

CS2109S Finals

AY24/25 SEM 1
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1 Solving Problems by Searching

1.1 Designing an Agent

- Assumptions:** Goal-based agent | Env is fully observable, deterministic, static, discrete
- Problem-solving Agent:** Agent that plans ahead (considers a seq. of actions that form a path to a goal state), undertakes SEARCH process
- Steps:**
 - Goal Formulation: (*What do we want?*)
 - Problem Formulation: (*How the world works?*) → States (state space), Initial State(initial state of agent), Goal State/Test (goal state of agent), Actions (things that agent can do in a given state), Transition Model (specifies outcome of an action to a given state & how it leads to new states), Action Cost Function (cost of performing an action)
 - Search: (*How to achieve it?*) → Path (seq. of actions), Solution (path to a goal)
 - Execute
- Representation Invariant:** A condition that must be true over all valid concrete representations of a class

1.2 Search Algorithms (Introduction)

- Search Algorithm:** Takes in search problem (input), returns solution/failure (output) | Defined by Order of Expansion (FRONTIER)
- Evaluation Criteria:**
 - Time Complexity: # of nodes generated/expanded
 - Space Complexity: Max # of nodes in memory
 - Completeness: Does it return solution if it exists?
 - Optimality: Does it always find least cost solution?
- Checking of Goal State:**
 - New state is checked for goal state before new states are PUSHED to frontier → Expand less states, may skip states with less cost
 - State is checked for goal state after state is POPPED from frontier → Expand more states, will not skip states with less cost

1.3 Search Algorithms (Uninformed Search)

- Key Idea:** Search Algo is given no clue about how close a state is to the goal | Can be Tree or Graph Search
- BFS:** Queue Frontier | Time Complexity: $O(b^d) = 1 + b + b^2 + \dots + b^d$, where b is branching factor, d is depth of optimal solution | Space Complexity: $O(b^d)$ when expanded until last child in worst case | Completeness: Complete if b is finite | Optimality: Optimal if step cost is same everywhere
- UCS:** Priority Queue (path cost) Frontier, where path cost == cost from root to state | Time Complexity: $O(b^{C^*}/\epsilon)$, where C^* = cost of optimal solution, ϵ is minimum edge cost → C^*/ϵ is est. depth of optimal solution in worst case | Completeness: Complete if $\epsilon > 0$ and C^* is finite (if $\epsilon = 0$, zero cost cycle may occur) | Optimality: Optimal if $\epsilon > 0$ *Note: BFS is special case of UCS where step cost == 1 for every edge*
- DFS:** Stack Frontier | Time Complexity: $O(b^m)$ where b is branching factor, m is max depth | Space Complexity: $O(bm)$ as only 1 path is expanded at one time | Completeness: Not complete (when depth is infinite or can go back or forth) | Optimality: Not optimal (there can be paths with less cost not explored yet)
- DLS (Depth Limited Search):** Limit the search depth to l where $l < m$, backtrack once depth limit is reached | Time Complexity: $O(b^l)$ | Space Complexity: $O(b \cdot l)$ | Completeness: Not complete when soln lies deeper l | Optimality: Not optimal when soln lies deeper than l *Note: We dk the depth of solution, which is a downside*
- IDS (Iterative Deepening Search):** Do DLS with max depth of $0, \dots, \infty$ → return soln if found, otherwise increase depth | Time Complexity: $O(b^d)$, *Overhead* = $(n_{IDS} - n_{DLS})/n_{DLS}$ | Space Complexity: $O(b \cdot d)$ | Completeness: Complete | Optimality: Optimal if step cost is same everywhere *Note: IDS is not always faster than DFS → Consider state space s.t. each state have only single successor & goal node is at depth $n \rightarrow IDS$ will run in $O(n^2)$, DFS will run in $O(n)$*
- Backward Search:** Search from goal
- Bidirectional Search:** Combine forward search & backward search, stop when 2 searches meet | Time Complexity: $2 * O(b^{d/2}) < O(b^d)$

