CSE 417T
Introduction to Machine Learning

Review of Exam 2

Instructor: Chien-Ju (CJ) Ho

- Homework 5: Due **Apr 30 (Tomorrow).**
  - Keep track of your late days

- Exam 1: **May 4 (Tuesday)**
  - Duration: 75+5 Minutes
  - Content: Focus on the content of 2nd half of the semester
    - Though knowledge is cumulative
  - Time: Lecture time (unless you have requested for exceptions last week)
  - Format: Gradescope online exam + Zoom (with camera on)
  - Information access during exam:
    - Allowed: Textbook, slides, hardcopy materials (e.g., your own notes)
    - Not allowed: search for information online during exam, talk to any other persons
  - Other notes
    - Practice questions are now on Gradescope (get familiar with interface)
    - **Follow Piazza announcements**

More Exam Information

- Join **Zoom** (on mycanvas) and **turn on camera** before starting the exam
  - Won't be recorded
  - Students taking the exam at a different time need to do so as well
  - The Zoom + Camera policy is "softly" enforced
    - I might ask you for reasons for not following
    - No penalty as long as there are legitimate reasons

- We won't be able to answer questions during the exam
  - I don't answer individual questions even during in-person exams for fairness concerns
  - Will take into account of potential mistakes on our end
  - E.g., if there are multiple feasible answers for the multi-choice questions
    - Will give points if you choose one of the feasible ones

More Exam Information

- Please do not discuss the exam within 24 hours of the exam
  - Some students take the exam at a different time
  - Piazza will be locked (no public posts) next Tuesday
- Get familiar with how to submit math-heavy answers on Gradescope
  - prepare blank papers, having a smooth process of taking photos and upload file
- No office hours after (including) next Tuesdays

- Again, follow Piazza for the latest announcements

Plans for Today

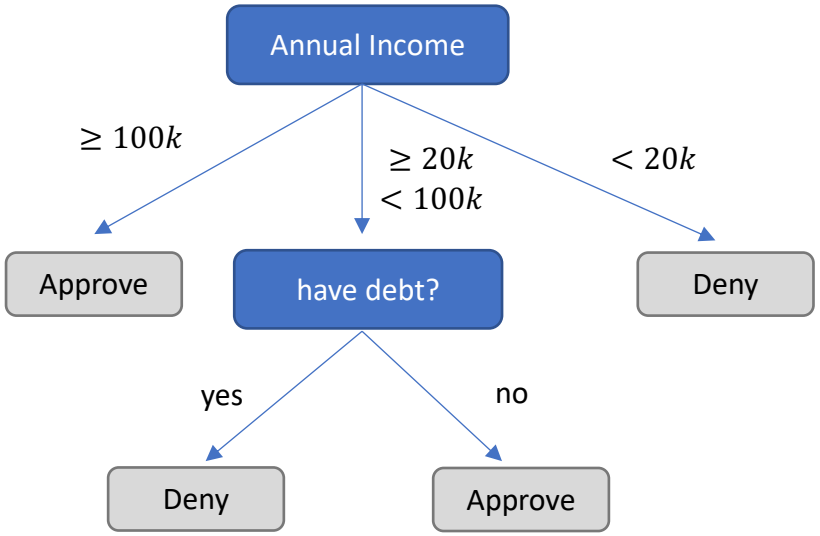
- Brief review of course content.
- Discussion of the practice questions.
- Discussion of any other questions you might have.

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)
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- 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 preference:	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 $\bar{g}(\vec{x}) = sign\left(\frac{1}{M}\sum_{m=1}^{M} g_m(\vec{x})\right)$
  - 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 weighted-aggregate$(g_1, \dots, g_T)$
  - Classification: $G(\vec{x}) = \bar{g}(\vec{x}) = sign\left(\frac{1}{T}\sum_{t=1}^{T} \alpha_t g_t(\vec{x})\right)$

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

- 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 $G(\vec{x}) = sign(\sum_{t=1}^{T} \alpha_t g_t(\vec{x}))$

