Lecture 10: Deep Learning Multiclass Classification

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Announcements

- Midterm on 11/3
  - Online open book exam
  - Exam time: 100 min
- Hw1 is due today!
  - 24 hour late credit
- Quiz 3 is due today!

What you will learn today

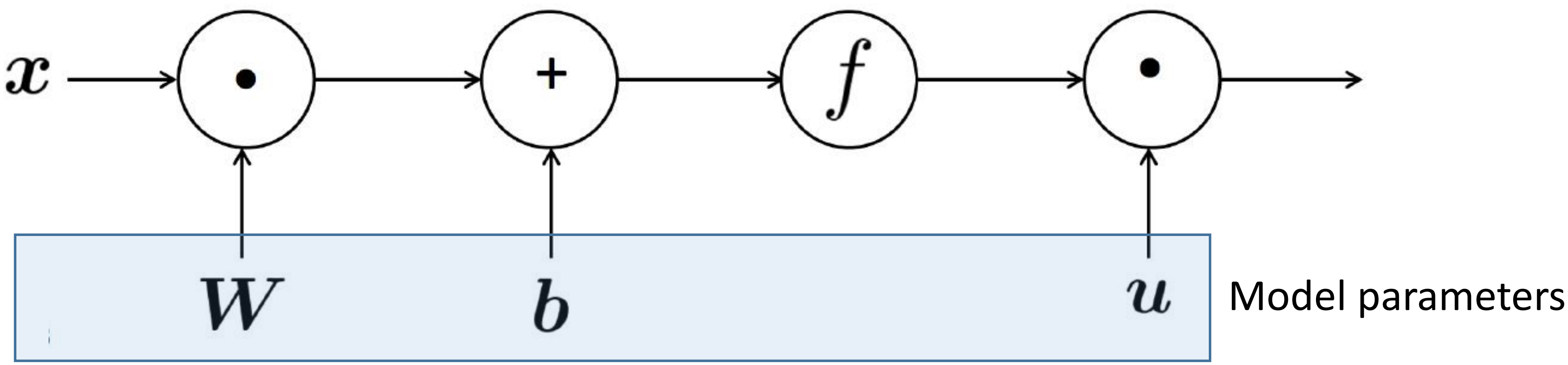
- Deep Learning architectures (not in exam)
- Multiclass Classification
  - One against all
  - One vs one
  - Multinomial Logistic Regression
    - Softmax function

Backpropagation through Computation Graphs

Computation Graphs and Backpropagation

- Consider the NN on the right
- We represent NN as a graph

$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad \text{(input)}$$

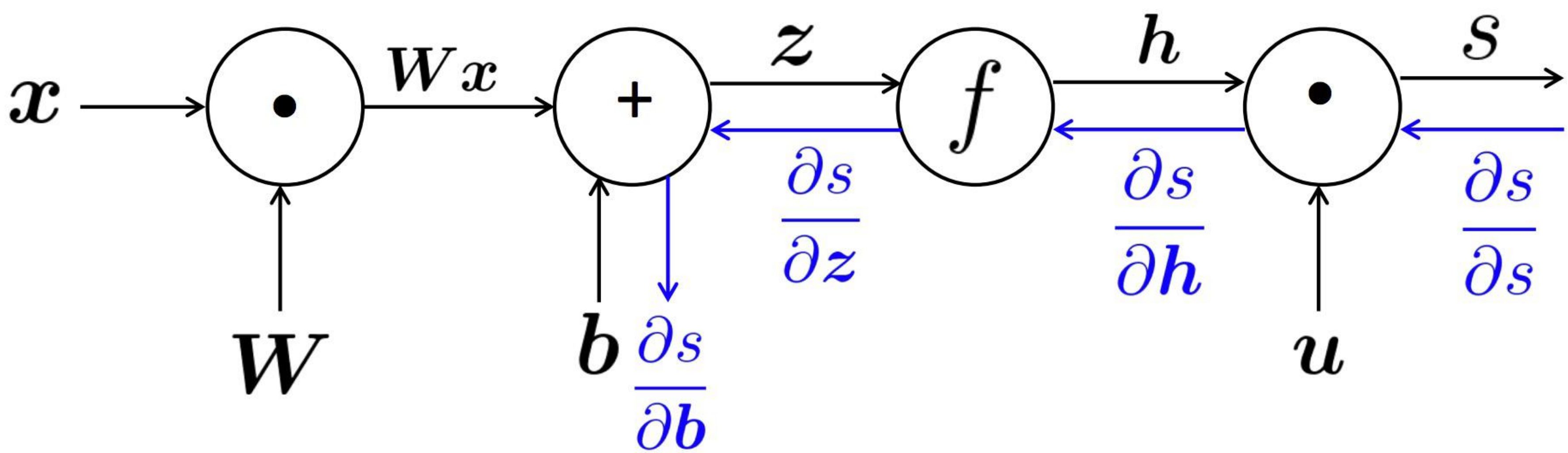


Back Propagation

$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad \text{(input)}$$

- Compute $\frac{\partial s}{\partial \boldsymbol{b}}$

Chain Rule: $\frac{\partial s}{\partial b} = \frac{\partial s}{\partial z}\frac{\partial z}{\partial b} = \cdots$

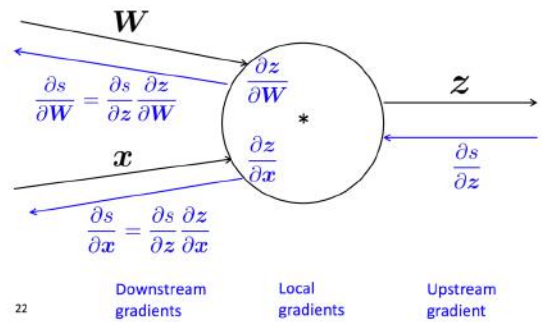


Why you should understand Backprop

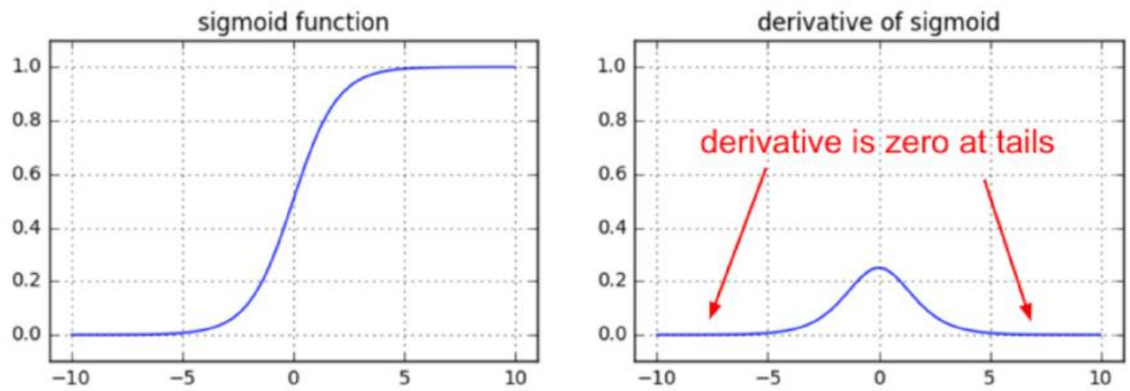
- Modern deep learning library implements backprop as a black-box for you
  - You can take a plane without knowing why it flies
  - but you're designing aircraft…
- Backpropagation doesn't always work perfectly.
  - Understanding why is crucial for debugging and improving models

https://medium.com/@karpathy/yes-you-should-understand-backprop-e2f06eab496b

Example: Gradient of sigmoid




```
z = 1/(1 + np.exp(-np.dot(W, x))) # forward pass
dx = np.dot(W.T, z*(1-z)) # backward pass: local gradient for x
dW = np.outer(z*(1-z), x) # backward pass: local gradient for W
```



