

CSE 417T

Introduction to Machine Learning

Review of Exam 2

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Logistics: Exam 2

- Exam 2 Date: December 8, 2022 (Thursday)
 - In-class exam (the same time/location as the lecture)
 - Exam duration: 75 minutes
 - Content
 - Focus on the content of 2nd half of the semester
 - However, knowledge is cumulative, and you are still expected to know the concepts earlier
- 2 sections of questions
 - 4~6 long questions (written response questions with explanations required)
 - 10 multiple choice questions (no explanations needed)
- Closed-book exam. You can bring two cheat-sheets
 - Up to letter size, front and back (up to 4 pages)
 - No format limitations (it can be typed, written, or a combination)
- No calculators (you don't need them)

Logistics: Exam Policies

- Similar to Exam 1, I might arrange random seat assignments
 - Will be announced on Piazza the night before the exam if I do
- If you prefer a left-handed seat, input your id on the following form:
 - <https://forms.gle/23247jWkqWmSSj8r7>
 - Please submit by Wednesday noon
 - The same form as in Exam 1
 - If you have done so in Exam 1, no need to do it again
 - The link is on a pinned Piazza post

Logistics: Exam Policies

- Please arrive on time. No extensions will be given if you arrive late.
- During the exam, if you have a question or if you finish before time is up:
 - **Do not get up**
 - Raise your hand and I will come to you
 - I most likely will not answer questions to individual students
 - But I'll give clarifications to everyone if multiple students ask the same question
- When time is called:
 - **Stop writing**
 - **Do not get up**
 - We will come around and collect your exam

Homework

- Solution Sketch of HW5 has been posted on Gradescope
 - Not intended to be comprehensive

Plans for Today

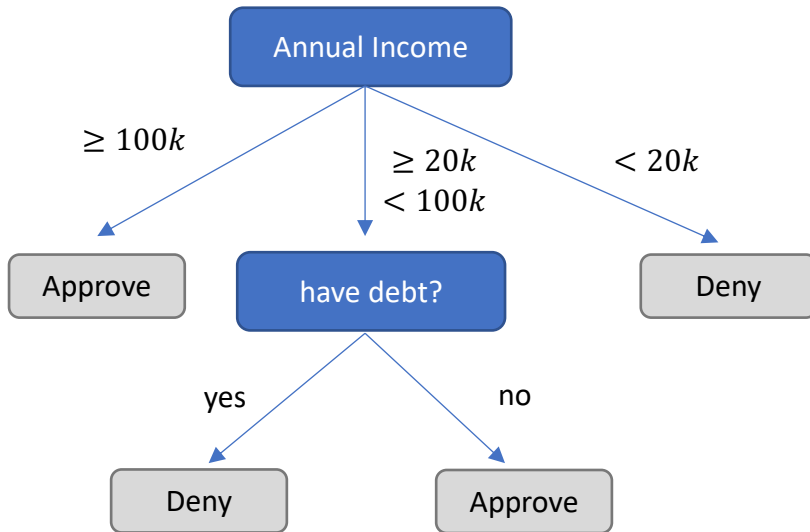
- Brief review of course content.
- Discussion of the practice questions.
- Discussion of any other questions you might have.

Brief Review

A quick review brushed over what we talked about.

Not guaranteed (and not likely) to cover everything in the exam.

Decision Tree Hypothesis



- Pros
 - Easy to interpret, handle multi-type data, easy to implement
- Cons
 - **bad generalization**
 - VC dimension is infinity, high variance, easily overfit
- Why we care?
 - One of the classical model
 - **Building block for other models** (e.g., random forest)

- Decision tree learning:

Goal:

minimize E_{in}
subject to $size(tree) \leq C$

approximately

General_DecisionTreeLearn(D)

Create a root node r

If **termination conditions** are met

return a single node tree with **leaf prediction** based on

Else: Greedily find a feature A to split according to **split criteria**

For each possible value v_i of A

Let D_i be the dataset containing data with value v_i for feature A

Create a subtree DecisionTreeLearn(D_i) that being the child of root r

ID3: Using Information Gain as Selection Criteria

- Information gain of choosing feature A to split
 - $Gain(D, A) = H(D) - \sum_i \frac{|D_i|}{|D|} H(D_i)$ [The amount of decrease in entropy]
- ID3: Choose the split that maximize $Gain(D, A)$

Notations:

$H(D)$: Entropy of D

$|D|$ is the number of points in D

General_DecisionTreeLearn(D)