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

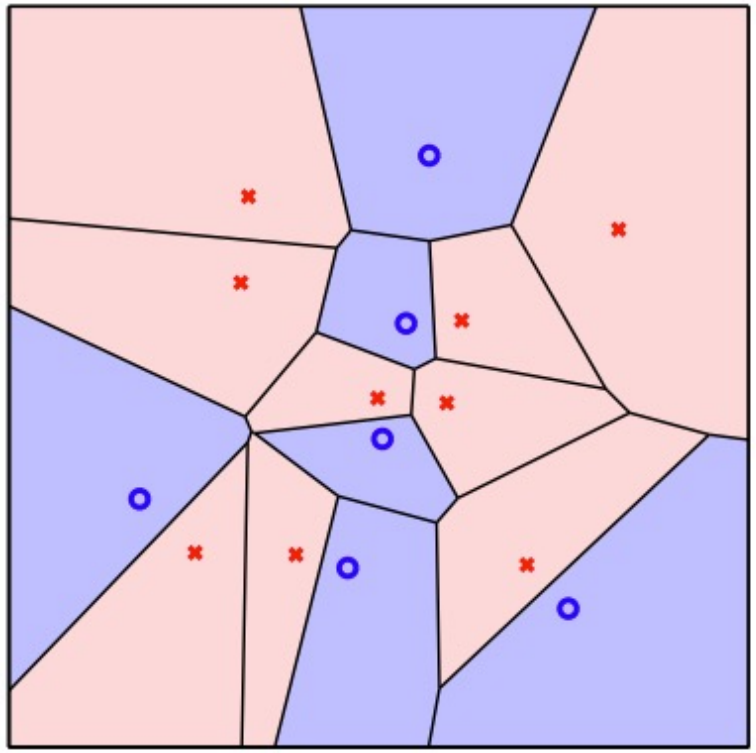
$$g(\vec{x}) = y_{[1]}(\vec{x})$$

- k-nearest neighbor (K-NN)

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

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: $E_{out} \leq E_{in}$ + 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 $N \to \infty$, 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.

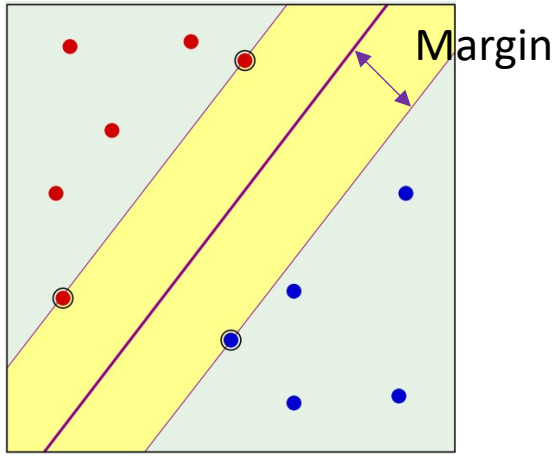
- k-NN:
  - Tuning k moderates the tradeoff of **generalization vs approximation**

Support Vector Machines

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

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

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

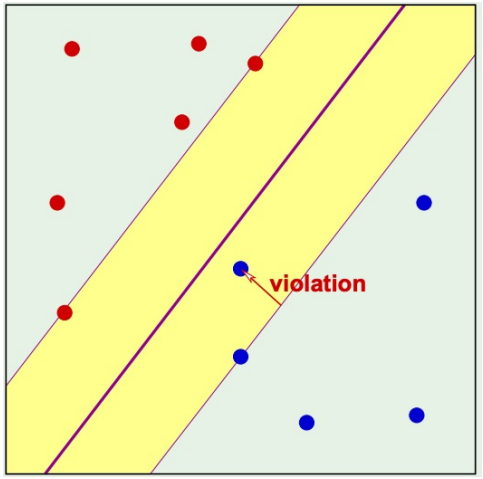


- If the data is not linearly separable
  - Soft-margin SVM
  - Nonlinear transformation – Dual Formulation and Kernel Tricks

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 $C\sum_{n=1}^{N}\xi_n$

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



Remarks:

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

Primal-Dual Formulations of Hard-Margin SVM

- Primal

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

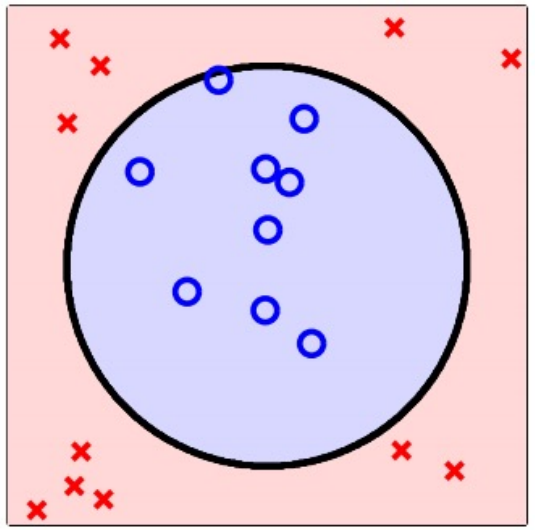
Given optimal $\vec{\alpha}^*$:

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

- Dual + Kernel Trick

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

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

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

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

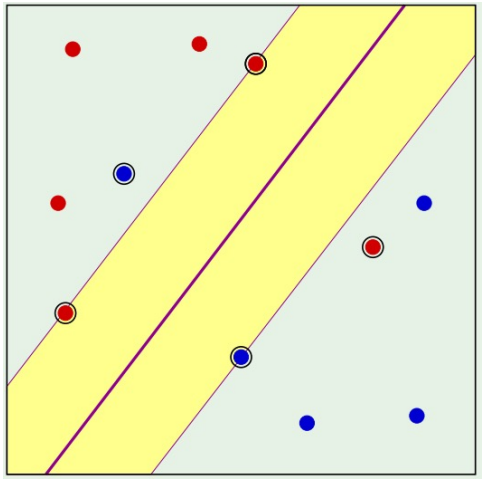
  - Still can be computed in the $\vec{x}$ space!