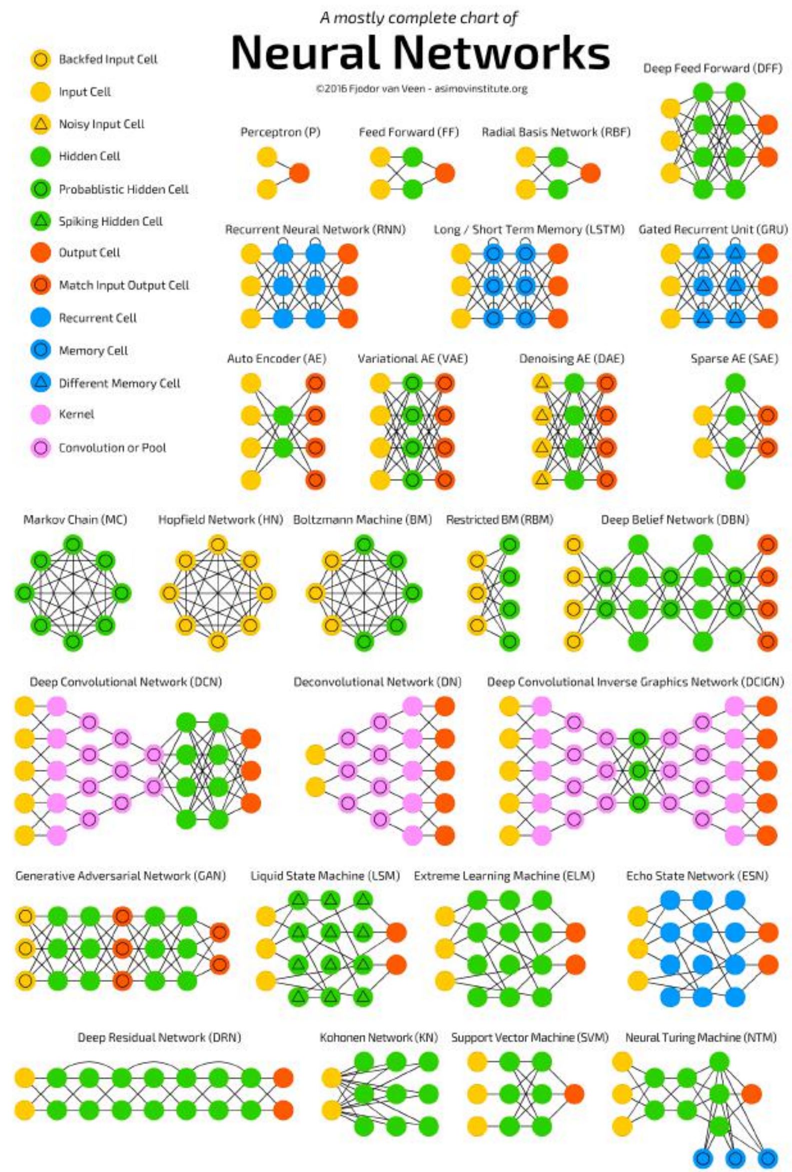
vanish gradient issue

More Details

- Parameter Initialization
  - Normally initialize weights to small random values; various designs
- Optimizer
  - Usually SGD works
  - Several SGD variants (e.g,. ADAM) automatically adjust learning rate based on an accumulated gradient

A neural network zoo

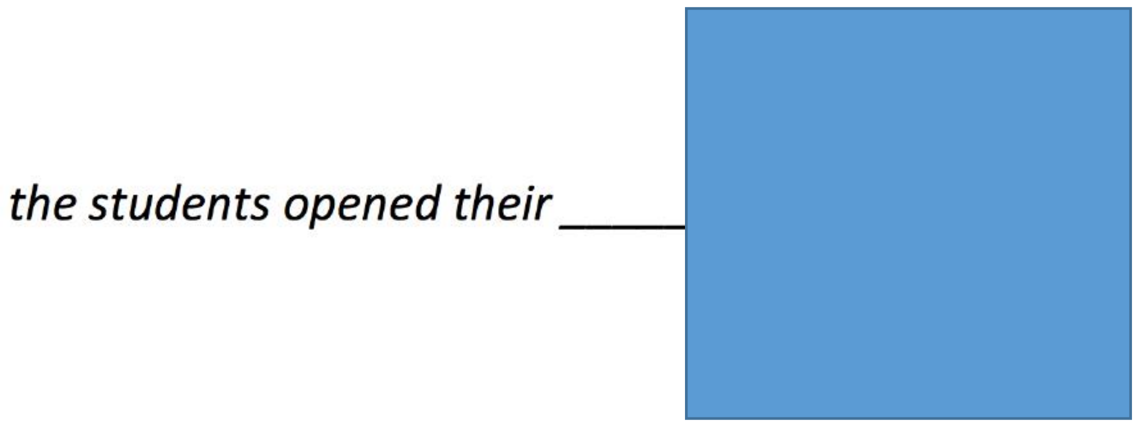
- The flexibility of NN allows us to try out different ideas
- However,
  there is no magic



Modeling with Neural Networks
(Advanced Topic/Not Included in Final)

Example – Language Model

- Predict next word



Idea 1:
A fixed-window neural Language Model

output distribution

$$\hat{\boldsymbol{y}} = \mathrm{softmax}(\boldsymbol{U}\boldsymbol{h} + \boldsymbol{b}_2) \in \mathbb{R}^{|V|}$$

hidden layer

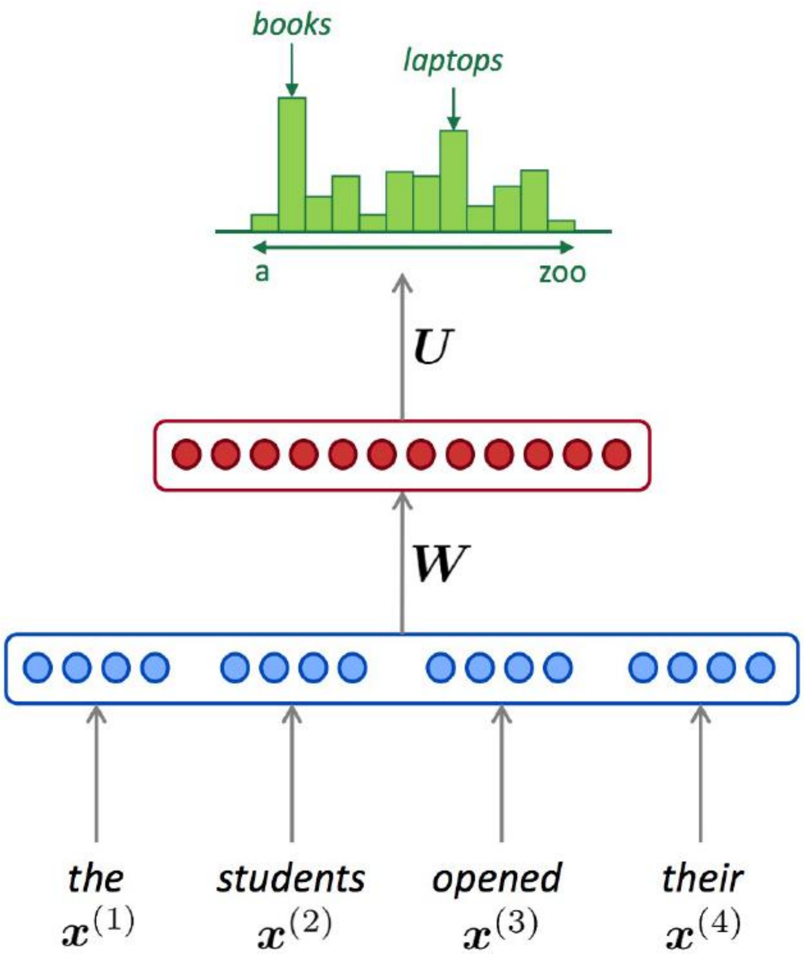
$$\boldsymbol{h} = f(\boldsymbol{W}\boldsymbol{e} + \boldsymbol{b}_1)$$