Create a root node r

If **termination conditions** are met

return a single node tree with **leaf prediction** based on

Else: Greedily find a feature A to split according to **split criteria**

For each possible value v_i of A

Let D_i be the dataset containing data with value v_i for feature A

Create a subtree DecisionTreeLearn(D_i) that being the child of root r

- ID3 termination conditions
 - If all labels are the same
 - If all features are the same
 - If dataset is empty
- ID3 leaf predictions
 - Most common labels (majority voting)
- ID3 split criteria
 - Information gain

Ensemble Learning

- Goal: Utilize a set of **weak learners** to obtain a **strong learner**.
- Format of ensemble learning
 - **Construct** many **diverse** weak learners
 - **Aggregate** the weak learners

Bagging:

- Construct diverse weak learners
 - (**Simultaneously**) bootstrapping datasets
 - Train weak learners on them
- Aggregate the weak learners
 - **Uniform** aggregation

Boosting

- Construct diverse weak learners
 - **Adaptively** generating datasets
 - Train weak learners on them
- Aggregate the weak learners
 - **Weighted** aggregation

Weak learner
choice:

Fully-grown decision trees
(low bias, high variance)

Decision stumps
(high bias, low variance)

Bagging and Random Forest

- Construct many random trees
 - Bootstrapping datasets (Sample with replacement from D)
 - Learn a **max-depth tree** for each of them
 - Other randomizations
 - When choosing split features, choose from a random subset (instead of all features)
 - Randomly project features (similar to non-linear transformation) for each tree
- Aggregate the random trees
 - Classification: Majority vote $\bar{g}(\vec{x}) = \text{sign} \left(\frac{1}{M} \sum_{m=1}^M g_m(\vec{x}) \right)$
 - Regression: Average $\bar{g}(\vec{x}) = \frac{1}{M} \sum_{m=1}^M g_m(\vec{x})$

Outline of a Boosting Algorithm

- Initialize D_1
- For $t = 1$ to T
 - Learn g_t from D_t
 - Reweight the distribution and obtain D_{t+1} based on g_t and D_t
- Output $\text{weighted-aggregate}(g_1, \dots, g_T)$
 - Classification: $G(\vec{x}) = \bar{g}(\vec{x}) = \text{sign}\left(\frac{1}{T} \sum_{t=1}^T \alpha_t g_t(\vec{x})\right)$

Questions

How to learn g_t from D_t

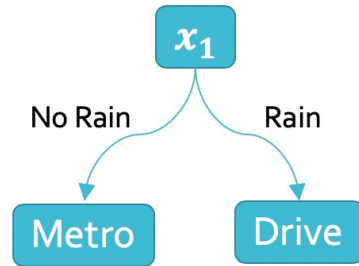
How to reweight the distribution and obtain D_{t+1}

How to perform weighted aggregation

AdaBoost Algorithm

How to learn g_t from D_t

- Decision stump



How to reweight D_{t+1}

- Make $E_{in}^{(D_{t+1})}(g_t) = 0.5$
- So g_t and g_{t+1} are “diverse”

How to weighted aggregation

- More weights on better g_t
- Lower ϵ_t : proxy for better g_t

- Given $D = \{(\vec{x}_1, y_1), \dots, (\vec{x}_N, y_N)\}$
- Initialize $D_1(n) = 1/N$ for all $n = 1, \dots, N$
- For $t = 1, \dots, T$
 - Learn g_t from D_t (using decision stumps)
 - Calculate $\epsilon_t = E_{in}^{(D_t)}(g_t)$
 - Set $\alpha_t = \frac{1}{2} \ln \left(\frac{1-\epsilon_t}{\epsilon_t} \right)$
 - Update $D_{t+1}(n) = \frac{1}{Z_t} D_t(n) e^{-\alpha_t y_n g_t(\vec{x}_n)}$
- Output $G(\vec{x}) = \text{sign}(\sum_{t=1}^T \alpha_t g_t(\vec{x}))$

Nearest Neighbors

- Predict \vec{x} according to its nearest neighbor
 - Given $D = \{(\vec{x}_1, y_1), (\vec{x}_2, y_2), \dots, (\vec{x}_N, y_N)\}$
 - Let $\vec{x}_{[1]}$ be \vec{x} 's nearest neighbor, i.e., the closest point to \vec{x} in D
 - Let $y_{[i]}(\vec{x})$ or $y_{[i]}$ be the label of $\vec{x}_{[i]}$