1.4 Search Algorithms (Informed Search)

- Key Idea:** Search Algo has a clue on how close a state is to the goal
- Best First Search:** Priority Queue ($f(n)$) Frontier, where $f(n)$ estimates the goodness of a state (Node with lowest $f(n)$ is selected first to be expanded) | $f(n)$ can be purely heuristic (estimated cost from n to goal) or a combi of path cost & heuristic
- Greedy Best First Search:** Priority Queue ($f(n) = h(n)$) Frontier, where $h(n)$ is heuristic function that est. cost from n to goal (Expands node that seems closest to goal according to $h(n)$ without considering path cost so far) | Time Complexity: $O(b^{m'})$ | Space Complexity: $O(b^{m'})$ | Completeness: Not complete since GBFS might keep expanding nodes based on $h(n)$ without ever finding goal | Optimality: Not optimal since GBFS selects nodes based on $h(n)$ without considering path cost
- A* Search:** Priority Queue ($f(n) = g(n) + h(n)$) where $g(n)$ is cost so far to reach n | Time Complexity: $O(b^{m'})$ | Space Complexity: $O(b^{m'})$ | Completeness: Complete | Optimality: Optimal
 - If $h(n)$ is admissible → A* using Tree search is optimal
 - If $h(n)$ is consistent → A* using Graph search is optimal
 - Note: UCS is special case of A* search where $h(n) = 0$*

1.5 Heuristics

- Estimate cost from node n to goal
- Admissible Heuristics:** For every node n , $h(n) \leq h^*(n)$, where $h^*(n)$ is true cost to reach goal state from n (Never over-estimate)
- Consistent Heuristics:** For every node n , every successor n' generated by action a , $h(n) \leq c(n, a, n') + h(n')$ and $h(G) = 0$ (Proof $h(n) - h(n') \leq c(n, a, n')$) *Note: If $h(n)$ is consistent, $f(n') \geq f(n) \rightarrow f(n)$ is non-decreasing along any path → Nodes are expanded in order of increasing f cost*
- Dominance:** If $h_2(n) \geq h_1(n)$ for all $n \rightarrow h_2$ dominates h_1 | If h_2 is admissible → h_2 is better for search
- Creating Admissible Heuristics:**
 - Problem with fewer restrictions on actions is called a relaxed problem
 - Cost of an optimal soln to a relaxed problem is an admissible h for original problem
- Consistent heuristic is admissible, Non-admissible heuristic is not consistent

2 Local Search & Adversarial Search

2.1 Local Search

- Assumptions:** Agent is a Goal/Utility-based agent, Env has a very large state space
- Informed & Uninformed Search VS Local Search**
 - IUS:** Low to moderate state space | Optimal or no soln | Search path is usually the soln
 - LS:** Very large state space | Good enuf soln is preferable rather than no soln | State is the soln (don't care about search path)

Local Search Overview:

- Basic Idea:** Start somewhere in state space, move towards a better spot
- Problem Formulation:** States(state space), Initial State(initial state of agent), Goal (optimal, coz we actually dk the goal state, rely on eval function instead), Successor Function (possible states from a state), Evaluation Function (Output value/goodness of a state)
- Hill Climbing Algorithm** **current** = Initial state

while True:

- neighbor** = a **highest-valued** successor of **current**
- if **value(neighbor) <= value(current)**:
 - return current**
 - current** = **neighbor**
- Known as Greedy Local Search (pick best amongst neighbors, repeat)
- Best Soln:** State space where eval. function has a max value (global max)
- Disadvantages: Cannot reach global max if it enters local max, plateau | Sensitive to choice of initial state, poor initial state may result in poor final state (Can overcome with random restarts, walks)

Simulated Annealing

- current** = initial state
- is** = a large positive value
- while **T** > 0:
 - next** = a randomly selected successor of **current**
 - if **value(next) > value(current)**: **current** = **next**
 - else with probability **P(current, next, T)**: **current** = **next**
 - decrease **T**
- P(current, next, T)** = $e^{(value(next) - value(current))/T}$
- More exploration of bad states is allowed when T is high, more exploitation is done when T is low → basically choosing worse successor may lead to a better max
- Theorem:** If T decreases slowly enough, SA will find global optimum with high probability

2.2 Adversarial Search

- Assumptions:** Agent is Utility-based | Env is a game (game cannot be single player, partially observable, stochastic, but must be fully observable, deterministic, discrete, terminal states exist, 2 players, zero-sum, turn taking)
- Minimax Algorithm:**

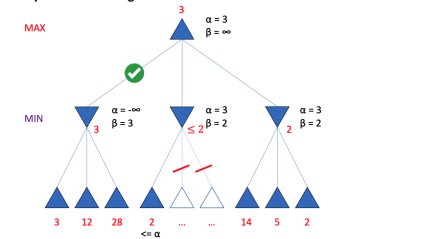
```
def minimax(curr):
    v = max_value(curr)
    return action in success(curr) with value v

def max_value(curr):
    if len(success(curr)) == 0:
        v = -inf
        for action, next_state in success(curr):
            v = max(v, min_value(next_state))
        return v

def min_value(curr):
    if len(success(curr)) == 0:
        v = inf
        for action, next_state in success(curr):
            v = min(v, max_value(next_state))
        return v
```

