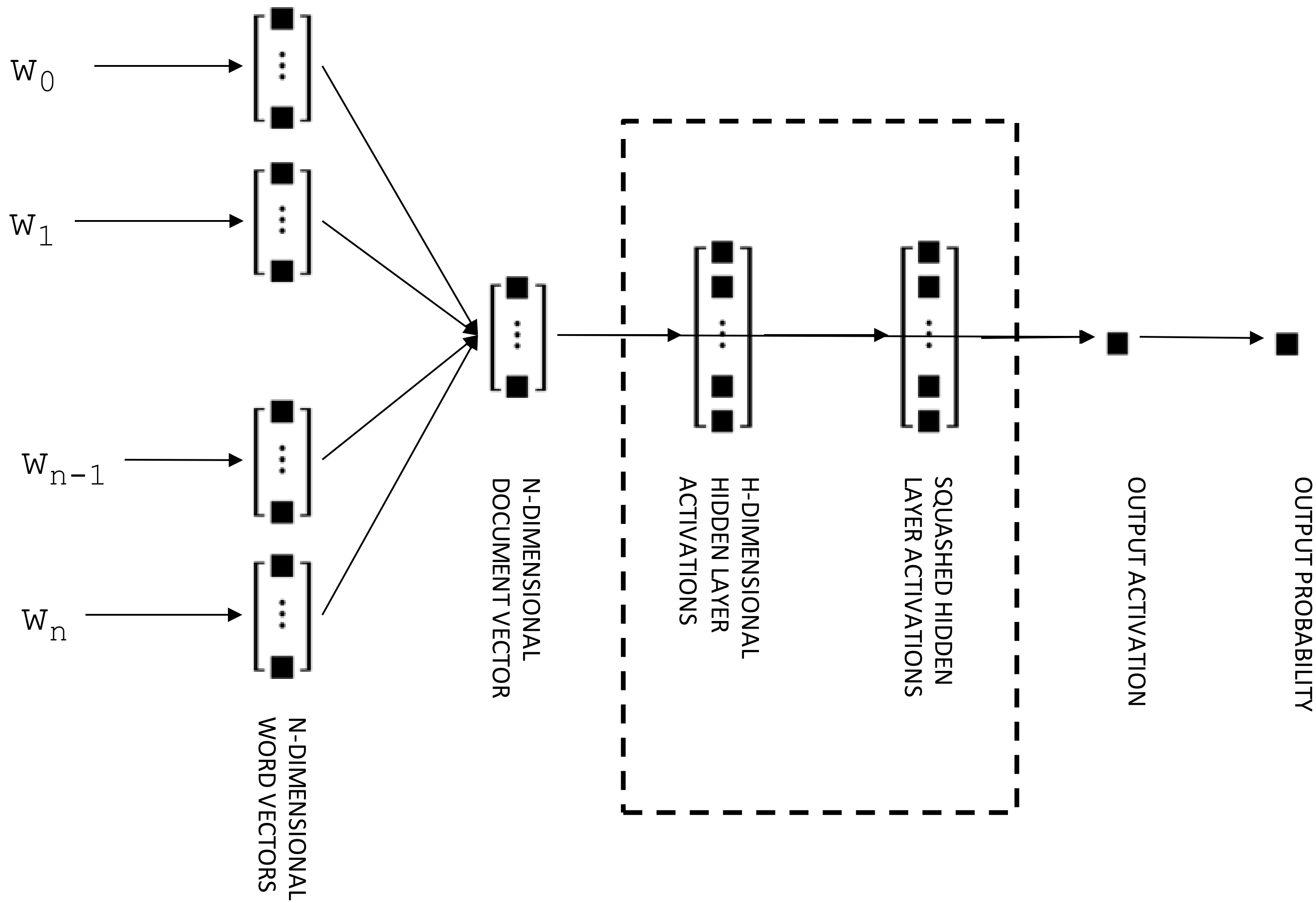
Document representation → hidden layer

$$h = Sigmoid(d^T W_1) = \frac{e^{d^T W_1}}{1 + e^{d^T W_1}}$$

Hidden layer → output probability

$$p = Sigmoid(h^T o) = \frac{e^{h^T o}}{1 + e^{h^T o}}$$