- Nearest neighbor hypothesis

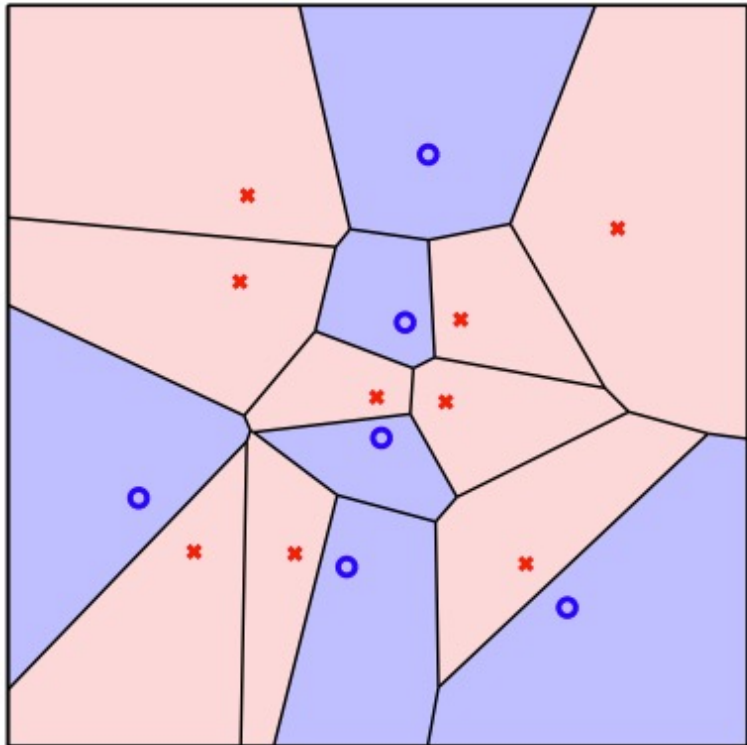
$$g(\vec{x}) = y_{[1]}(\vec{x})$$

- k -nearest neighbor (K-NN)

$$g(\vec{x}) = \text{sign}\left(\sum_{i=1}^k y_{[i]}(\vec{x})\right)$$

1-Nearest Neighbor

$g(\vec{x})$ looks like a Voronoi diagram



- Properties of 1-Nearest Neighbor (NN)
 - No training is needed
 - Good interpretability
 - In-sample error $E_{in} = 0$
 - VC dimension is ∞
- This seems to imply bad learning models from what we talk about so far? Why we care?
- What we really care about is E_{out}
 - VC analysis: $E_{out} \leq E_{in} + \text{Generalization error}$
 - We can infer E_{out} through E_{in} and model complexity
 - NN has nice guarantees outside of VC analysis

Properties of Nearest Neighbors

- 1-NN

- Given mild conditions, for 1-nearest neighbor, when $N \rightarrow \infty$, with high probability,

$$E_{out} \leq 2E_{out}^*$$

- That is, we can not infer E_{out} from E_{in} , but we know it cannot be much worse than the **best anyone can do**.

- k-NN:

- Tuning k moderates the tradeoff of **generalization vs approximation**

Radial Basis Function

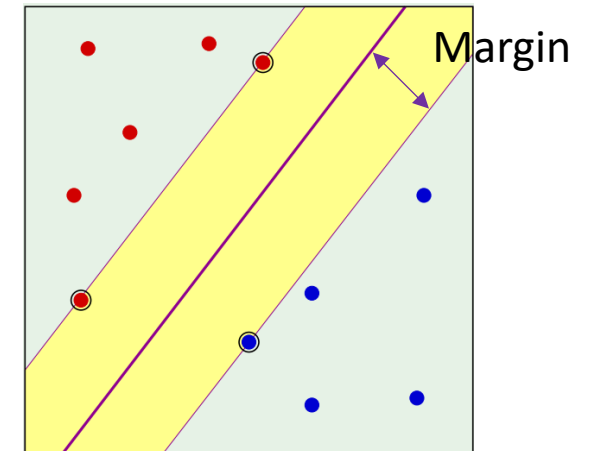
- $h(\vec{x}) = \sum_{k=1}^K w_k \phi\left(\frac{\|\vec{x} - \vec{\mu}_k\|}{r}\right)$
- Connection to linear models
 - Parametric RBF is essentially linear model with nonlinear transformation
- Connection to nearest neighbor
 - RBF is based on the similarity to a set of points
- Connection to SVM with RBF Kernel
 - Using K representative points vs. using support vectors
- Connection to Neural Networks
 - RBF can be graphically represented as a one-hidden layer network