Assumes opponent play optimally, trying to minimize player's value
 - Intuition:** MAX wins when utility is high, MIN wins when utility is low | Assign utility values to all terminal states & start tracing from terminal states → Eventually, all states will have utility values, starting player can choose a state that will max/min his utility
 - Analysis:** Completeness: Complete if tree is finite | Time Complexity: $O(b^{m'})$ | Space Complexity: $O(bm)$ depth first exploration | Optimality: Optimal against optimal opponent

Alpha-beta Pruning

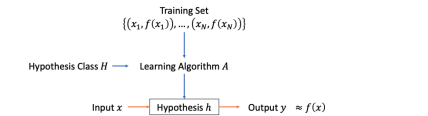


- Definitions:** α is best explored option to the root for MAX player (Highest value for MAX) | β is best explored option along path to the root for MIN player (Lowest value for MIN)
- Procedure:** 1. Assign $\alpha = -\infty$, $\beta = \infty$ for root 2. Propagate values down to the terminal node 3. Update α value at MAX node, β value at MIN node 4. Propagate values up 5. Prune branches of nodes where $\alpha \geq \beta$
- Minimax with Cutoff**
 - Instead of calling *is terminal*, call *is cutoff* which returns TRUE if (1): State is terminal or (2): Cut-off is reached
 - Instead of using *utility*, call *eval* which is an eval. function that returns (1): Utility for terminal states or (2): Heuristic value for non-terminal states

3 Introduction to ML & Decision Trees

3.1 Introduction to ML

- Definitions:** Computer program is said to learn from experience E w.r.t. some class of tasks T & performance measure P , if its performance at tasks in T , as measured by P , improves with experience E
- Types of Feedback:**
 - Supervised Learning: Involves training a model on a labeled dataset, where input data is paired with correct output → Model learns to map inputs to outputs based on this labeled data, allowing it to make predictions on new data
 - Regression: Predict continuous input
 - Classification: Predict discrete input
 - Unsupervised Learning: Deals with dataset that do not have labeled outputs → Goal is to identify patterns & structures within data
 - Reinforcement Learning: Agent learns to make decisions by interacting with an environment → Agent receives feedback in the form of rewards or penalties based on its actions → Learns optimal behaviors over time
- Formal Definitions:**



3.2 Performance Measure

- Accuracy:** $\frac{TP+TN}{TP+FN+FP+TN}$
- Precision:** $\frac{TP}{TP+FP}$ (How many selected items are relevant, maximise if FP is costly)
- Recall:** $\frac{TP}{TP+FN}$ (How many relevant items are selected, maximise if FN is dangerous)
- F1 Score:** $\frac{2}{1/precision+1/recall}$

3.3 Decision Trees

- Traits of Decision Trees:**
 - Decision Trees can express any function of input attributes
 - Consistent Decision Tree for any training set, but probably will not generalize to new examples
- # of distinct decision trees with n boolean attributes = 2^{2^n}**
- Decision Tree Learning Algorithm** **DTL(examples, attributes, default):**
 - if **examples** is empty: return **default**
 - if **examples** have the same classification: return **classification**
 - if **attributes** is empty: return **mode(examples)**
 - best** = **choose_attribute(attributes, examples)**
 - tree** = a new decision tree with root **best**
 - for each value v_i of **best**:
 - examples_i** = [rows in **examples** with **best** = v_i]
 - subtree** = **DTL(examples_i, attributes - best, mode(examples_i))**
 - add a branch to **tree** with label v_i and subtree **subtree**

- mode:** Category with the highest number
- choose attribute:** Chooses attribute with the highest information gain
- Choosing an attribute:**
 - Ideally select an attribute that splits examples into "all positive" or "all negative"
 - Entropy** (Measure of randomness):
$$I(P(v_1), \dots, P(v_n)) = -\sum_{i=1}^n P(v_i) \log_2 P(v_i)$$
where for data set containing p positive & n negative examples,
$$I\left(\frac{p}{p+n}, \frac{n}{p+n}\right) = -\frac{p}{p+n} \log_2 \frac{p}{p+n} - \frac{n}{p+n} \log_2 \frac{n}{p+n}$$
Note: $I(1,0) = I(0,1) = 0$, $I(0.5, 0.5) = 1$
 - Information Gain** (Entropy of curr. node - Total Entropy of children nodes):
$$IG(A) = I\left(\frac{p}{p+n}, \frac{n}{p+n}\right) - remainder(A)$$
$$remainder(A) = \sum_{i=1}^v \frac{p_i + n_i}{p+n} I\left(\frac{p_i}{p_i + n_i}, \frac{n_i}{p_i + n_i}\right)$$
, where examples are split into v subsets by attribute A