Comparison to logistic regression



Logistic regression: summary

Words → document representation

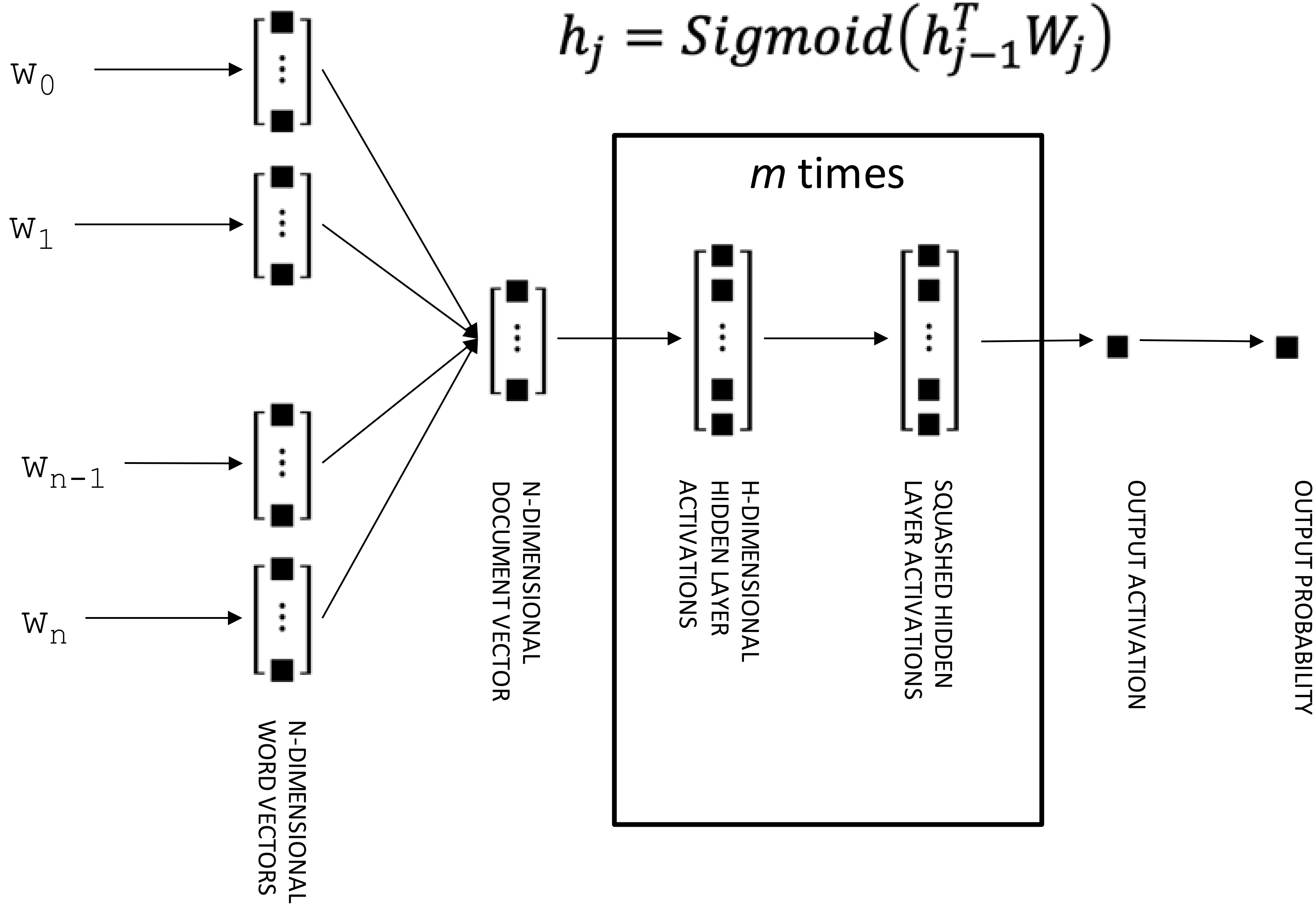
$$d = \sum_{i=1}^{n} \frac{E_{w_i}}{n}$$