Support Vector Machines

- Goal: Find the **max-margin** linear separator
- If the data is **linearly separable**
 - **Hard-Margin SVM**

$$\begin{array}{ll} \text{minimize}_{\vec{w}, b} & \frac{1}{2} \vec{w}^T \vec{w} \\ \text{subject to} & y_n (\vec{w}^T \vec{x}_n + b) \geq 1, \forall n \end{array}$$

- $g(\vec{x}) = \text{sign}(\vec{w}^{*T} \vec{x} + b^*)$

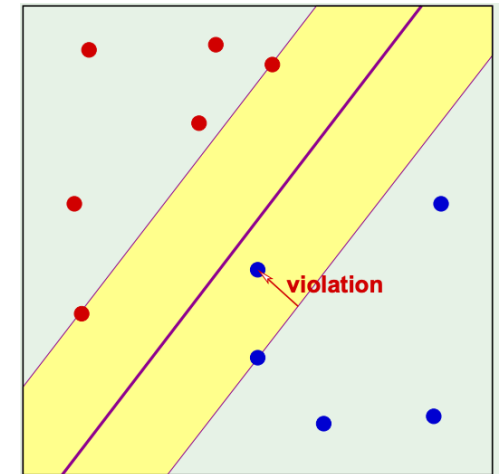


- If the data is not linearly separable
 - **Soft-margin SVM**
 - Nonlinear transformation – **Dual Formulation** and **Kernel Tricks**

Soft-Margin SVM

- For each point (\vec{x}_n, y_n) , we allow a deviation $\xi_n \geq 0$
 - The constraint becomes: $y_n(\vec{w}^T \vec{x}_n + b) \geq 1 - \xi_n$
 - We add a penalty for each deviation: Total penalty $C \sum_{n=1}^N \xi_n$

$$\begin{aligned} &\text{minimize}_{\vec{w}, b, \xi} \quad \frac{1}{2} \vec{w}^T \vec{w} + C \sum_{n=1}^N \xi_n \\ &\text{subject to} \quad y_n(\vec{w}^T \vec{x}_n + b) \geq 1 - \xi_n, \forall n \\ &\quad \quad \quad \xi_n \geq 0, \forall n \end{aligned}$$



Remarks:

- C is a hyper-parameter we can choose, e.g., using validation
 - Larger C \Rightarrow less tolerable to noise \Rightarrow smaller margin
- Soft-margin SVM is still a Quadratic Program, with efficient solvers

Primal-Dual Formulations of Hard-Margin SVM

- Primal

$$\begin{aligned} & \text{minimize}_{\vec{w}, b} \quad \frac{1}{2} \vec{w}^T \vec{w} \\ & \text{subject to} \quad y_n (\vec{w}^T \vec{x}_n + b) \geq 1, \forall n \end{aligned}$$

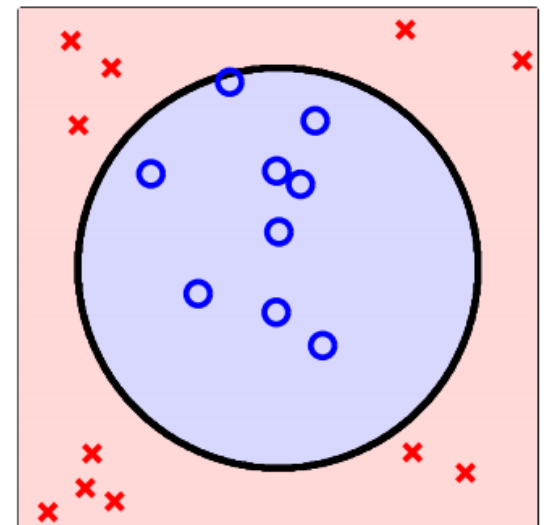
Given optimal $\vec{\alpha}^*$:

- $\vec{w}^* = \sum_{\alpha_n^* > 0} \alpha_n^* y_n \vec{x}_n$
- Find a $\alpha_n^* > 0$, $b^* = y_n - \vec{x}_n^T \vec{w}^*$

- Dual + Kernel Trick

$$\begin{aligned} & \text{maximize}_{\vec{\alpha}} \quad \sum_{n=1}^N \alpha_n - \frac{1}{2} \sum_{n=1}^N \sum_{m=1}^N \alpha_n \alpha_m y_n y_m K(\vec{x}_n, \vec{x}_m) \\ & \text{subject to} \quad \sum_{n=1}^N \alpha_n y_n = 0 \\ & \quad \quad \quad \alpha_n \geq 0, \forall n \end{aligned}$$