concatenated word embeddings

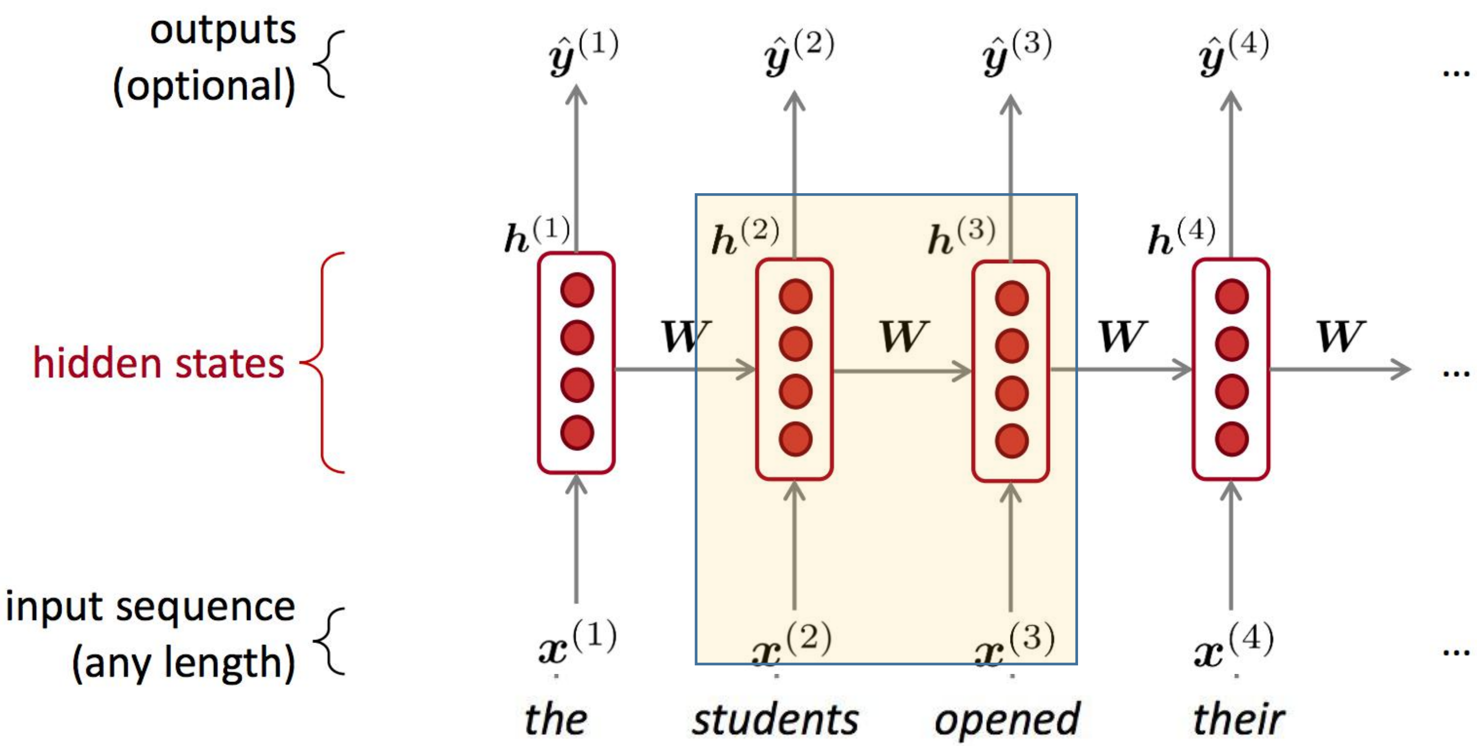
$$\boldsymbol{e} = [\boldsymbol{e}^{(1)}; \boldsymbol{e}^{(2)}; \boldsymbol{e}^{(3)}; \boldsymbol{e}^{(4)}]$$

words / one-hot vectors

$$\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \boldsymbol{x}^{(3)}, \boldsymbol{x}^{(4)}$$

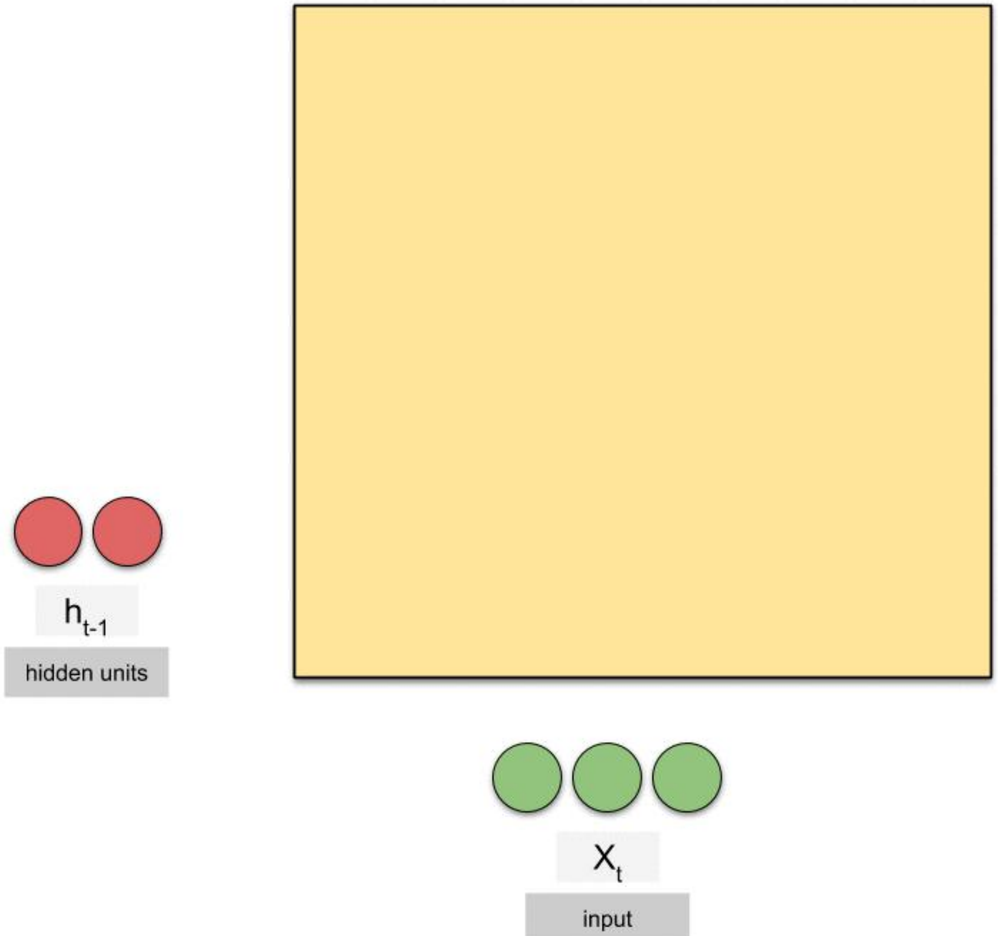


Idea 2:
Recurrent Neural Networks (RNN)