- Dealing with continuous valued attributes:** Define a discrete valued input attribute to partition values into discrete set of intervals
- Dealing with missing values:** Assign most common value of attribute, assign probability to each value and sample, drop attribute, drop rows
- Overfitting:** Decision Tree is perfect on training data, but worse on test data
- Occam Razor:** Prefer short/simple hypothesis (long/complex hypothesis that fits data may be coincidental)
- Pruning:** Prevents nodes from being split even when it fails to cleanly separate examples (Min samples left: Merge until leaf node is above min. samples number | Max depth: Merge until leaf nodes are at depth less than max depth)

4 Linear Regression

4.1 Linear Regression Basics

- Purpose:** Given $h(w) = w_0 + w_1x + \dots$, find a w that fits the data well
- Mean Squared Error (Loss Function):**
$$J_{MSE}(w) = \frac{1}{2m} \sum_{i=1}^m (h(w(x^{(i)})) - y^{(i)})^2$$
 - m is the number of training examples
 - $h(w(x^{(i)})) = \hat{y}^{(i)}$
 - $y^{(i)}$ is actual y value for the i th training example
- Partial Derivative:**
$$\frac{\partial J_{MSE}(w)}{\partial w_1} = \frac{1}{m} \sum_{i=1}^m (w_1 x^{(i)} - y^{(i)}) x^{(i)}$$
(when we differentiate $J_{MSE}(w)$ wrt. particular weight, i.e. w_1)

4.2 Gradient Descent

- Gradient Definition:** $\begin{bmatrix} \frac{\partial J(w)}{\partial w_0} \\ \frac{\partial J(w)}{\partial w_1} \end{bmatrix}$, where each expression is a partial derivative wrt. different weights
- Gradient Descent Algorithm:**
 - Start at some w
 - Pick a nearby w that reduces $J(w)$:
$$w_j \leftarrow w_j - \gamma \frac{\partial J(w_0, w_1, \dots)}{\partial w_j}$$
 - Repeat until minimum is reached
 - Gradient Descent with 2 parameters:** Always store gradient in intermediate variable, then conduct gradient descent on each weight separately → Do not conduct gradient descent on all weights concurrently (or else a new weight will be updating another weight unknowingly)
 - Theorem:** $J_{MSE}(w)$ is convex for linear regression → 1 minimum, global minimum only
- Gradient Descent Variants**
 - Batch Gradient Descent:** All training examples involved
 - Mini-batch Gradient Descent:** Subset of training examples at a time; Cheaper (faster); Random, may escape local minima for non-convex function
 - Stochastic Gradient Descent:** 1 random data point at a time (Order which we use the samples should be randomly decided); Cheapest (fastest); More random, may escape local minima for non-convex function
- 4.2 Extension of Linear Regression**
 - Features of different scales:** A feature with smaller magnitude will take much smaller steps each update than another feature with larger magnitude → Converging becomes slower
 - Solution 1:** Have different learning rates for each weight

- Solution 2:** Conduct mean normalization $x_j \leftarrow \frac{x_j - \mu_j}{\sigma_j}$, where σ_j is the standard deviation of the feature across all training examples & μ_j is the mean of the feature across all training examples
- Non-linear relationship:** Use polynomial regression for non-linear relationship (transform features) | Terms that are raised to a power more than 1 might need to be scaled as they can become too big | Max degree of polynomial needed to fit any set of n points is $n - 1$ (otherwise will overfit)

4.5 Normal Equation

- Normal Equation Procedure:**
$$X = \begin{bmatrix} 1 & x_1^{(1)} & \dots & x_n^{(1)} \\ 1 & x_1^{(2)} & \dots & x_n^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(m)} & \dots & x_n^{(m)} \end{bmatrix} \quad w = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_n \end{bmatrix} \quad y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$
$$h_w(x) = Xw$$

Annotations: A red arrow points to the '1' in the first column of X, labeled 'Bias'. A red arrow points to the matrix multiplication, labeled 'A bunch of math...'. A red arrow points to the equation $w = (X^T X)^{-1} X^T Y$, labeled 'Assume invertible'.