- Both can be efficiently solved using QP solver.
- We can infer the solution from one to the other



Recover (\vec{w}^*, b^*) from $\vec{\alpha}^*$ with Kernel Tricks

- Note that $\vec{\alpha}^*$ is solved in the \vec{z} space
 - $\vec{w}^* = \sum_{\alpha_n^* > 0} \alpha_n^* y_n \Phi(\vec{x}_n)$
 - Find a $\alpha_n^* > 0$, $b^* = y_n - \vec{w}^{*T} \Phi(\vec{x}_n)$
 - We want to avoid the transformation!
- Let's look at the hypothesis
 - $g(\vec{x}) = \text{sign}(\vec{w}^{*T} \Phi(\vec{x}) + b^*)$

$$\begin{aligned}\vec{w}^{*T} \Phi(\vec{x}) &= \left(\sum_{\alpha_n^* > 0} \alpha_n^* y_n \Phi(\vec{x}_n) \right)^T \Phi(\vec{x}) \\ &= \sum_{\alpha_n^* > 0} \alpha_n^* y_n \Phi(\vec{x}_n)^T \Phi(\vec{x}) \\ &= \sum_{\alpha_n^* > 0} \alpha_n^* y_n K(\vec{x}_n, \vec{x})\end{aligned}$$

$$\begin{aligned}b^* &= y_n - \vec{w}^{*T} \Phi(\vec{x}_n) \\ &= y_n - \left(\sum_{\alpha_m^* > 0} \alpha_m^* y_m \Phi(\vec{x}_m) \right)^T \Phi(\vec{x}_n) \\ &= y_n - \sum_{\alpha_m^* > 0} \alpha_m^* y_m K(\vec{x}_m, \vec{x}_n)\end{aligned}$$

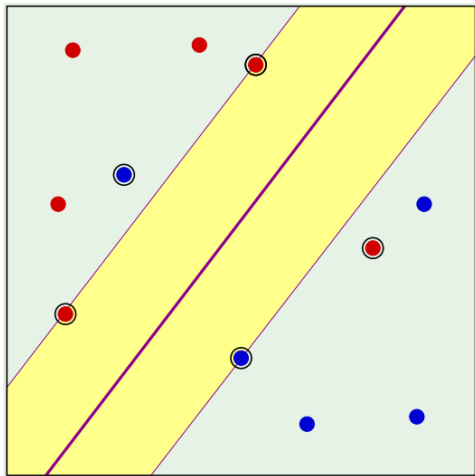
- Still can be computed in the \vec{x} space!

