CSE 417T
Introduction to Machine Learning

Review of Exam 2
Instructor: Chien-Ju (CJ) Ho

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

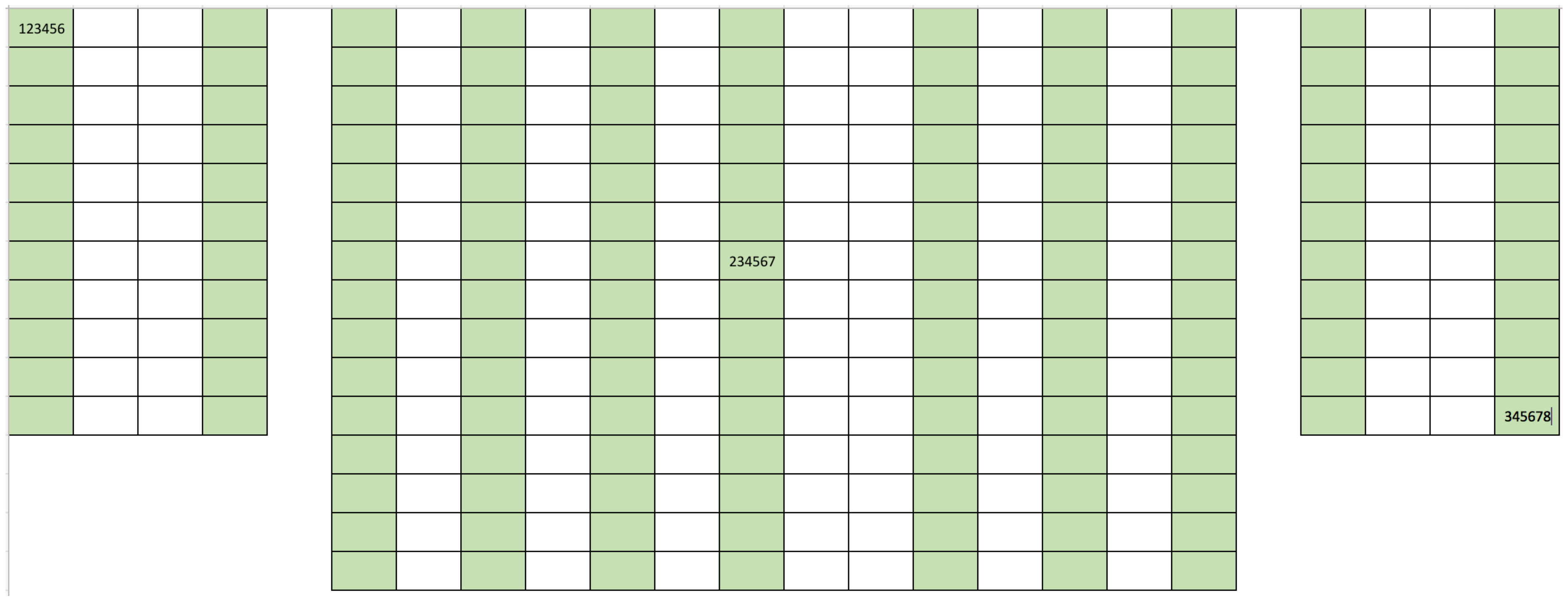
  - 2 sections of questions
    - ~5 long questions (written response questions with explanations required)
    - 10 multiple choice questions (no explanations needed)

  - 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

- I might arrange random seat assignments
  - Will be announced on Piazza the night before the exam if I do



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

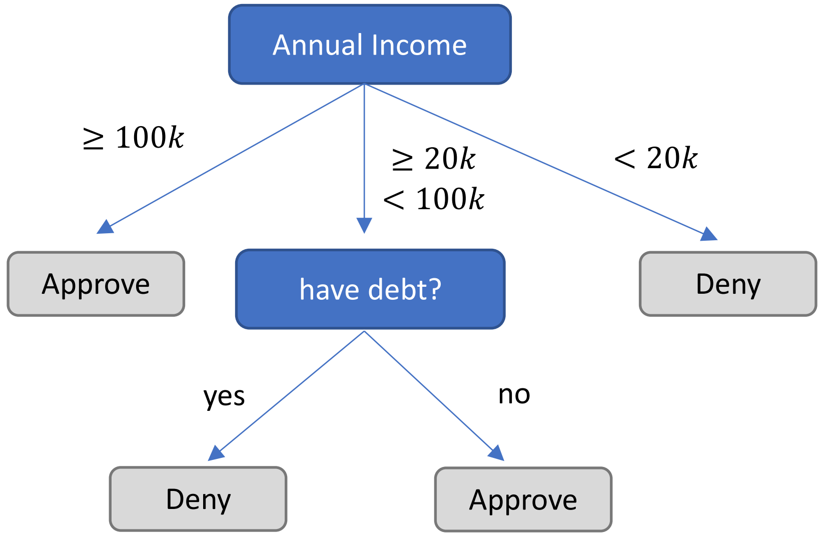
- Brief review of course content.
- Discussion of the practice questions.
- Discussion of any other questions you might have.