Document representation → output probability

$$p = Sigmoid(d^T o) = \frac{e^{d^T o}}{1 + e^{d^T o}}$$

Feed-forward neural network: multiple hidden layers

$$h_j = Sigmoid\left(h_{j-1}^T W_j\right)$$



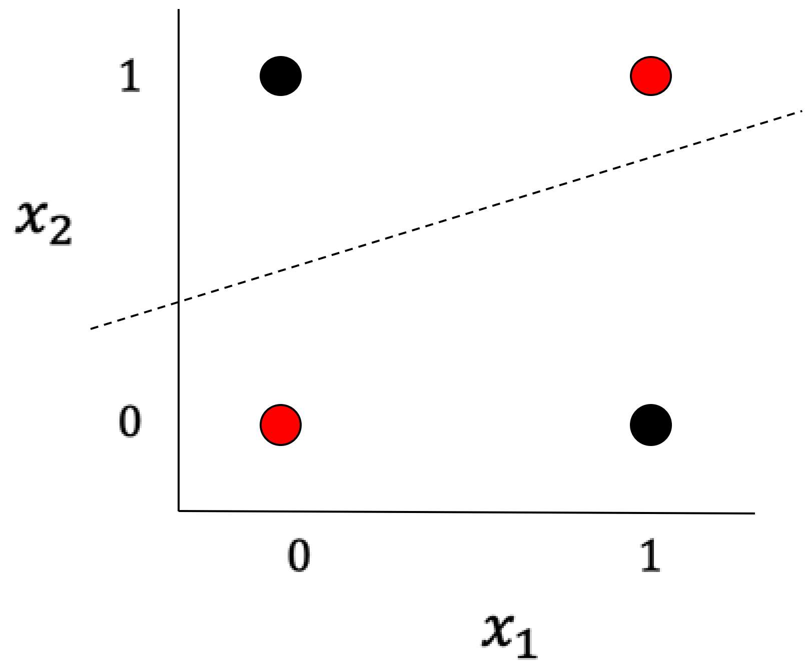
What is the point of nonlinearities?

Expressive capacity

- Some functions cannot be expressed / represented / learned without them

XOR - "Exclusive Or"

- Matrix multiplication is just a linear operation, and XOR requires a non-linear decision boundary



Expressive capacity of neural networks

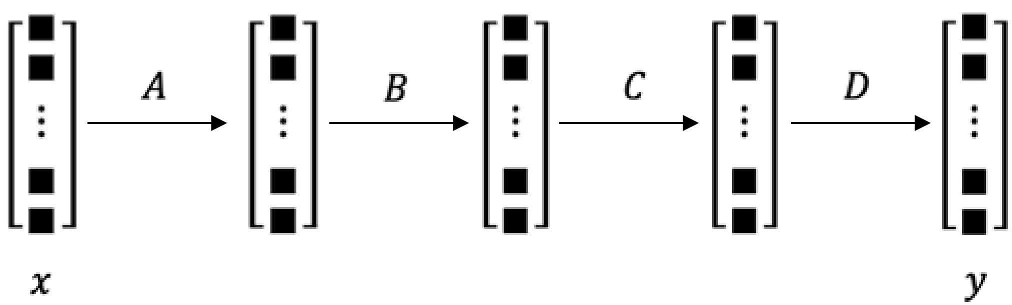
- A feed-forward neural network with fully-connected layers, at least one hidden layer with nonlinear activations (such as sigmoid) can represent any function of its inputs with arbitrary precision
  - Depends only on number of hidden nodes in the network
- Can be thought of as a “universal function approximator”

What is the point of multiple hidden layers?

- A network with a single hidden layer can represent any function as well as a network with multiple hidden layers
- **But** it may require an exponentially greater number of nodes
- Deeper networks are better for representing complex relationships between inputs and outputs
- **But** they can introduce difficulties for optimization
  - Regularization helps
  - Also residual connections (advanced topic)

Hidden layers are only useful with nonlinearities

- Remember that without nonlinear activation functions, each layer of a feedforward neural network is just a linear transform of the previous layer (matrix multiplication)
- And successive matrix multiplications are always expressible as a single matrix multiplication



$$y = x^T ABCD = x^T(ABCD)$$

$$M \stackrel{\text{def}}{=} ABCD$$
$$y = x^T M$$

Multilabel vs. multiclass

- Multilabel classification
  - Labels are not mutually exclusive
  - E.g., document may be labeled as <u>both</u> "space" and "electronics"
  - Probabilities do not sum to one
  - Logistic **sigmoid** nonlinearity at output layer
- Multiclass classification
  - Labels are mutually exclusive
  - Probabilities must sum to one
  - **Softmax** nonlinearity at output layer

REVISITING: GRADIENT DESCENT

Loss functions

Loss function	Usage	Formula
Binary cross-entropy	Binary or multilabel classification	$\mathcal{L} = -y_i \log \hat{y}_i - (1 - y_i) \log(1 - \hat{y}_i)$
Categorical cross-entropy	Multiclass classification	$\mathcal{L} = -\sum_i y_i \log \hat{y}_i$
Squared error	Regression (prediction of a real-valued output)	$\mathcal{L} = \sum_i (y_i - \hat{y}_i)^2$