Kernel Functions

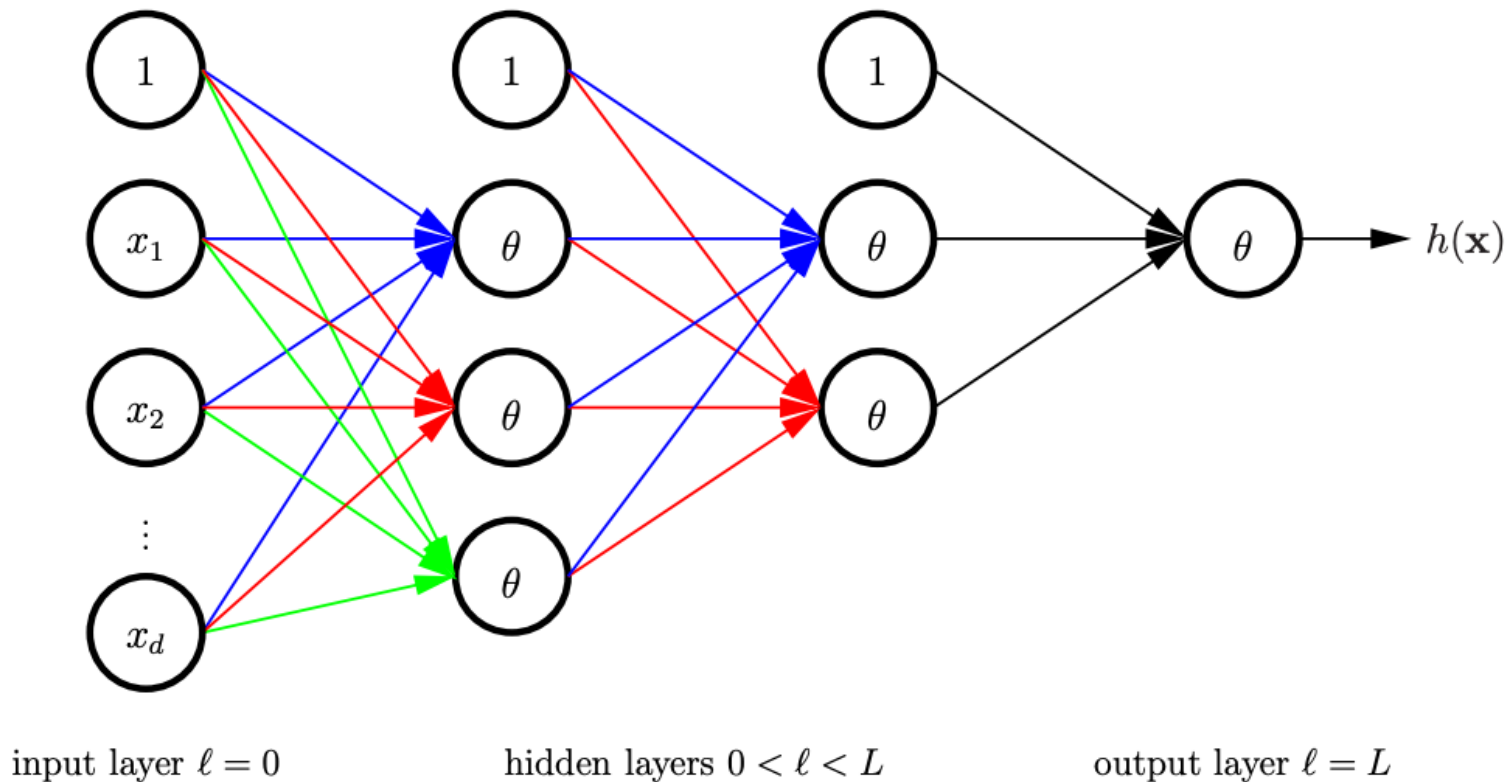
- Q-th order Polynomial kernel $K_{\Phi_Q}(\vec{x}, \vec{x}') = (1 + \vec{x}^T \vec{x}')^Q$
 - The corresponding $\Phi(x)$: Q-th order polynomial transform
- Gaussian RBF Kernel $K_{\Phi}(\vec{x}, \vec{x}') = e^{-\gamma \|\vec{x} - \vec{x}'\|^2}$
 - The corresponding $\Phi(x) = e^{-x^2} \left(1, \sqrt{\frac{2}{1}} x, \sqrt{\frac{2^2}{2!}} x^2, \dots \right)$
- When we plug in $K(\vec{x}, \vec{x}')$ in dual SVM
 - We are finding the **max-margin** separator in an **infinite dimensional** space
 - Seems to introduce infinite generalization error?
 - Maximizing margin help mitigate this issue
 - The number of support vectors provides indicators on the generalization

Support Vectors

- $\alpha_n^* > 0 \Rightarrow (\vec{x}_n, y_n)$ is a support vector
 - $y_n(\vec{w}^{*T} \vec{x}_n + b^*) = 1 - \xi_n$
- SVM classifier can be expressed using support vectors
 - $g(\vec{x}) = \text{sign}(\sum_{\alpha_n^* > 0} \alpha_n^* y_n K(\vec{x}_n, \vec{x}) + b^*)$
- Connection to generalization error through **LOOCV**