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 $\longrightarrow$

```
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
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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

<u>Bagging:</u>

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

<u>Boosting</u>

- 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 $\bar{g}(\vec{x}) = sign\left(\frac{1}{M}\sum_{m=1}^{M} g_m(\vec{x})\right)$
  - 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$(g_1, \ldots, g_T)$
  - 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

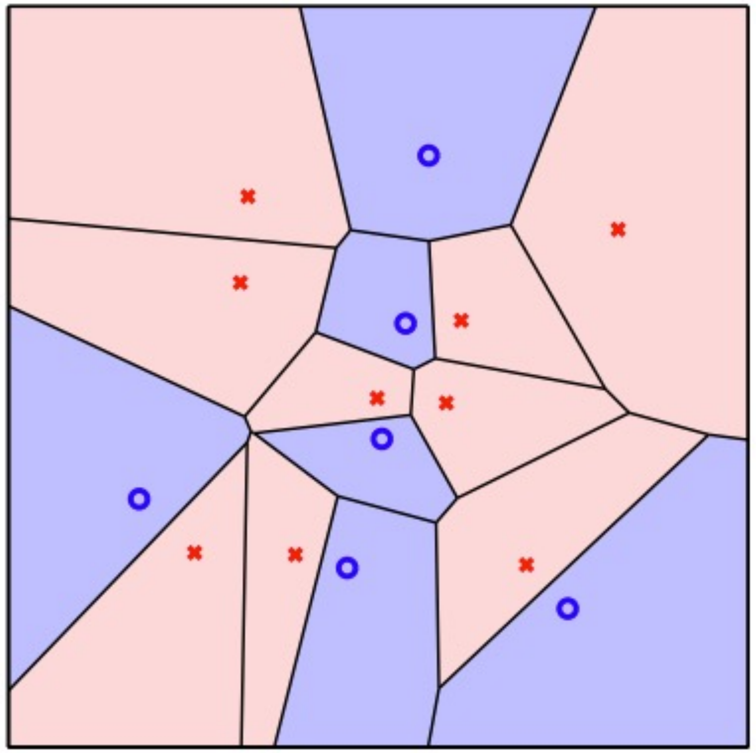
$$g(\vec{x}) = y_{[1]}(\vec{x})$$

- 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**

Radial Basis Function

- $h(\vec{x}) = \sum_{k=1}^{K} w_k \, \phi\left(\frac{\|\vec{x}-\vec{\mu}_k\|}{r}\right)$

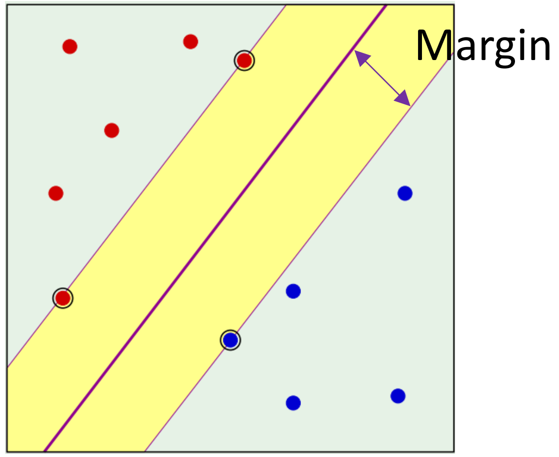
- Connection to linear models