Other Loss functions are available: (e.g., absolute error, hinge loss)

Gradient descent

1. Define a loss function to be minimized. For Logistic regression this is cross entropy loss (logistic loss)

$$\ell_{\text{LogReg}}(\boldsymbol{\theta}; \boldsymbol{x}^{(i)}, y^{(i)}) = -\boldsymbol{\theta} \cdot \boldsymbol{f}(\boldsymbol{x}^{(i)}, y^{(i)}) + \log \sum_{y' \in \mathcal{Y}} \exp(\boldsymbol{\theta} \cdot \boldsymbol{f}(\boldsymbol{x}^{(i)}, y'))$$

[E-NLP 2.59]

2. Compute **gradient of loss** with respect to parameters

3. Update parameters in the direction of gradient

Formula: E-NLP 2.5

Gradient descent

- <u>Batch</u> gradient descent: accumulate updates across entire dataset before applying

η: Learning rate

$$\Theta_{t+1} \leftarrow \Theta_t - \eta \sum_{i=1}^{|D|} \nabla \log L(\Theta; \vec{x_i}; y_i)$$

slow!

- <u>Stochastic</u> gradient descent: update parameters after gradient calculated for each training exemplar

$$\Theta_{t+1} \leftarrow \Theta_t - \eta \nabla \log L(\Theta; \vec{x_i}; y_i)$$

fast!
but less stable

- <u>Minibatch</u>: Process updates for smaller samples of dataset (16-1024)

$$\Theta_{t+1} \leftarrow \Theta_t - \eta \sum_{i=1}^{n} \nabla \log L(\Theta; \vec{x_i}; y_i)$$

faster, more stable

More complex optimization

- Gradient descent:

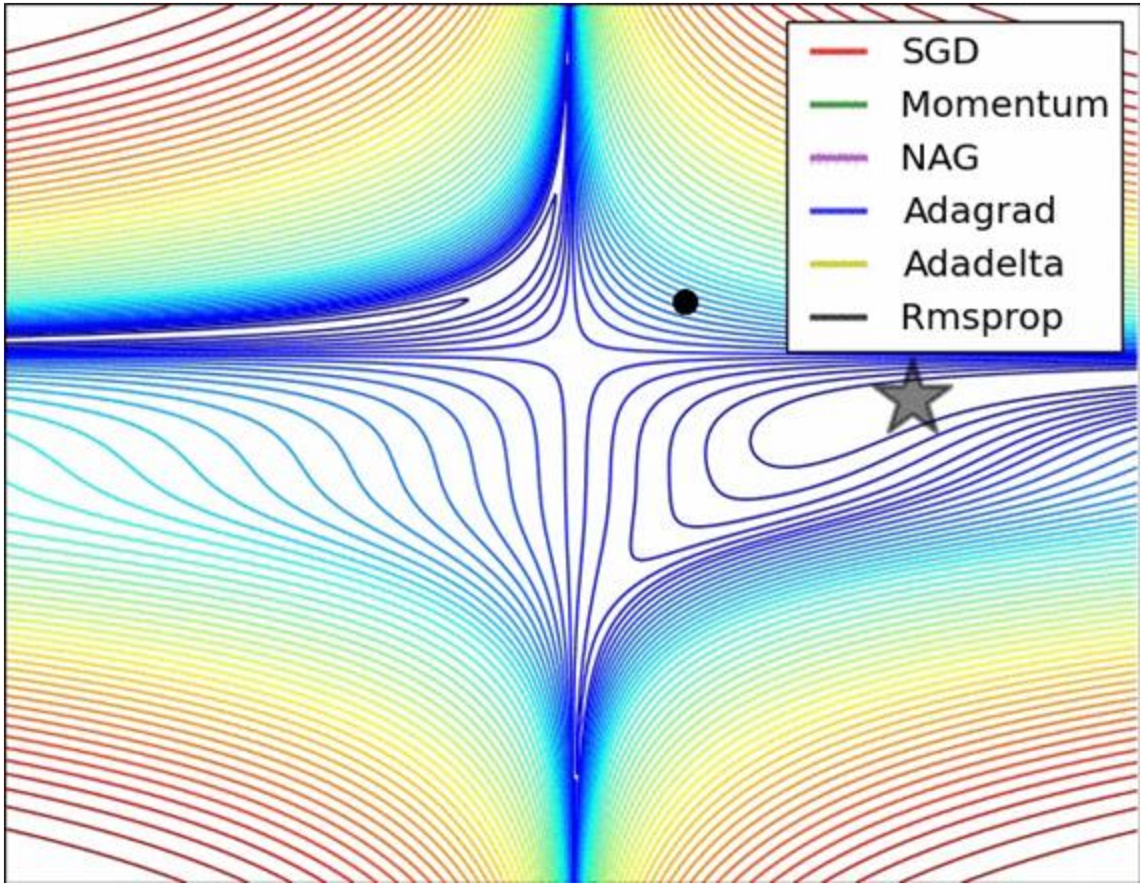
$$\Theta_{t+1} \leftarrow \Theta_t - \eta \nabla \log L(\Theta)$$