Neural Networks



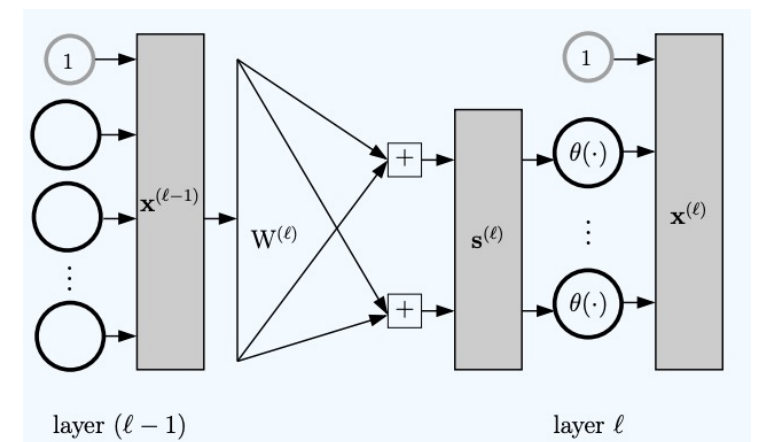
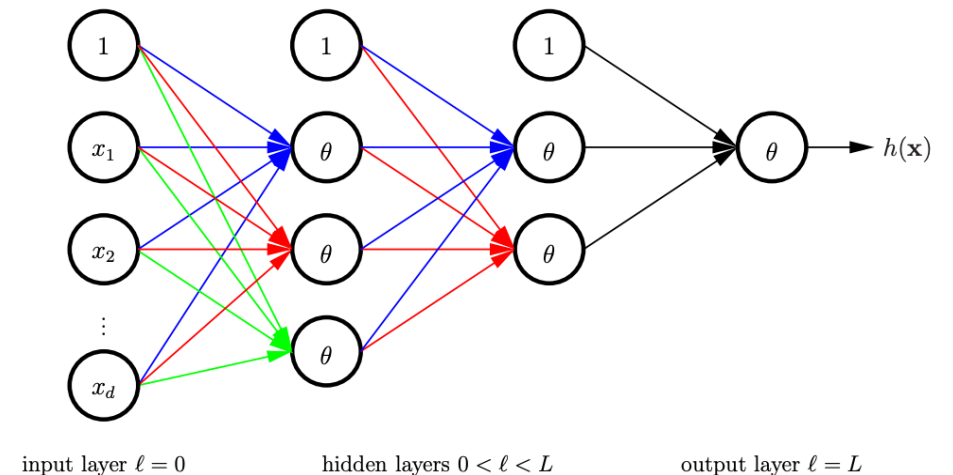
θ : **activation function**
(Specify the “activation” of the neuron)



We mostly focus on **feed-forward** network structure

Notations of Neural Networks (NN)

- Notations:
 - $\ell = 0$ to L : layer
 - $d^{(\ell)}$: dimension of layer ℓ
 - $\vec{x}^{(\ell)}$: the nodes in layer ℓ
 - $w_{i,j}^{(\ell)}$: weights; characterize hypothesis in NN
 - $s_j^{(\ell)} = \sum_{i=0}^{d^{(\ell-1)}} w_{i,j}^{(\ell)} x_i^{(\ell-1)}$: linear signals
 - θ : activation function
 - $x_j^{(\ell)} = \theta(s_j^{(\ell)})$



Forward Propagation (evaluate $h(\vec{x})$)

- A Neural network hypothesis h is characterized by $\{w_{i,j}^{(\ell)}\}$
- How to evaluate $h(\vec{x})$?

$$\mathbf{x} = \mathbf{x}^{(0)} \xrightarrow{w^{(1)}} \mathbf{s}^{(1)} \xrightarrow{\theta} \mathbf{x}^{(1)} \xrightarrow{w^{(2)}} \mathbf{s}^{(2)} \xrightarrow{\theta} \mathbf{x}^{(2)} \dots \xrightarrow{w^{(L)}} \mathbf{s}^{(L)} \xrightarrow{\theta} \mathbf{x}^{(L)} = h(\mathbf{x}).$$

Forward propagation to compute $h(\mathbf{x})$:

```
1:  $\mathbf{x}^{(0)} \leftarrow \mathbf{x}$                                 [Initialization]
2: for  $\ell = 1$  to  $L$  do                                [Forward Propagation]
3:    $\mathbf{s}^{(\ell)} \leftarrow (\mathbf{W}^{(\ell)})^T \mathbf{x}^{(\ell-1)}$ 
4:    $\mathbf{x}^{(\ell)} \leftarrow \begin{bmatrix} 1 \\ \theta(\mathbf{s}^{(\ell)}) \end{bmatrix}$ 
5: end for
6:  $h(\mathbf{x}) = \mathbf{x}^{(L)}$                                 [Output]
```

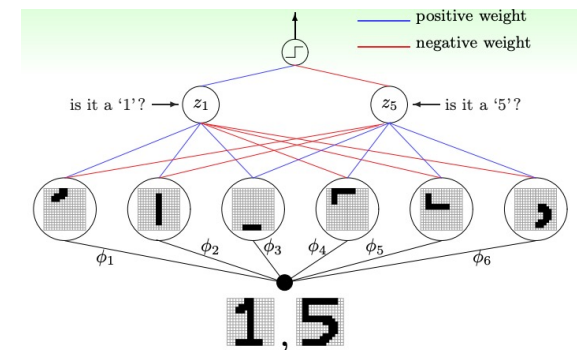
Given weights $w_{i,j}^{(\ell)}$ and $\vec{x}^{(0)} = \vec{x}$, we can calculate all $\vec{x}^{(\ell)}$ and $\vec{s}^{(\ell)}$ through forward propagation.