Kernel Functions

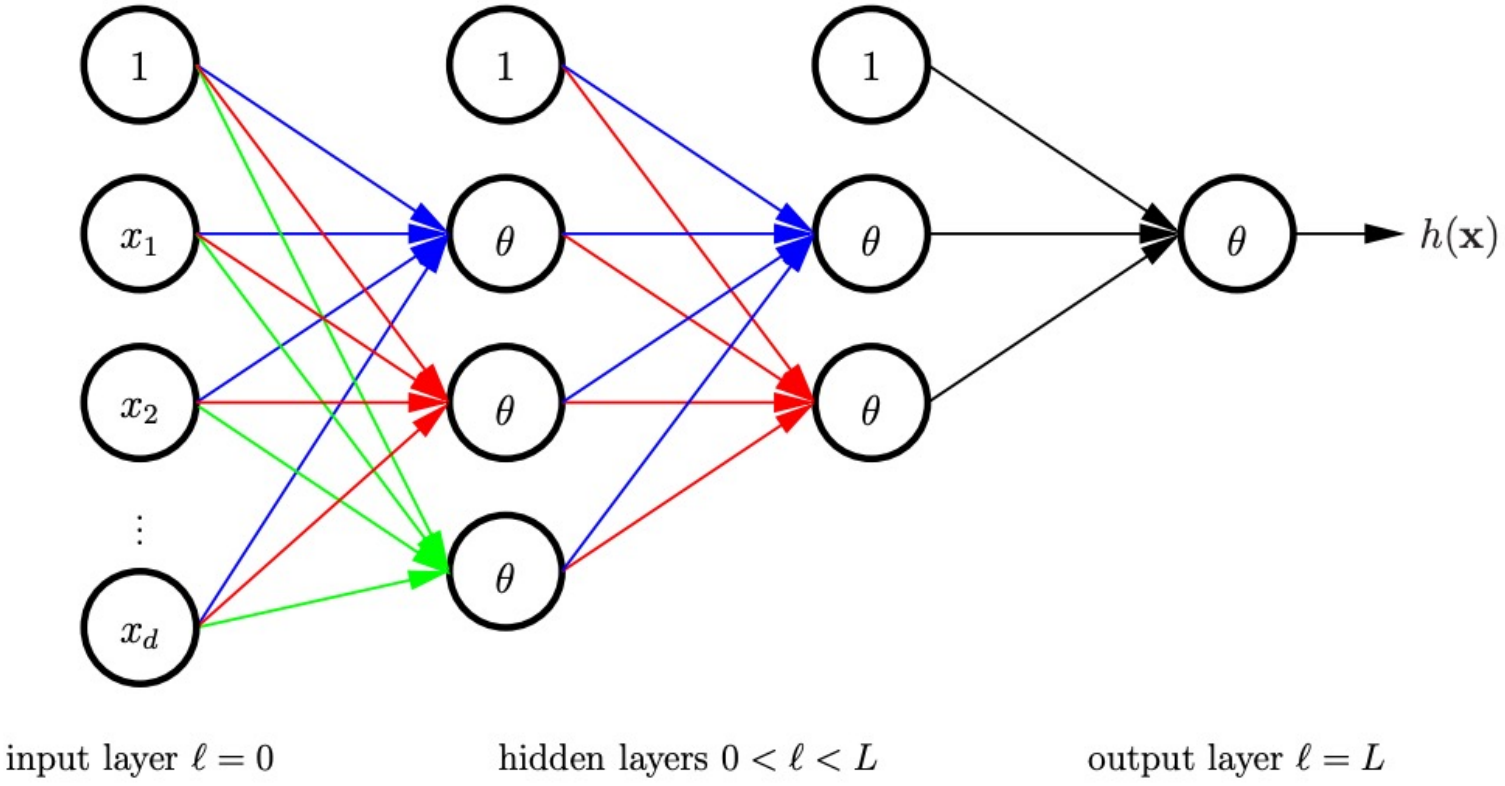
- Q-th order Polynomial kernel $K_{\Phi_Q}(\vec{x}, \vec{x}') = (1 + \vec{x}^T \vec{x}')^Q$
  - The corresponding $\Phi(x)$: Q-th order polynomial transform
- Gaussian RBF Kernel $K_\Phi(\vec{x}, \vec{x}') = e^{-\gamma \|\vec{x} - \vec{x}'\|^2}$
  - The corresponding $\Phi(x) = e^{-x^2}\left(1, \sqrt{\frac{2}{1}}x, \sqrt{\frac{2^2}{2!}}x^2, \ldots\right)$
- 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