$X^T X$ becomes non-invertible when it is singular, which occurs when its rows (repeated or identical data points) or columns (redundant or highly correlated features) are linearly dependent

Gradient Descent VS Normal Equation:

	Gradient Descent	Normal Equation
Need to choose γ	Yes	No
Iterational	Yes	None
Large number of features n	Many	None
Large number of features n	No problem	Slow ($O(n^3) \rightarrow O(n^2)$)
Feature scaling?	May be necessary	Not necessary
Constraints	<	if it needs to be invertible

5 Logistic Regression

5.1 Logistic Regression Basics

- Used for classification problems
- Logistic Regression (1D)**
 - Logistic Function: $\sigma(z) = \frac{1}{1 + e^{-z}}$, where $z = wx$
 - Output of $\sigma(z)$ aka. $h_w(x)$ is in $[0, 1]$ and treated as a probability → If $\sigma(z) > \alpha$, then label as 1
- Logistic Regression (2D):** Decision boundary is a line of intersection between prediction boundary plane and plane containing all the prediction points → Decision boundary is perpendicular to w

5.2 Measuring Fit

- Why MSE is bad for Logistic Regression:** J_{MSE} for logistic regression would not work well as it is non-linear → non-convex → multiple local minima
- Cross Entropy for C classes:** $CE(y, \hat{y}) = -\sum_{i=1}^C y_i \log(\hat{y}_i)$ (Measures the average number of bits required to identify an event from 1 probability distribution → measures the difference between discovered probability distribution of a classification model & predicted values)
- Binary Cross Entropy for 2 classes:** $BCE(y, \hat{y}) = -\log(\hat{y}) - (1 - y) \log(1 - \hat{y})$
 - Given $y = 1$ & value of \hat{y} is high, model will be rewarded for making a correct prediction
 - Given $y = 1$ & value of \hat{y} is low, model will be penalized for making a wrong prediction
- BCE Loss Function:** $J_{BCE}(w) = \frac{1}{m} \sum_{i=1}^m BCE(y^{(i)}, h_w(x^{(i)}))$, which is convex for logistic regression → Can find global minimum during gradient descent

5.3 Gradient Descent

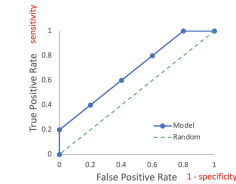
- Partial Derivative:**
$$\frac{\partial J_{BCE}(w)}{\partial w_0} = \frac{1}{m} \sum_{i=1}^m (h_w(x^{(i)}) - y^{(i)})$$
$$\frac{\partial J_{BCE}(w)}{\partial w_1} = \frac{1}{m} \sum_{i=1}^m (h_w(x^{(i)}) - y^{(i)}) x_1^{(i)}$$

5.4 Multi-Class Classification

- Split the multi-class dataset into multiple binary classification problems → Binary classifier is then trained on each binary classification problem & predictions are made using the model that is the most confident
- One VS All:** Fit 1 classifier per class, fit against all other classes → Pick the highest probability (Eg. 3 classes of cat, dog, rabbit → Classifier of cat against all other classes gives the highest probability → Predict as cat)
- One VS One:** Fit 1 classifier per class pair → Pick the most wins (Eg. Cat wins Dog, Rabbit wins Cat, Rabbit wins Dog → Predict as Rabbit)

5.5 Performance Measure

- True Positive Rate & False Positive Rate:** $TPR = \frac{TP}{TP+FN}$, $FPR = \frac{FP}{FP+TN}$
- Receiver Operator Characteristics (ROC) Curve:**
 - Graphical plot that illustrates performance of a binary classifier
 - Different data plots are for different α threshold values
 - If ROC curve is above diagonal random line → Model is more accurate than random chance
 - Area under curve (AUC) of ROC: AUC > 0.5 means model is better than chance, AUC ≈ 1 means model is very accurate, AUC = 0 means model is predicting opposite class for each data



5.6 Model Evaluation & Selection, Hyper-parameter Tuning

- Model Selection (based on error function):**
 - Train each model h_i on training set D_{train}
 - Run the models on validation set D_{val} → Choose model with MINIMUM $J_{D_{val}}$
 - Test that model on a test set D_{test} & assess the model by computing $J_{D_{test}}$

Model Evaluation: When comparing a logistic regression model's output with target label, use Accuracy or AUC-ROC, but not loss functions such as MSE, MAE, BCE