Backpropagation Algorithm

- Recall that $\frac{\partial e_n(W)}{\partial w_{i,j}^{(\ell)}} = \delta_j^{(\ell)} x_i^{(\ell-1)}$
- Backpropagation Algorithm
 - Initialize $w_{i,j}^{(\ell)}$ randomly
 - For $t = 1$ to T
 - Randomly pick a point from D (for stochastic gradient descent)
 - Forward propagation: Calculate all $x_i^{(\ell)}$ and $s_i^{(\ell)}$
 - Backward propagation: Calculate all $\delta_j^{(\ell)}$
 - Update the weights $w_{i,j}^{(\ell)} \leftarrow w_{i,j}^{(\ell)} - \eta \delta_j^{(\ell)} x_i^{(\ell-1)}$
 - Return the weights

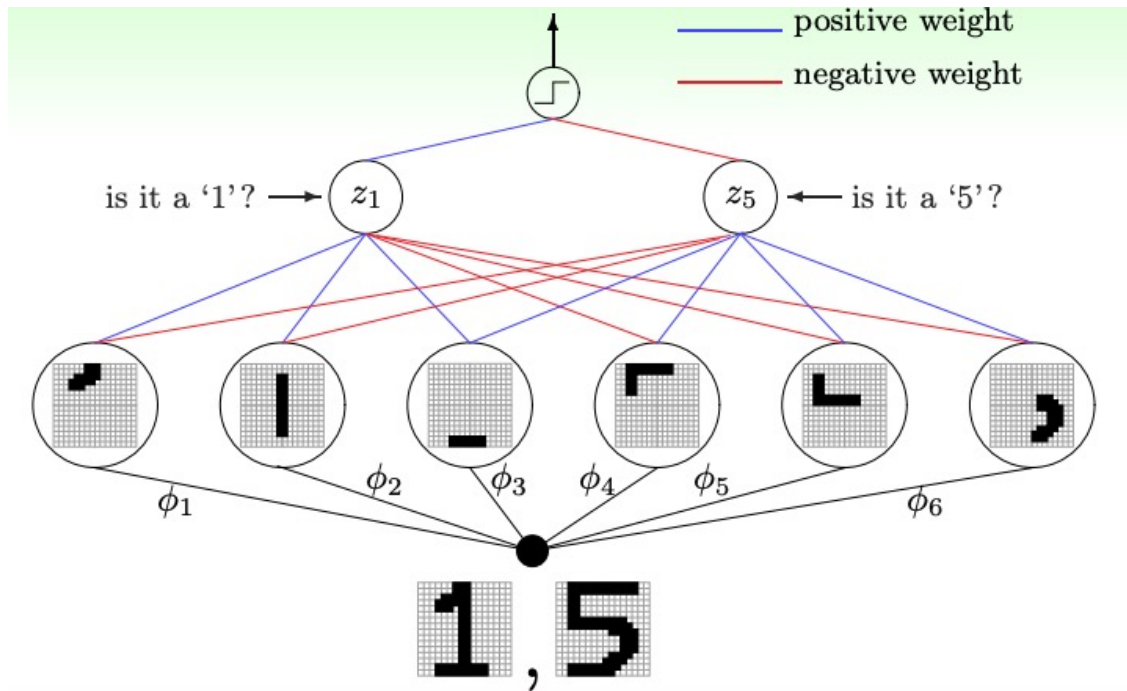
Discussion

- Backpropagation
 - gradient descent with efficient gradient computation
 - E_{in} is not convex in weights
 - Gradient descent doesn't guarantee to converge to global optimal
 - Run it many times, each with a different initialization (initialization matters)
- Regularization
 - Weight-based regularization, early stopping, dropout, adding noise, etc
- Deep learning
 - Neural Networks with many layers
 - Enable hierarchical representations of data



Deep Neural Network

- “Shallow” neural network is powerful (universal approximation theorem holds with a single hidden layer). Why “deep” neural networks?



Each layer captures **features** of the previous layers.

We can use “raw data” (e.g., pixels of an image) as input. The hidden layer are extracting the **features**.

Design different **network architectures** to incorporate domain knowledge.

Some Techniques in Improving Deep Learning

- Regularization to mitigate overfitting
 - Weight-based, early stopping, dropout, etc
- Incorporating domain knowledges
 - Network architectures (e.g., Convolutional Neural Nets)
- Improving computation with huge amount of data
 - Hardware architecture to improve parallel computation
- Improving gradient-based optimization
 - Choosing better **initialization** points

Practice Questions