  - Parametric RBF is essentially linear model with nonlinear transformation
- Connection to nearest neighbor
  - RBF is based on the similarity to a set of points
- Connection to SVM with RBF Kernel
  - Using K representative points vs. using support vectors
- Connection 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

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

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

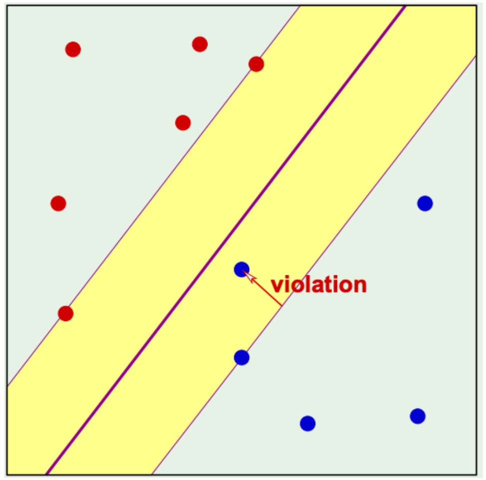


- If the data is not linearly separable
  - Soft-margin SVM
  - Nonlinear transformation – Dual Formulation and Kernel Tricks

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

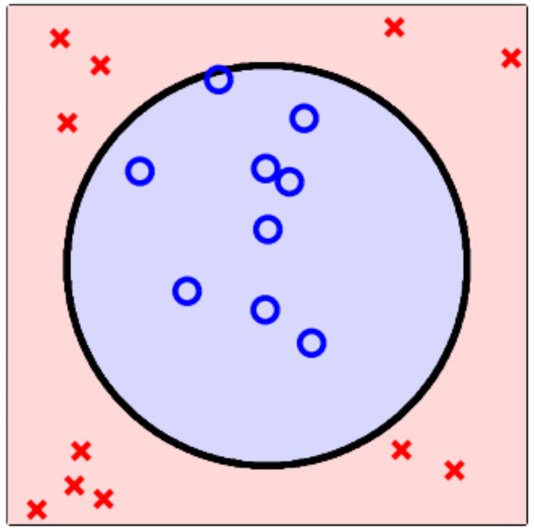
$$\begin{array}{ll} \text{minimize}_{\vec{w},b} & \frac{1}{2}\vec{w}^T\vec{w} \\ \text{subject to} & y_n(\vec{w}^T\vec{x}_n + b) \geq 1, \forall n \end{array}$$

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