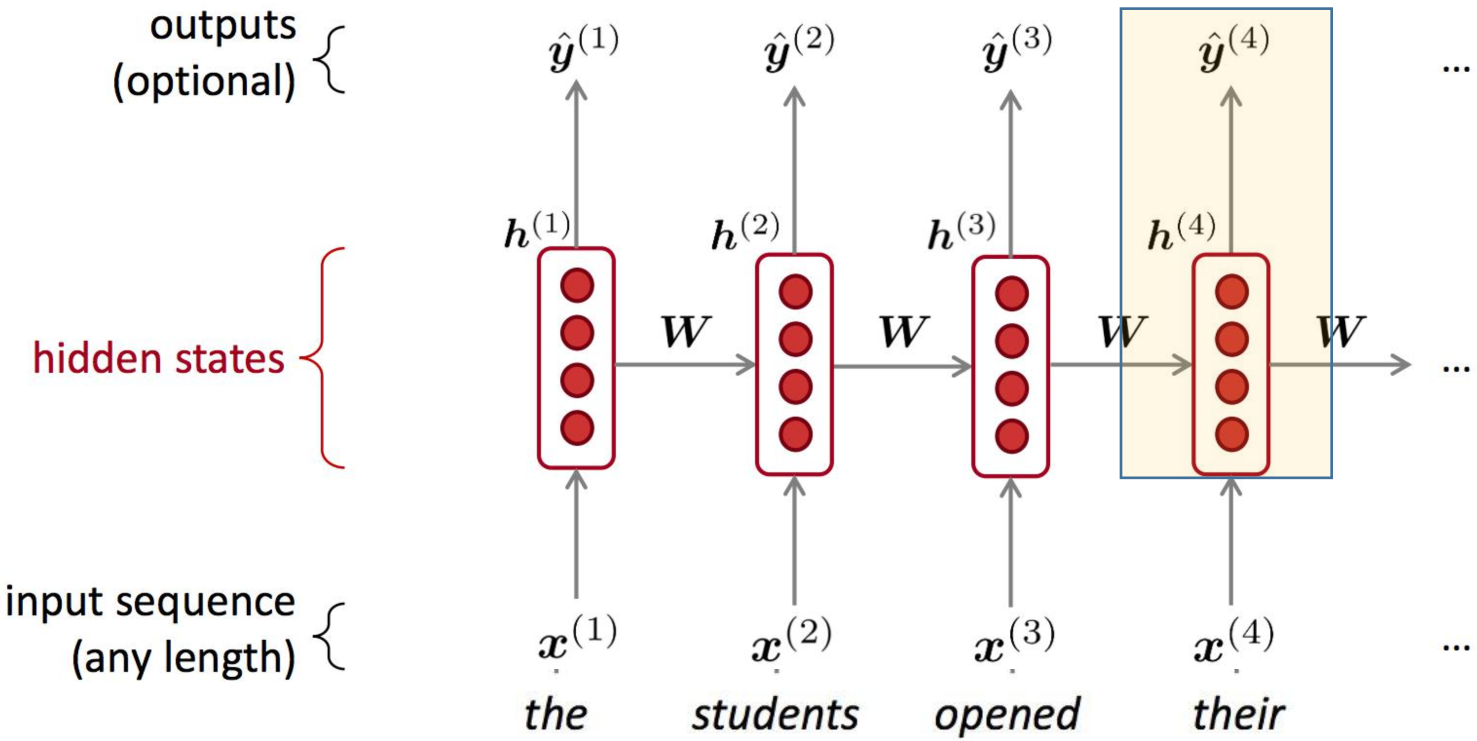
Core idea: Apply the same weights W *repeatedly*

Recurrent Neural Network



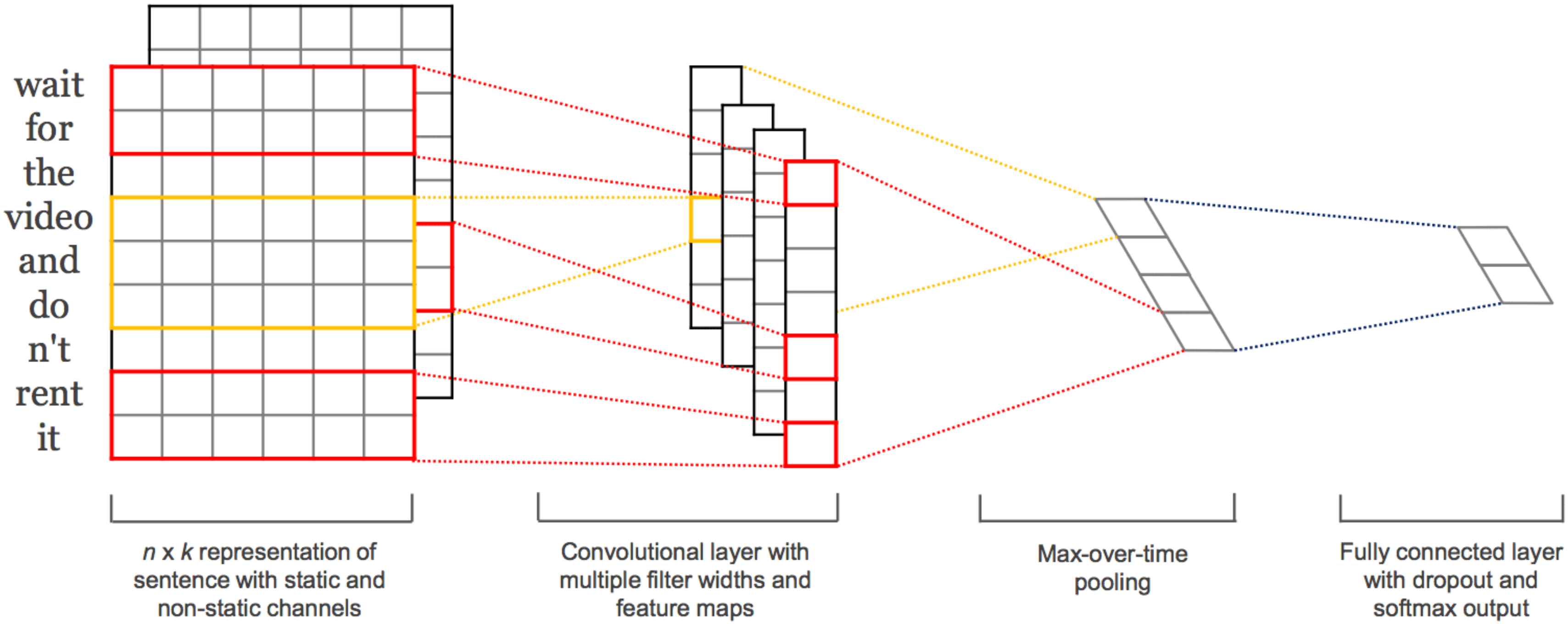
https://towardsdatascience.com/animated-rnn-lstm-and-gru-ef124d06cf45