- Momentum:
  - Preferentially continue parameter search in direction of previous gradients; accelerate in directions of consistent updates

$$v_{t+1} = \gamma v_t + \eta \nabla \log L(\Theta)$$
$$\Theta_{t+1} \leftarrow \Theta_t - v_{t+1}$$

- Adaptive gradient:
  - Adagrad and Adadelta: move faster in selected directions of the gradient, for parameters (words) that occur infrequently
  - Cf. E-NLP 2.6.2

More complex optimization



Alec Radford: https://imgur.com/a/Hqolp

NEURAL NETWORK TOOL CHEST

Nonlinearities

- Softmax and logistic sigmoid are the most common nonlinearities used in neural networks for NLP, but there are a few others to be familiar with.
- The general constraints on nonlinearities (or *activation functions*) is that they be **monotonic** (continuously increasing or decreasing) and **differentiable** (smooth)
- The primary nonlinear functions used are
  - Softmax
  - Logistic sigmoid
  - Hyperbolic tangent (`tanh`)
  - Rectified linear (ReLU)

Nonlinearities: softmax

- Softmax is typically only used at the output layer of a network in order to get probabilistic/normalized outputs for multiclass classification problems
- It is sometimes treated as part of the loss function, rather than part of the network per se.

TensorFlow 2.0 RC is available Learn more

TensorFlow > API > TensorFlow Core r1.14 > Python

tf.losses.softmax_cross_entropy

View source on GitHub

Creates a cross-entropy loss using tf.nn.softmax_cross_entropy_with_logits_v2.

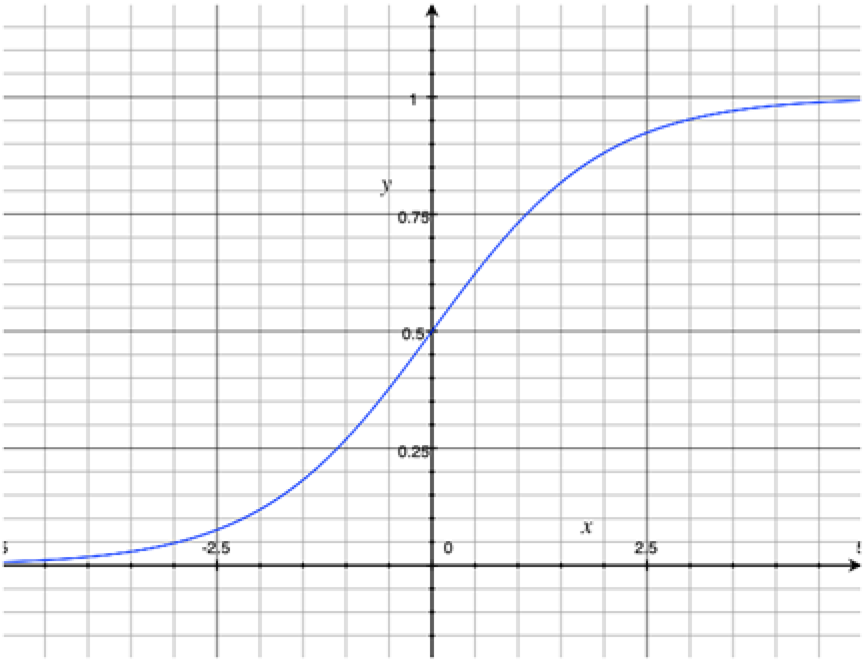
$$Softmax(\vec{x}) = \left[\frac{e^{\vec{x}_i}}{\sum_{\forall j} e^{\vec{x}_j}}\right]_{\forall i}$$