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



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

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

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

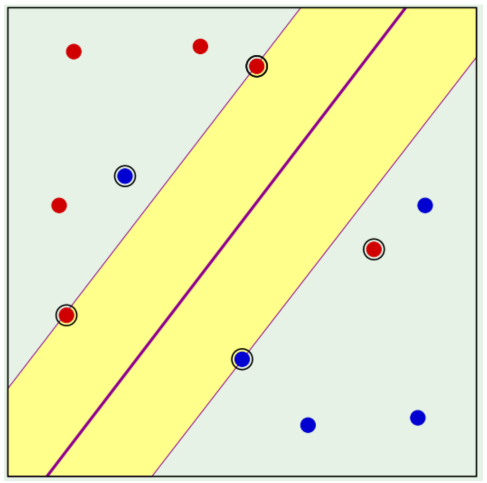
- Still can be computed in the $\vec{x}$ space!

Kernel Functions

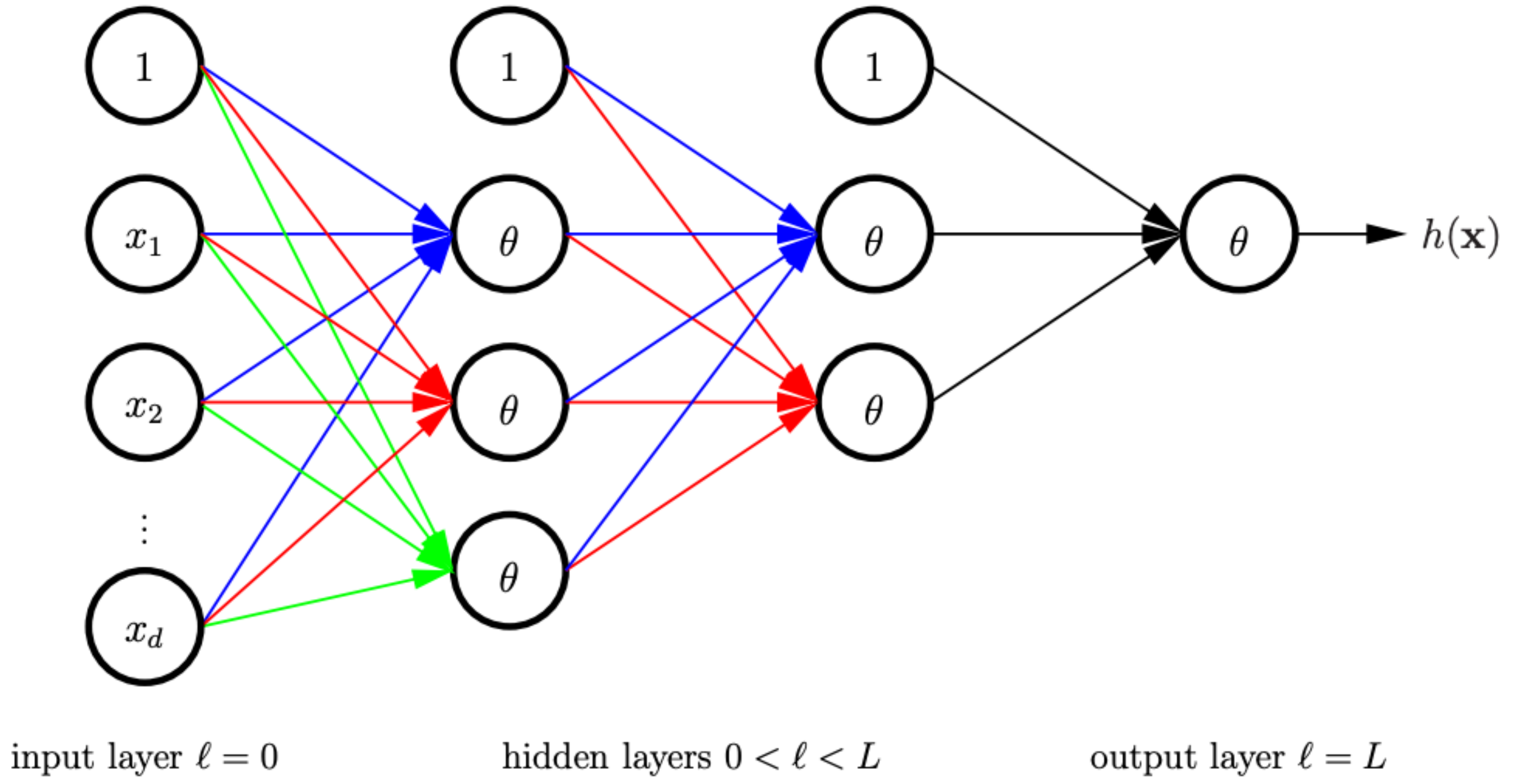
- Q-th order Polynomial kernel $K_{\Phi_Q}(\vec{x}, \vec{x}') = (1 + \vec{x}^T \vec{x}')^Q$
  - The corresponding $\Phi(x)$: Q-th order polynomial transform
- Gaussian RBF Kernel $K_{\Phi}(\vec{x}, \vec{x}') = e^{-\gamma \|\vec{x} - \vec{x}'\|^2}$
  - The corresponding $\Phi(x) = e^{-x^2}\left(1, \sqrt{\frac{2}{1}}x,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



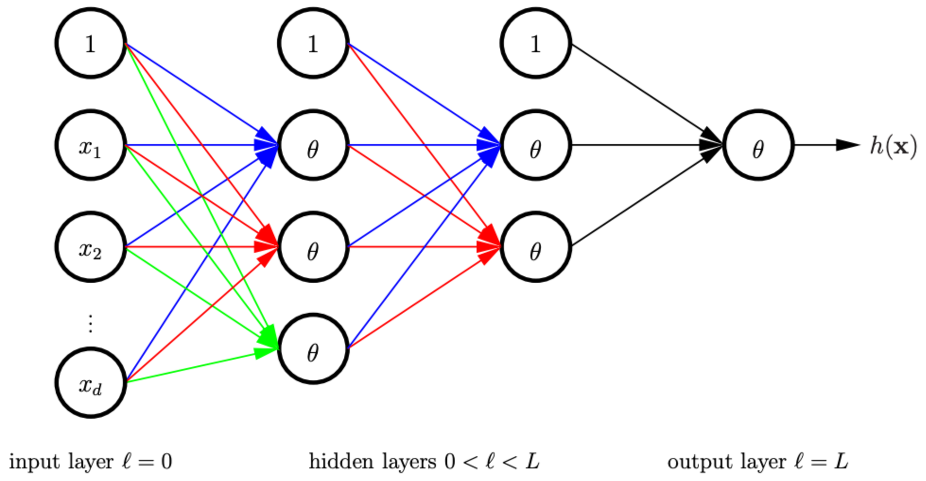
θ: activation function

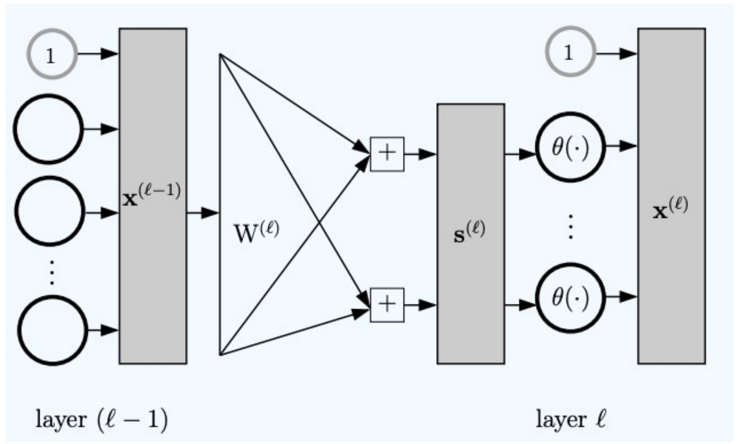
(Specify the "activation" of the neuron)

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]
```