Prediction using Latent State



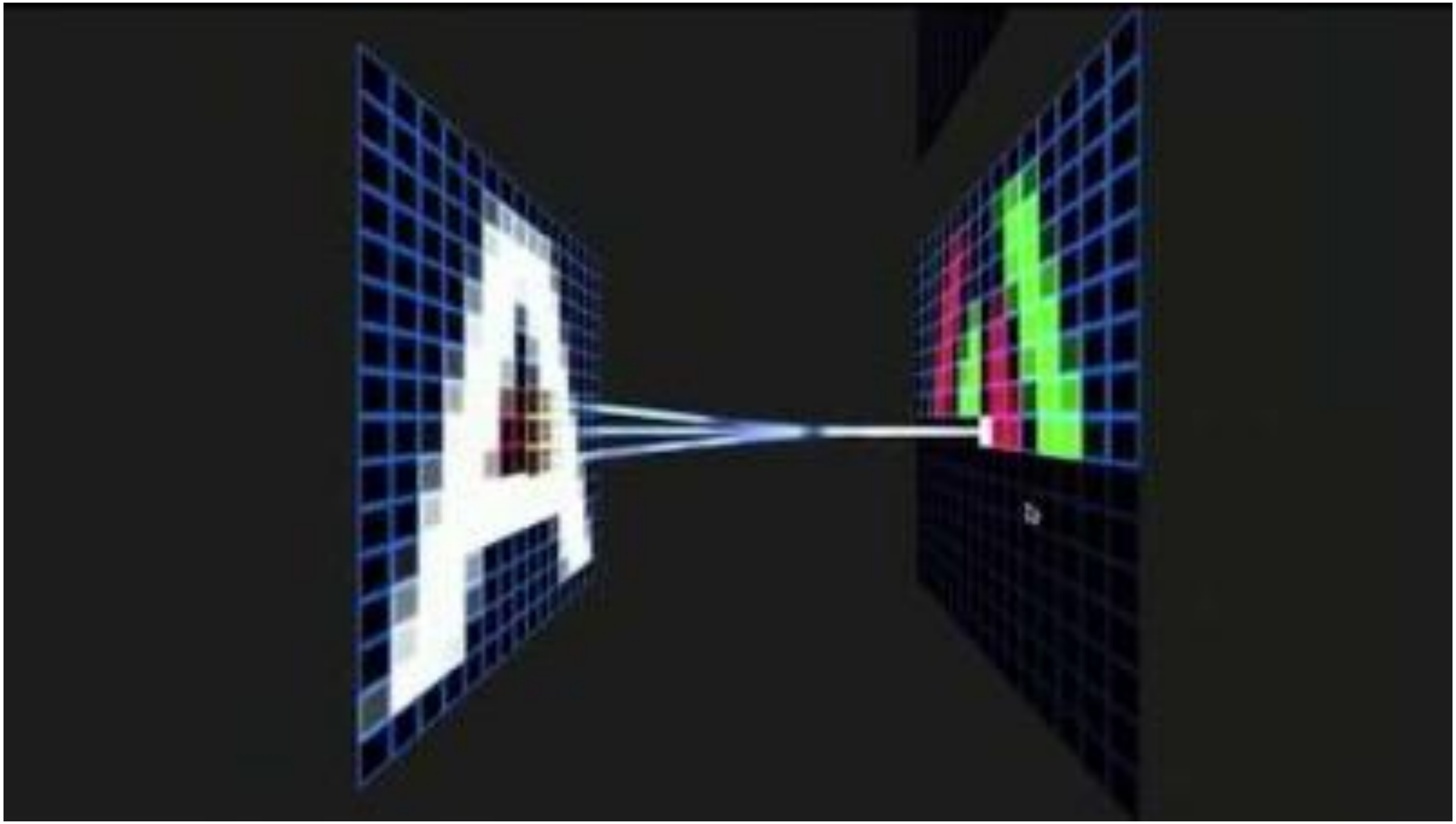
<u>**Core idea:**</u> Apply the same weights W *repeatedly*

Idea 3: Convolutional NN



"Convolutional Neural Networks for Sentence Classification", 2014.