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



Neural Networks



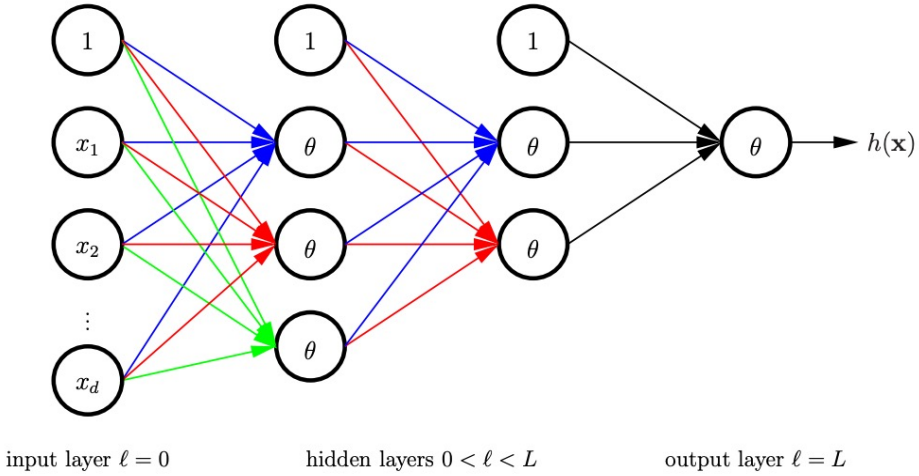
θ: activation function

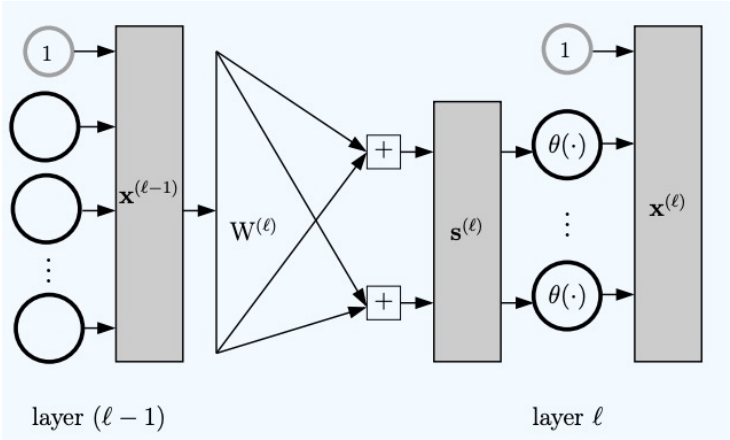
(Specify the "activation" of the neuron)

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
    - $x_j^{(\ell)} = \theta\left(s_j^{(\ell)}\right)$





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

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

$$\mathbf{x} = \mathbf{x}^{(0)} \xrightarrow{\mathrm{W}^{(1)}} \mathbf{s}^{(1)} \xrightarrow{\theta} \mathbf{x}^{(1)} \xrightarrow{\mathrm{W}^{(2)}} \mathbf{s}^{(2)} \xrightarrow{\theta} \mathbf{x}^{(2)} \cdots \xrightarrow{\mathrm{W}^{(L)}} \mathbf{s}^{(L)} \xrightarrow{\theta} \mathbf{x}^{(L)} = h(\mathbf{x}).$$

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: $\mathbf{s}^{(\ell)} \leftarrow (\mathrm{W}^{(\ell)})^{\mathrm{T}}\mathbf{x}^{(\ell-1)}$

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]

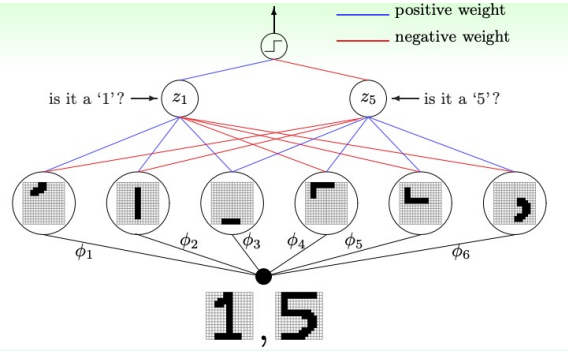
Given weights $w_{i,j}^{(\ell)}$ and $\vec{x}^{(0)} = \vec{x}$, we can calculate all $\vec{x}^{(\ell)}$ and $\vec{s}^{(\ell)}$ through forward propagation.

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



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

Practice Questions