CROSSENTROPYLOSS

CLASS `torch.nn.CrossEntropyLoss(weight=None, size_average=None, ignore_index=- 100, reduce=None, reduction='mean', label_smoothing=0.0)` [SOURCE]

Nonlinearities: logistic sigmoid

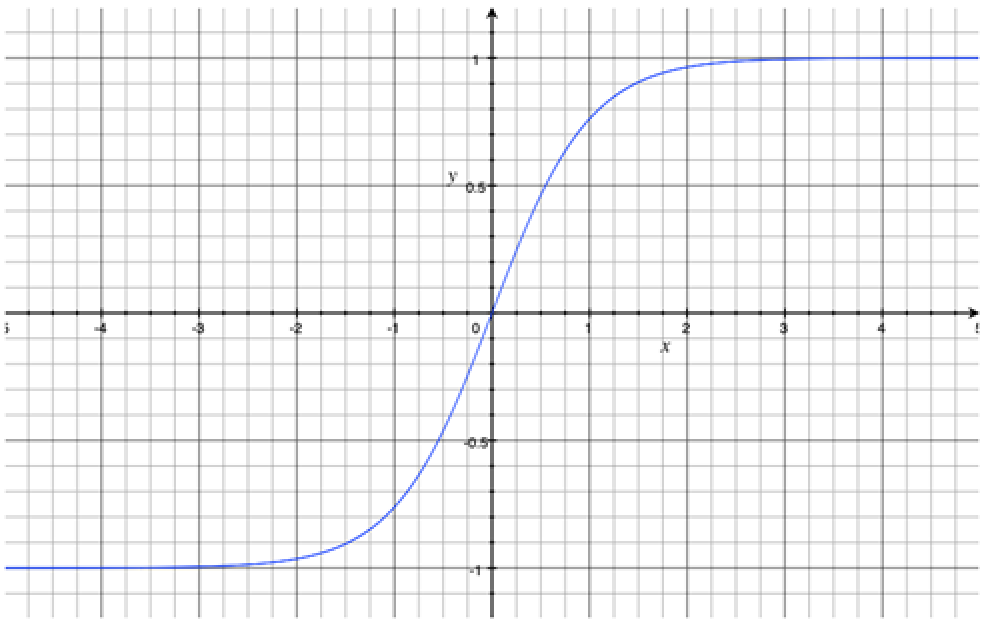
- Most commonly-used activation function for hidden layer of network
- Also at output layer for binary classification tasks
- Produces activations constrained to range [0,1]



$$Sigmoid(\vec{x}) = \frac{e^{\vec{x}}}{1 + e^{\vec{x}}}$$

Nonlinearities: hyperbolic tangent

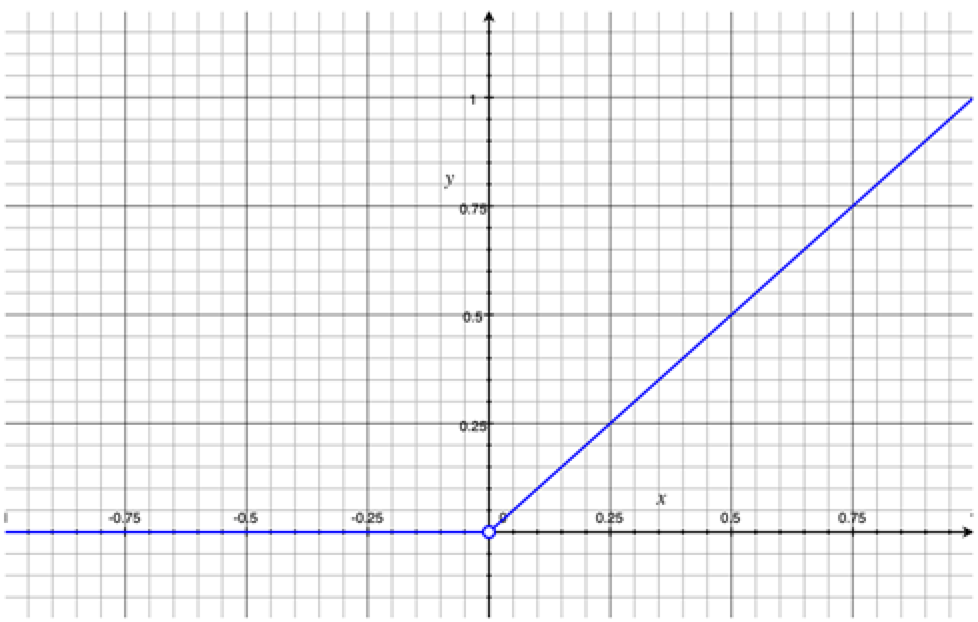
- Sigmoid-like activation function that allows negative outputs
- Used in LSTMs (later this semester)
- Produces activations constrained to range $[-1,1]$



$$\text{htan}(\vec{x}) = \frac{e^{\vec{x}} - e^{-\vec{x}}}{e^{\vec{x}} + e^{-\vec{x}}}$$