Convolutional NN



https://www.youtube.com/watch?v=f0t-OCG79-U

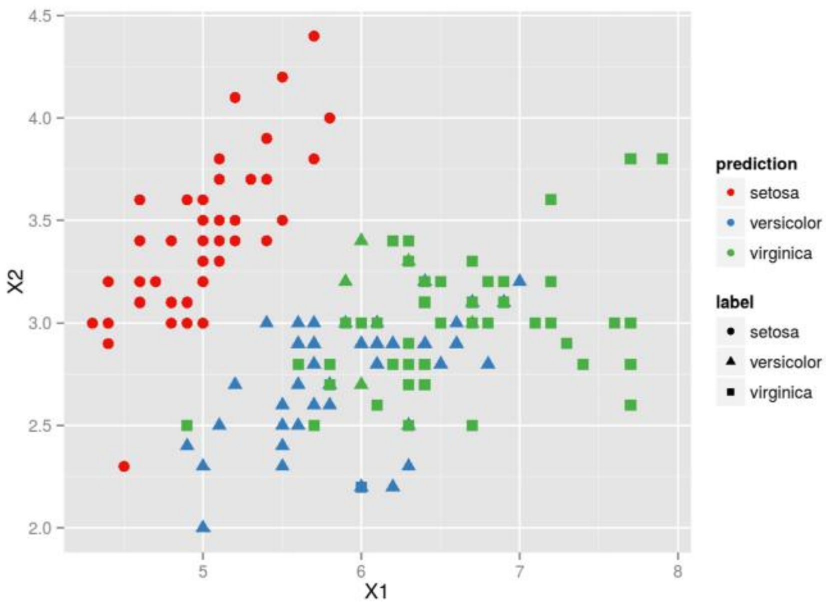
Multi-Class Classification

This Lecture

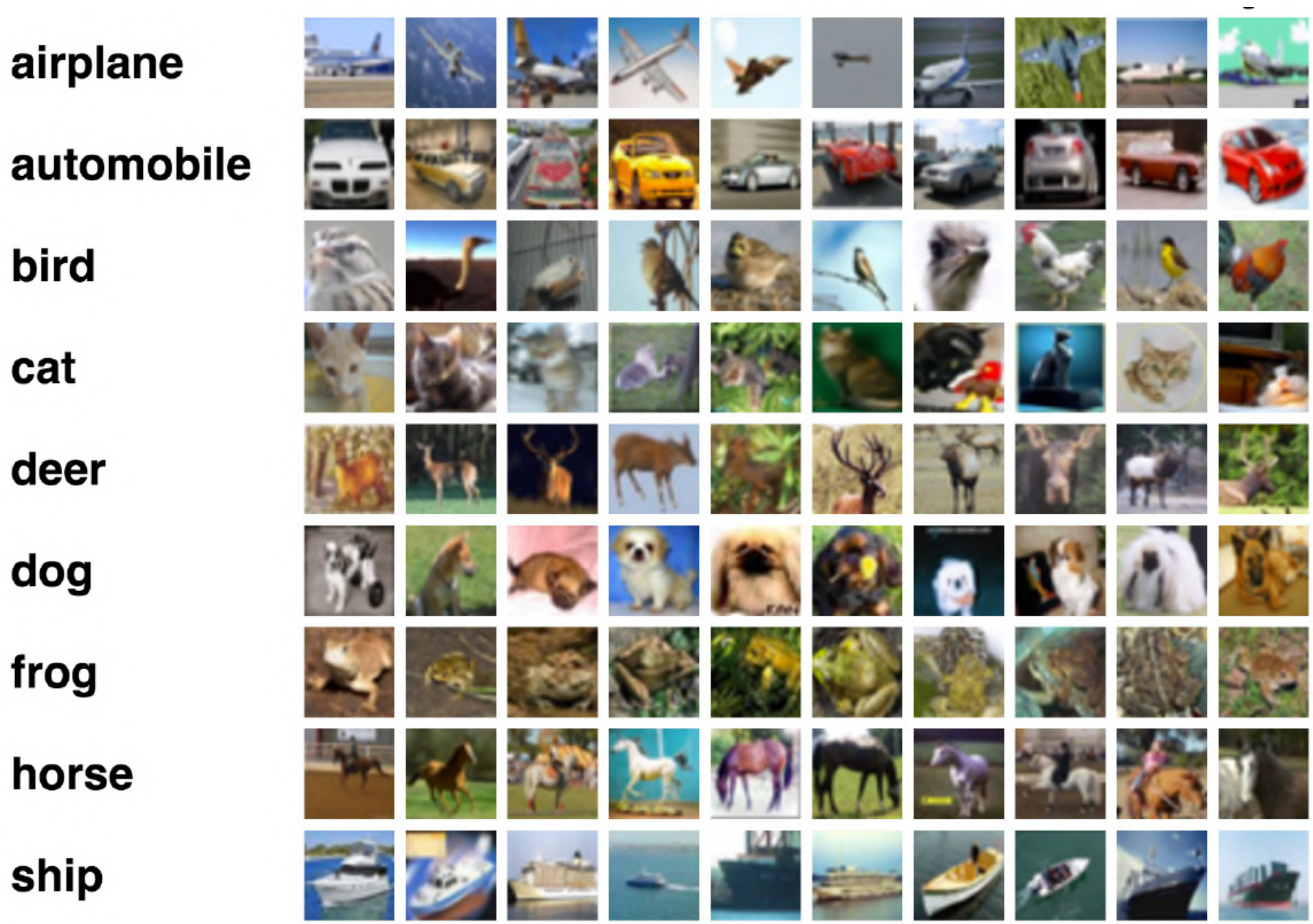
- Multiclass classification overview
- Reducing multiclass to binary
  - One-against-all & One-vs-one
- One classifier approach
  - Multiclass logistic regression

What is multiclass

- Output $\in \{1,2,3, \ldots K\}$
  - In some cases, output space can be very large (i.e., K is very large)
- Each input belongs to exactly one class
  (c.f. in multilabel, input belongs to many classes)



Example applications



Two key ideas to solve multiclass

- Reducing multiclass to binary
  - Decompose the multiclass prediction into multiple binary decisions
  - Make the final decision based on these binary classifiers
- Training a single classifier
  - Consider all classes simultaneously

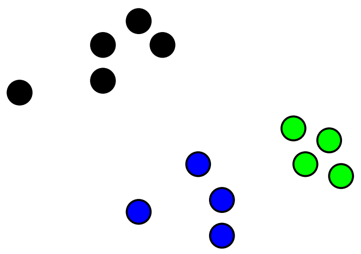
This Lecture

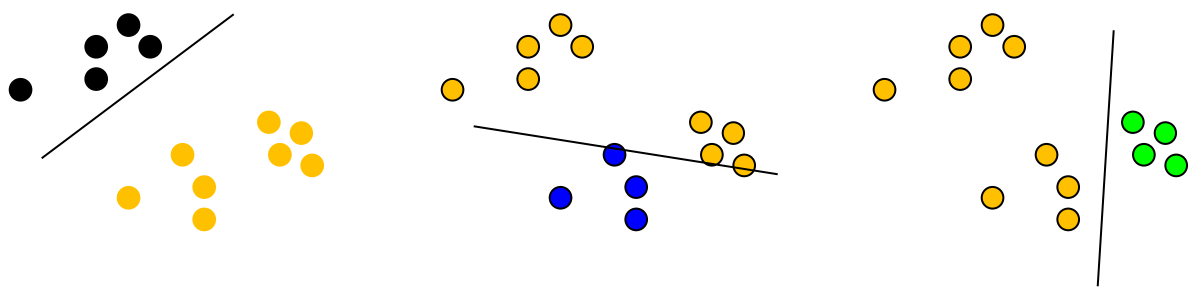
- Multiclass classification overview
- Reducing multiclass to binary
  - One-against-all & One-vs-one

One against all strategy

One against All learning

- Multiclass classifier
  - Function $f : R^n \rightarrow \{1,2,3,...,k\}$
- Decompose into binary problems

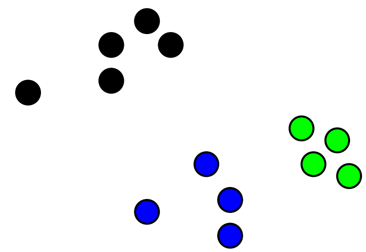




One-against-All learning algorithm

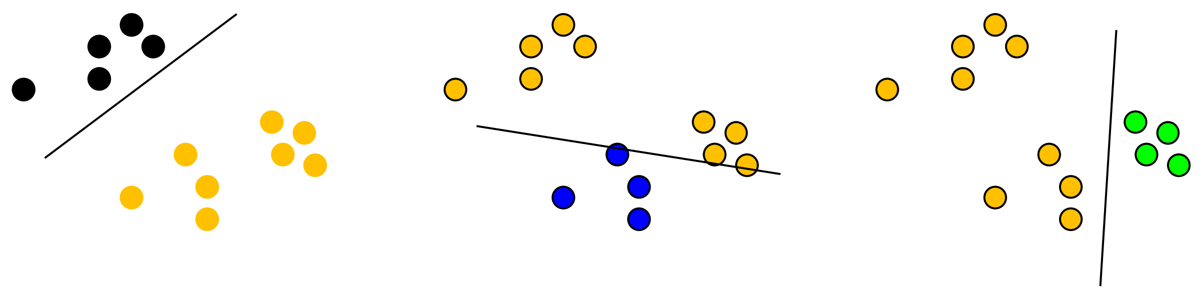
- Learning: Given a dataset $D = \{(x_i, y_i)\}$
  $x_i \in R^n, y_i \in \{1,2,3, \dots K\}$
- Decompose into K binary classification tasks
  - Learn K models: $w_1, w_2, w_3, \dots w_K$
  - For class k, construct a binary classification task as:
    - Positive examples: Elements of D with label k
    - Negative examples: All other elements of D
  - The binary classification can be solved by any algorithm we have seen

One against All learning



- Multiclass classifier
  - Function $f : R^n \rightarrow \{1,2,3,...,k\}$
- Decompose into binary problems

Ideal case: only the correct label will have a positive score



$w_{black}^T x > 0$ $\quad$ $w_{blue}^T x > 0$ $\quad$ $w_{green}^T x > 0$

One-against-All Inference

- Learning: Given a dataset $D = \{(x_i, y_i)\}$
  $x_i \in R^n, y_i \in \{1,2,3, \dots K\}$
- Decompose into K binary classification tasks
  - Learn K models: $w_1, w_2, w_3, \dots w_K$
- Inference: "Winner takes all"
  - $\hat{y} = \mathrm{argmax}_{y \in \{1,2,\dots K\}}\, w_y^T\, x$

For example: $y = \mathrm{argmax}(w_{black}^T\, x\,,\ w_{blue}^T\, x,\ w_{green}^T\, x)$

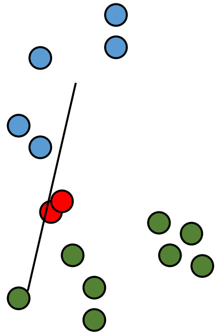
  - An instance of the general form

$$\hat{y} = \mathrm{argmax}_{\boldsymbol{y} \in \mathcal{Y}}\, f(\boldsymbol{y}; \boldsymbol{w}, \boldsymbol{x})$$