Bias: Error introduced by approximating a real-world problem (which may be very complex) with a simplified model → High bias is associated with Under-fitting & perform poorly on both training and test data, Bias does not improve with an increased number of data points

Variance: Error introduced by the model's sensitivity to small fluctuations in the training data → High variance is associated with Over-fitting & Perform well on the training data but poorly on test data. Obtaining more data points is likely to decrease variance

Hyperparameter Tuning: To find the best model by looping through:

- Pick hyperparameters (Eg. Learning rate of gradient descent, max depth of decision tree, min sample of decision tree, loss function of regression model)
- Train model with hyperparameters
- Evaluate model

6 Support Vector Machine

6.1 Regularisation

- Methods to address overfitting**
 - Reduce number of features from high degree to low degree polynomial
 - Regularisation: Keep all features but reduce magnitude of w_j → Done by adding the weights to cost function, but since we do not know which w_j to penalise, we penalise all w_j instead

- Linear Regression with Regularisation**
 - Cost Function:** $J(w) = \frac{1}{2m} \sum_{i=1}^m (h_w(x^{(i)}) - y^{(i)})^2 + \frac{\lambda}{2m} \sum_{j=1}^n w_j^2$
 - Gradient Descent:** $w_j \leftarrow w_j - \gamma \frac{1}{m} \sum_{i=1}^m (h_w(x^{(i)}) - y^{(i)}) x_j^{(i)} - \gamma \frac{\lambda}{m} w_j$

- When $\lambda = 0$, there is no regularisation, overfitting occurs
- When $\lambda = \text{high value}$, there is too much regularisation, under fitting occurs (line equation reduces to just w_0)

- Linear Regression with Regularisation (Normal Equation)**

$$J(w) = \frac{1}{2m} \sum_{i=1}^m (h_w(x^{(i)}) - y^{(i)})^2 + \frac{\lambda}{2m} \sum_{j=1}^n w_j^2$$

A few steps of math

$$w = (X^T X + \lambda I)^{-1} X^T Y$$

This works even if $X^T X$ is non-invertible if $\lambda > 0$

- Modify the regularisation matrix such that the 1st element (corresponding to bias term) is 0 instead of 1 → 1st row and column correspond to bias term w_0 and are set to 0 to not penalise the bias term

- Logistic Regression with Regularisation**
 - Cost Function:** $J(w) = -\frac{1}{m} \sum_{i=1}^m [y^{(i)} \log h_w(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_w(x^{(i)}))] + \frac{\lambda}{2m} \sum_{j=1}^n w_j^2$
 - Gradient Descent:** $w_j \leftarrow w_j - \gamma \frac{1}{m} \sum_{i=1}^m (h_w(x^{(i)}) - y^{(i)}) x_j^{(i)} - \gamma \frac{\lambda}{m} w_j$

6.2 Support Vector Machine

Background: We want to maximise the margin between all positive & negative points

Procedure (Hard Margin SVM):

- Define decision rule (what is positive point, what is negative point): $\bar{w} \cdot \bar{x} + b \geq 0$ then positive

2. Equation of margin: $margin = \frac{2}{\|w\|}$

3. Constrained Optimization Problem:

$$\min \frac{1}{2} \|w\|^2 \quad \text{s.t.} \quad y^{(i)} (w \cdot x^{(i)} + b) - 1 \geq 0$$

or $\max \alpha \geq 0 \sum_i \alpha^{(i)} - \sum_i \sum_j \alpha^{(i)} \alpha^{(j)} y^{(i)} y^{(j)} (x^{(i)} \cdot x^{(j)})$

4. Parameterization of decision boundary: Form system of equations using constraints and equation for the weights ($\sum_{i=1}^n \alpha^{(i)} y^{(i)} = 0$ and $w = \sum_{i=1}^n \alpha^{(i)} y^{(i)} x^{(i)}$) → Obtain values of $\alpha^{(i)}$ with GUE

Objective (Lagrange function):

$$L(w, b, \alpha) = \frac{1}{2} \|w\|^2 - \sum_i \alpha^{(i)} [y^{(i)} (w \cdot x^{(i)} + b) - 1], \quad \forall_i \alpha^{(i)} \geq 0$$