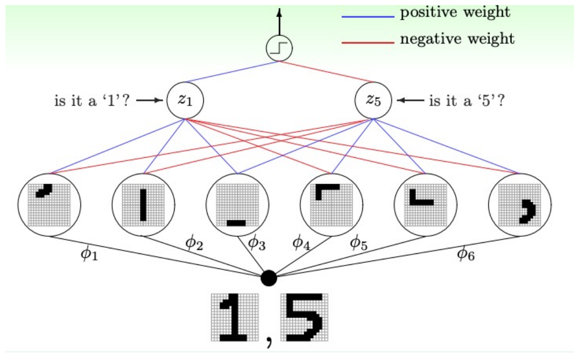
Given weights $w_{i,j}^{(\ell)}$ and $\vec{x}^{(0)} = \vec{x}$, we can calculate all $\vec{x}^{(\ell)}$ and $\vec{s}^{(\ell)}$ through forward propagation.

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

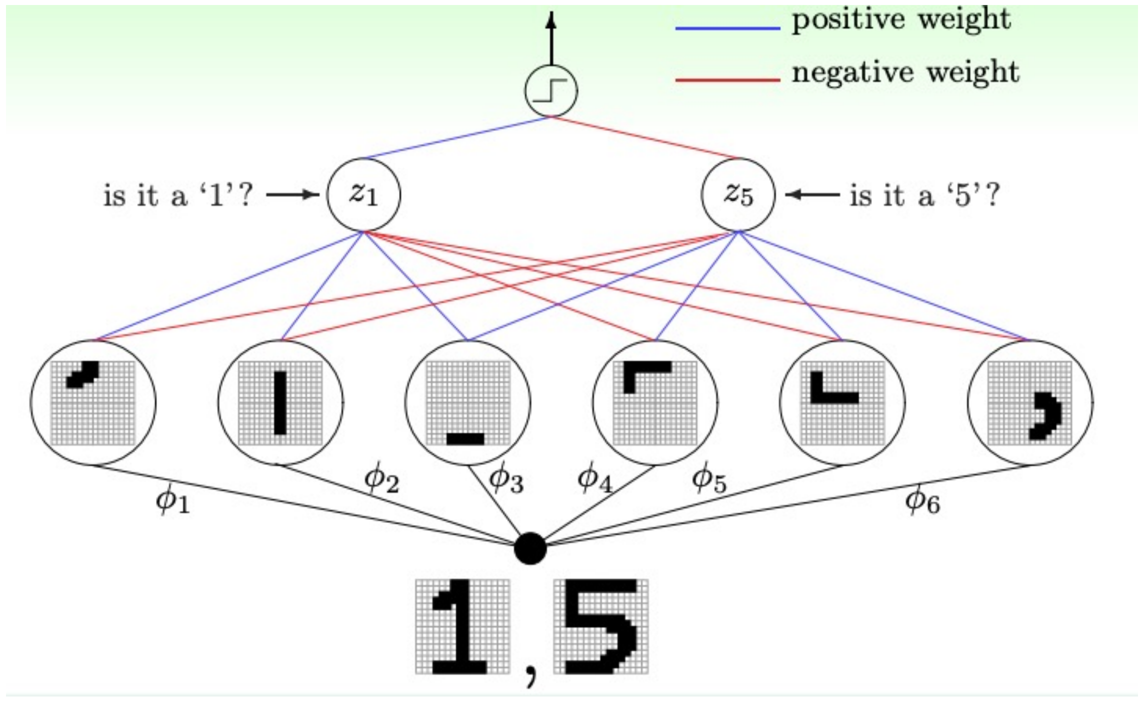
Discussion

- 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



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