$w = \{w_1, w_2, \dots w_K\},\ f(\boldsymbol{y}; \boldsymbol{w}, \boldsymbol{x}) = \boldsymbol{w}_y^T\, x$

One-against-All analysis

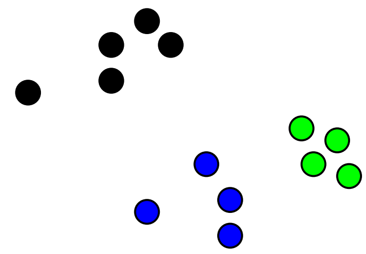
- Not always possible to learn
  - Assumption: each class individually separable from all the others
- Need to make sure the range of all classifiers is the same –K classifiers are trained independently.
- Easy to implement; work well in practice

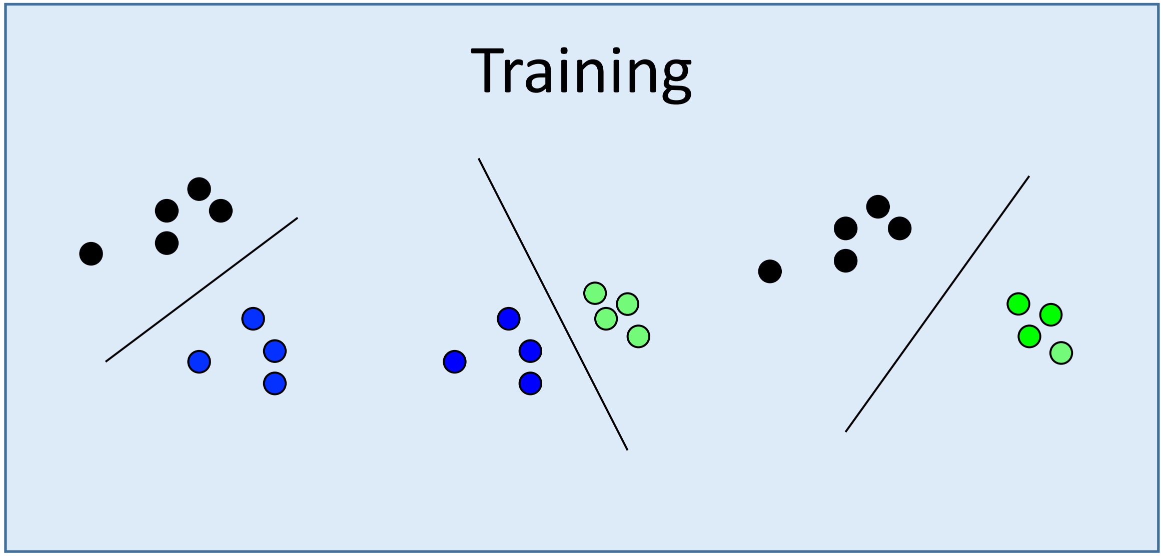


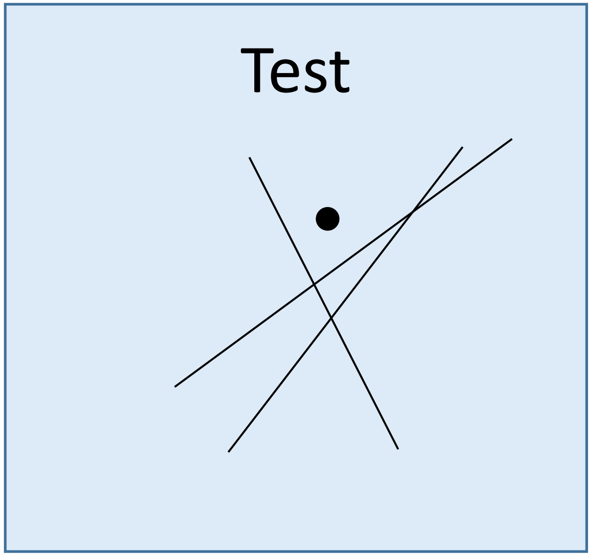
One v.s. One (All against All) strategy

One v.s. One learning

- Multiclass classifier
  - Function $f : R^n \rightarrow \{1,2,3,...,k\}$
- Decompose into binary problems





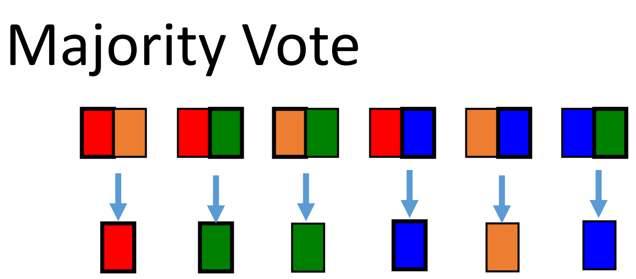


One-v.s-One learning algorithm

- Learning: Given a dataset $D = \{(x_i, y_i)\}$
  $x_i \in R^n, y_i \in \{1,2,3, \dots K\}$
- Decompose into C(K,2) binary classification tasks
  - Learn C(K,2) models: $w_1, w_2, w_3, \dots w_{K*(K-1)/2}$
  - For each class pair (i,j), construct a binary classification task as:
    - Positive examples: Elements of D with label i
    - Negative examples Elements of D with label j
    - The binary classification can be solved by any algorithm we have seen

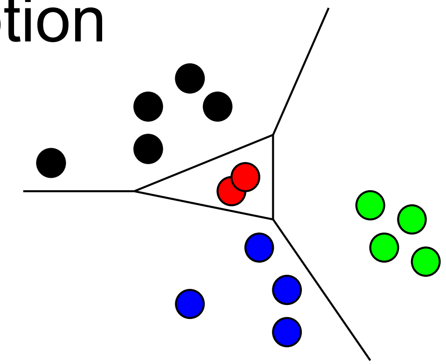
One-v.s-One Inference algorithm

- Decision Options:
  - More complex; each label gets k-1 votes
  - Output of the binary classifier may not coherent.
  - Majority: classify example x to take label i if i wins on x more often than j (j=1,…k)



Comparisons

- One against all
  - O(K) weight vectors to train and store
  - Training set of the binary classifiers may unbalanced
  - Less expressive; make a strong assumption



- One v.s. One (All v.s. All)
  - O(K^2) weight vectors to train and store
  - Size of training set for a pair of labels could be small
    ⇒ overfitting of the binary classifiers
  - Need large space to store model

Exercise

- Consider we have a 10-class classification problem with 29 features, each class has 1,000 examples.
- How many parameters are in total for linear models with one-vs-one?
- How many parameters are in total for linear models with one-against-all?
- How large is the training data for each one-vs-one classifier?
- How large is the training data for each one-against-all classifier?