Nonlinearities: ReLU

- *Rectified Linear Unit*
- Produces sparse activations (many zeroes)
- Technically not differentiable at 0, but can be dealt with computationally
- Produces activations constrained to range $[0, \infty]$



$$rectifier(\vec{x}) = \max(\vec{x}, 0)$$

THE ART OF NETWORK ENGINEERING

Parameters and Hyperparameters

- Parameters: model-internal values that are set through training in order to optimize against some loss function
  - Examples: word embeddings, weight matrices between network layers
- Hyperparameters: model architecture or optimization decisions that are fixed in advance of training
  - Examples: learning rate, number of hidden layers, number of nodes per layer, regularization hyperparameters

Hyperparameters in neural networks

- Many model types have hyperparameters
  - Naïve Bayes – Smoothing hyperparameter
  - Logistic Regression – L1/L2 penalty
  - KNN – k neighbors
- But neural networks have a *lot* of them. How to search?
  - Choose a value and hope for the best
  - Search many values and select the best one based on development data
- Performance may also vary across training runs with a different random seed

Regularization in neural networks

- **Regularization**: discouraging or regulating model complexity
  - Especially important for neural networks due to the *curse of dimensionality*
- In a high-dimensional space, there are many possible parameterizations (decision surfaces) that have equivalent performance according to our loss function (perhaps perfect accuracy on the training set)

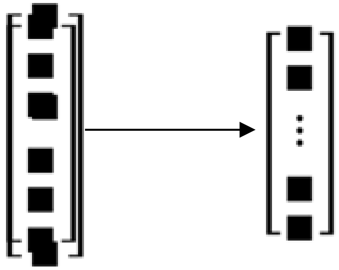
Regularization in neural networks

- L1 and L2 penalties we learned about in connection with logistic regression are used in neural networks as well
  - Different regularization penalties may be associated with weights at different layers
- Another regularization technique is *early stopping*—halting training before the loss has been fully minimized
  - Monitor performance on development dataset

Regularization in neural networks

Dropout is a regularization technique specific to neural networks

- During training, a **fixed percentage** of outputs at each layer are randomly set to zero
- This introduces noise into the inputs of the next layer, discouraging large weights
- It also discourages "co-adaptation" nodes in a layer that jointly perform a single function and can cause training to stall in a local minimum



Frozen and tied weights

- In a neural network, some weights may be fixed, rather than updating in the course of training. These are referred to as *frozen.*
  - For instance, word embeddings from word2vec may be used at the input layer of the network, but not updated in training a task-specific model
  - Alternatively, the embedding weights may be further refined through task-specific training. This is called *fine-tuning*
- *Tied* or *shared weights* are constrained to be the same within a network.
  - For instance, we could build a network to classify pairs of documents, and constrain the portions of the network specific to a single document to be the same across both.