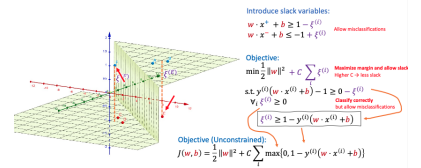
$$\frac{\partial L(w, b, \alpha)}{\partial w} = w - \sum_i \alpha^{(i)} y^{(i)} x^{(i)} = 0 \Rightarrow w = \sum_i \alpha^{(i)} y^{(i)} x^{(i)}$$

$$\frac{\partial L(w, b, \alpha)}{\partial b} = -\sum_i \alpha^{(i)} y^{(i)} = 0$$

More math: plug solution w into Lagrange function to obtain "dual" objective

$$L(\alpha) = \sum_i \alpha^{(i)} - \frac{1}{2} \sum_i \sum_j \alpha^{(i)} \alpha^{(j)} y^{(i)} y^{(j)} (x^{(i)} \cdot x^{(j)})$$

- Soft Margin SVM**



- Soft margin SVM is used when data is not linearly separable (allows for some misclassification of training data)
- Slack variable is introduced to handle instances where data points are either on wrong side of margin or even misclassified

 - $\xi_i = 0$ means data point lies either on or outside margin & is correctly classified
 - $0 < \xi_i \leq 1$ means data point is within margin, but still correctly classified
 - $\xi_i > 1$ means data point is on wrong side of decision boundary (misclassified)

- C is regularisation parameter that controls the trade-off between maximising the margin and minimising classification errors → Larger C gives more importance to minimising slack variables (fewer misclassifications are allowed), while smaller C allows for more margin violations

- Kernel Methods & Kernel Tricks**
 - Used when data is truly not linearly separable
 - Use a kernel to transform data into higher dimensional space for non-linearly separable data

7 Introduction to Neural Networks

7.1 Perceptron

- Formula:** $\hat{y} = h_w(x) = g(\sum_{i=1}^n w_i x_i)$, where g is the activation function & g is normally the sign function ($g(z) = +1 \text{ if } z \geq 0, \text{ else } -1$) for perceptrons
- Perceptron Learning Algorithm:**
 - Initialise $\forall_i w_i$ (set random initial weights)
 - Loop (until convergence aka, no misclassification or max steps reached)
 - For each instance $(x^{(i)}, y^{(i)})$, classify $\hat{y}^{(i)} = h_w(x^{(i)})$
 - Select 1 misclassified instance $(x^{(j)}, y^{(j)})$
 - Update weights: $w \leftarrow w + \gamma(y^{(j)} - \hat{y}^{(j)})x^{(j)}$ (remember to add bias term for x)

7.2 Neural Networks

- Single Layer Neural Network**
 - Same like perceptron, except g is normally non-linear (Eg. σ , tanh, ReLU, Leaky ReLU)
 - NOT, AND, OR, NOR functions can be modelled by single layer, but XOR, XNOR require multi-layer (data is not linearly separable)

- Matrix multiplication in Neural Network:** $\hat{y} = g(W^T x)$ in a single layer, where $\#$ of rows in $W = \#$ of inputs per perceptron, $\#$ of columns in $W = \#$ of perceptrons in layer
- Forward Propagation across multi-layer:** Basically repeated matrix multiplication from right to left

- Regression & Classification**
 - Activation function of perceptron(s) in final layer determines if we are doing regression (linear/no activation), binary classification (sigmoid) or multi-class classification (softmax)
 - Softmax activation:** $g(z) = \frac{e^{z_j}}{\sum_{j=1}^C e^{z_j}}$, where sum of outputs of all the final layer perceptrons is 1

7.3 Gradient Descent with Neural Network

- Derivative of Sigmoid function:** $\sigma(x) = \frac{1}{1 + e^{-x}}$, $\sigma'(x) = \sigma(x)(1 - \sigma(x))$
- Gradient Descent on Single Layer Neural Network:** Given $a = \sum_{i=0}^n w_i x_i$, $\hat{y} = \sigma(a)$, $L = \frac{1}{2} (\hat{y} - y)^2$ (MSE), Weight update is $w_i \leftarrow w_i - \gamma \frac{dL}{dw_i} = w_i - \gamma \frac{dL}{da} \frac{da}{dw_i}$
- $w_i \leftarrow w_i - \gamma (\hat{y} - y) \hat{y} (1 - \hat{y}) x_i$ (Derived with chain rule)