Problems with Decompositions

- Learning optimizes over *local* metrics
  - Does not guarantee good *global* performance
  - We don't care about the performance of the *local* classifiers
- Poor decomposition $\Rightarrow$ poor performance
  - Difficult local problems
  - Irrelevant local problems
- Efficiency: e.g., All vs. All vs. One vs. All

Decomposition methods: Summary

- General Ideas:
  - Decompose the multiclass problem into many binary problems
  - Prediction depends on the decomposition
    - Constructs the multiclass label from the output of the binary classifiers
- Learning optimizes local correctness
  - Each binary classifier don't need to be globally correct and isn't aware of the prediction procedure

Multi-class Logistic Regression

Recall: (binary) logistic regression

$$\min_{\boldsymbol{w}} \quad \frac{1}{2}\boldsymbol{w}^T\boldsymbol{w} + C\sum_i \log(1 + e^{-\mathrm{y_i}(\mathbf{w}^{\mathrm{T}}\mathbf{x}_{\mathrm{i}})})$$

Assume labels are generated using the following probability distribution:

$$P(y=1|\mathbf{x},\mathbf{w}) = \frac{e^{\mathbf{w}^T\mathbf{x}}}{1+e^{\mathbf{w}^T\mathbf{x}}} = \frac{1}{1+e^{-\mathbf{w}^T\mathbf{x}}}$$

$$P(y=-1|\mathbf{x},\mathbf{w}) = \frac{1}{1+e^{\mathbf{w}^T\mathbf{x}}}$$

(multi-class) log-linear model

- Assumption:

Partition function

$$P(y|x, w) = \frac{\exp(w_y^T x)}{\sum_{y' \in \{1,2,\ldots K\}} \exp(w_{y'}^T x)}$$

- This is a valid probability assumption. Why?

soft-max function

- Example

$$softmax\left(\begin{bmatrix} -1 \\ 0 \\ 3 \\ 5 \end{bmatrix}\right) = \begin{bmatrix} 0.368/169.87 \\ 1/169.87 \\ 20.09/169.87 \\ 148.41/169.87 \end{bmatrix} = \begin{bmatrix} 0.002 \\ 0.006 \\ 0.118 \\ 0.874 \end{bmatrix}$$

Softmax

- Softmax: let s(y) be the score for output y here s(y)=$w^T\phi(x, y)$ (or $w_y^T x$) but it can be computed by other function.

$$P(y) = \frac{\exp(s(y))}{\sum_{y\prime\in\{1,2,\ldots K\}} \exp(s(y))}$$

Why we call it softmax?

- Softmax: let s(y) be the score for output y
  here s(y)=$w^T\phi(x,y)$ (or $w_y^T x$) but it can be computed by other function.

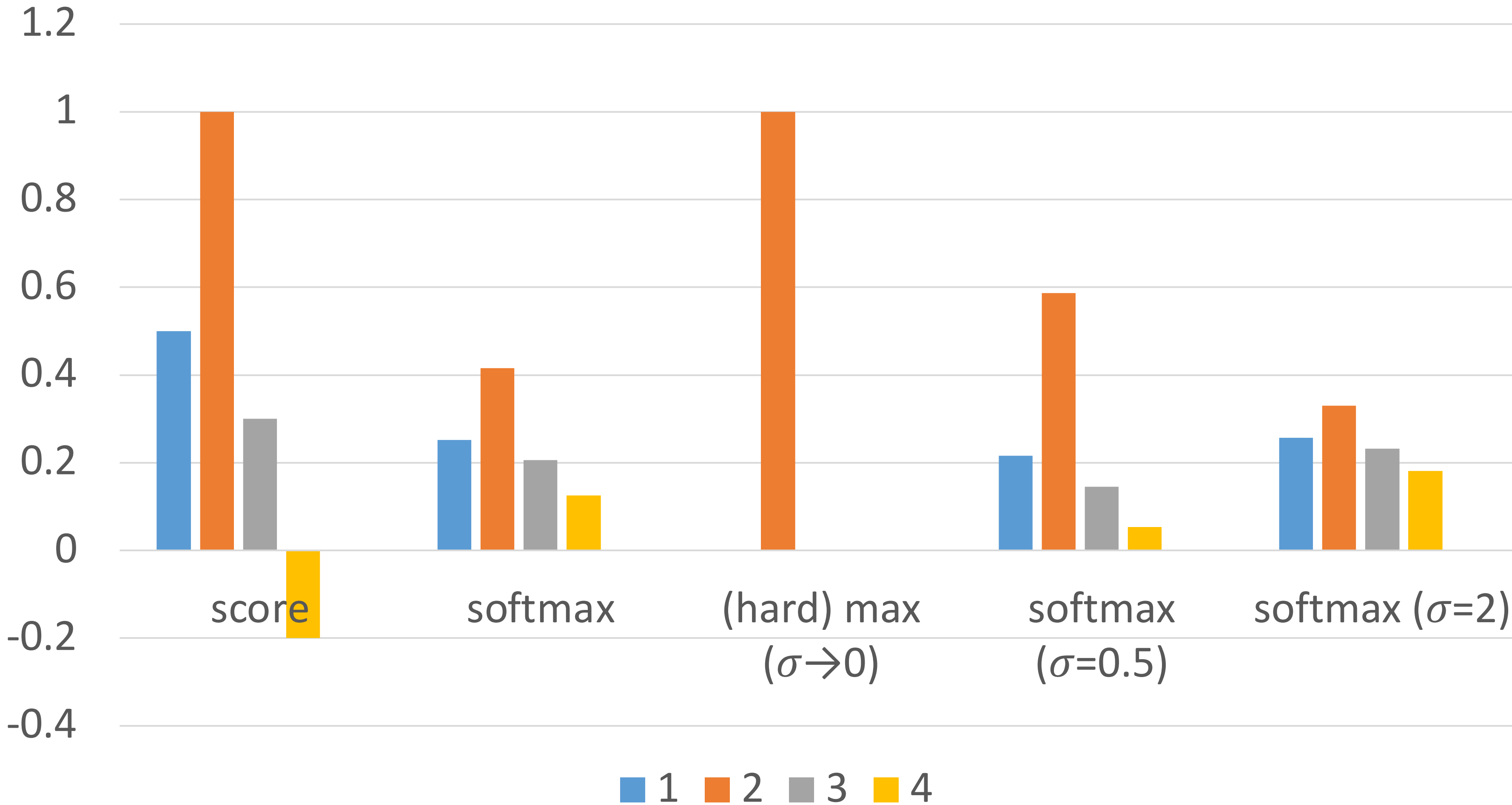
$$P(y) = \frac{\exp(s(y))}{\sum_{y' \in \{1,2,\ldots K\}} \exp(s(y))}$$

- We can control the peakedness of the distribution

$$P(y|\sigma) = \frac{\exp(s(y)/\sigma)}{\sum_{y' \in \{1,2,\ldots K\}} \exp(s(y/\sigma))}$$

Example

$S(1) = .5; \quad s(2)=1; \quad s(3)=0.3; \quad s(4)=-0.2$



Maximum log-likelihood estimation

- Training can be done by maximum log-likelihood estimation i.e. $\max_w \log P(D|w)$

$D=\{(x_i, y_i)\}$

$$P(D|w) = \Pi_i \frac{\exp\left(w_{y_i}^T x_i\right)}{\sum_{y' \in \{1,2,\ldots K\}} \exp(w_{y'}^T x_i)}$$

$$\log P(D|w) = \sum_i [w_{y_i}^T x_i - \log \sum_{y' \in \{1,2,\ldots K\}} \exp(w_{y'}^T x_i)]$$

Comparisons

- Log-linear model (multi-class)

$$\min_{w} \sum_i [\log \sum_{k\in\{1,2,\ldots K\}} \exp\left(w_k^T x_i\right) - w_{y_i}^T x_i]$$

- Log-linear mode (logistic regression)

$$\min_{\boldsymbol{w}} \quad \sum_i \log(1 + e^{-\mathrm{y}_\mathrm{i}(\mathbf{w}^\mathrm{T}\mathbf{x}_\mathrm{i})})$$

Reduction v.s. single classifier

- Reduction
  - Future-proof: if we improve the binary classification model ⇒ improve muti-class classifier
  - Easy to implement
- Single classifier
  - Global optimization: directly minimize the empirical loss; easier for joint prediction