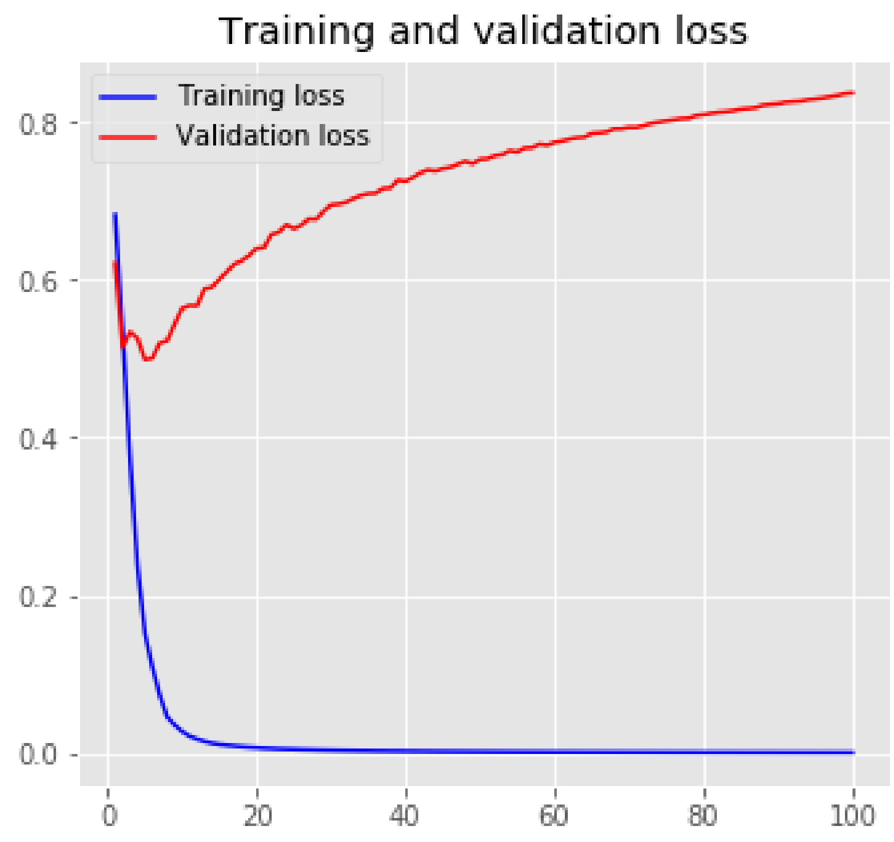
TROUBLESHOOTING NEURAL NETWORKS

Evaluation

- Neural networks have great expressive capacity
  - Therefore, we need to ensure that we monitor performance on held-out data to **avoid overtraining**
- Neural networks are difficult to optimize – non-convex error functions with local minima
  - Therefore, we need to monitor performance to ensure convergence

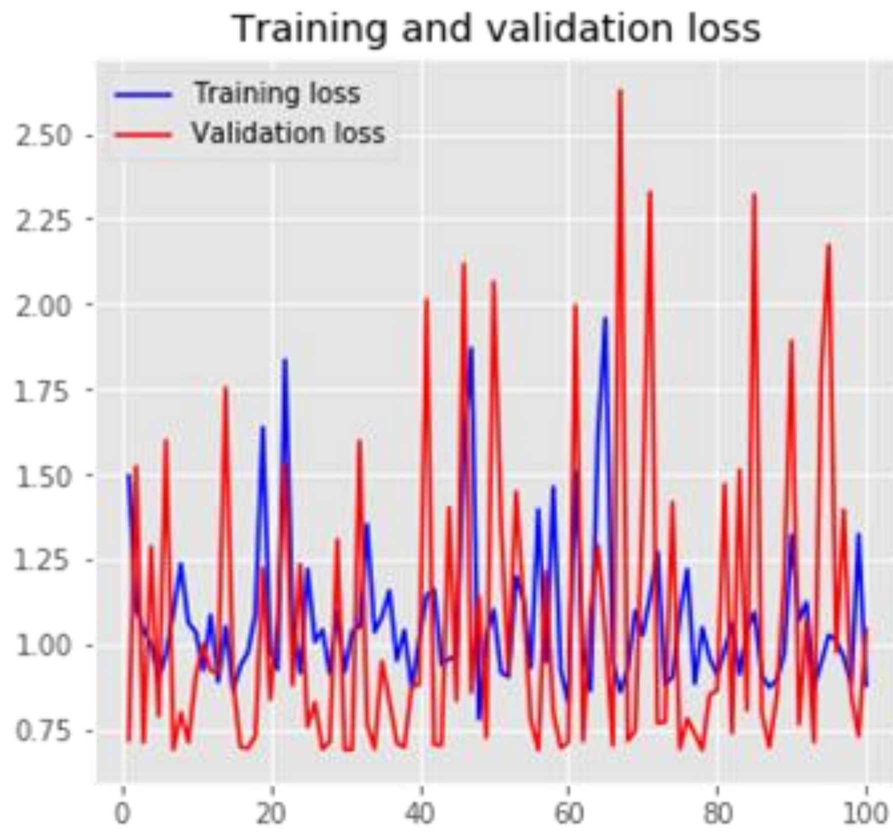
Common issues: overtraining

- Monitor performance on held-out set



Common issues: non-convergence

- Reduce learning rate
- If convergence is too slow, increase learning rate



Common issues: model complexity

- Start simple – remember, logistic regression is a neural network
- A single-layer bag-of-words model is a strong baseline!