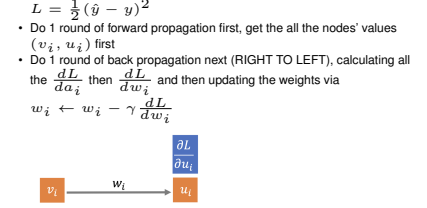
7.4 Neural Network VS Other models

- Logistic Regression:** Has Linear, Non-robust decision boundary (prone to misclassification since decision boundary can be too close to data points)
- Logistic Regression with Feature Mapping:** Has Non-linear, Non-robust decision boundary (prone to misclassification since decision boundary can be too close to data points)
- Support Vector Machine:** Has Non-linear, Robust decision boundary (decision boundary is guaranteed to be far from data points)
- Neural Networks:** Has Non-linear, non-robust decision boundary (prone to misclassification since decision boundary can be too close to data points)

7.5 Back Propagation

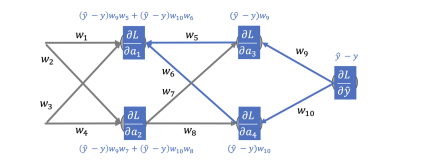
- Chain Rule Background:**

- 1 intermediate variable:** Given $a = f(x)$, $z = g(a)$, then $\frac{dz}{dx} = \frac{dz}{da} \frac{da}{dx}$
- 2 intermediate variables:** Given $a = f(x)$, $b = g(x)$, $z = h(a, b)$, then $\frac{dz}{dx} = \frac{dz}{da} \frac{da}{dx} + \frac{dz}{db} \frac{db}{dx}$
- Back Propagation with Linear Activation:**
 - Given linear activation $g(x) = x$ and loss function $L = \frac{1}{2} (\hat{y} - y)^2$
 - Do 1 round of forward propagation first, get the all the nodes' values (v_i, u_i) first
 - Do 1 round of back propagation next (RIGHT TO LEFT), calculating all the $\frac{dL}{da_i}$ then $\frac{dL}{dw_i}$, and then updating the weights via $w_i \leftarrow w_i - \gamma \frac{dL}{dw_i}$

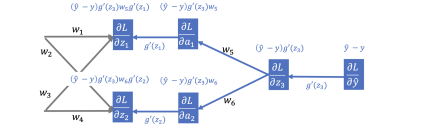


$$\frac{\partial L}{\partial w_i} = \frac{\partial L}{\partial u_i} v_i$$

$$\frac{dL}{dw_i} = \frac{dL}{du_i} \frac{du_i}{dw_i} = \frac{dL}{du_i} v_i$$



- Back Propagation with Non-linear Activation:**
 - Given non-linear activation $g(x)$ and loss function $L = \frac{1}{2} (\hat{y} - y)^2$
 - Same as linear activation, except need to account for $g'(z_i)$



8 Convolution Neural Network

8.1 Purpose

- Automatically & efficiently learn features from data while maintaining spatial relationships between pixels
- Does not make sense to have $800 \times 800 \times 100 = 64$ million weights for a neural network with 100 neurons for a 800×800 input pixel image → Use CNN instead

8.2 Convolution:2D

- Given image input X and kernel W → Multiply sliding input window with kernel then sum → Output a feature map
- If we want to detect 1 more feature, we use another kernel and form another feature map

8.3 Convolution Tricks

- Add Padding:** Add padding of 0s to image input → Resulting feature map can be same size as original image input → Without padding, size of feature maps would shrink with each layer, which could lead to loss of important information, especially near the edges of the image
- Add Strides:** Increase stride length, so that we slide the input window multiple pixels over a single step → Reduces the size of feature maps (manage computational costs) → Larger stride focuses on more global patterns rather than small, localized details (reduces risk of overfitting)
- Formula to get dimension of feature map:** Output Dimension = $[(\text{Input Dimension} - \text{Kernel Dimension} + 2 \times \text{Padding}) / \text{Stride}] + 1$
- Pooling layer:** Down-samples feature maps via Max pool, Average pool, Sum pool
- Receptive Field:** Area of the input that contributes the output of a neuron in a convolutional layer (gives us an idea of where we are getting our results from as data flows through the layers of the network) → Larger receptive field enables network to capture more global features

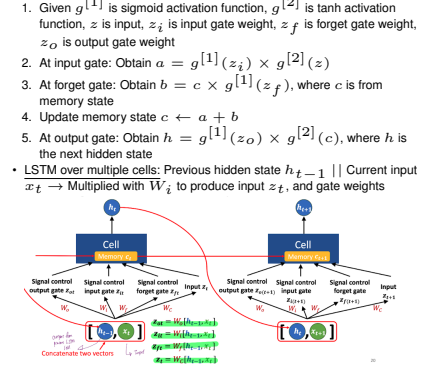
 - Let $r_0 = 1, j_0 = 1$
 - $r_i = r_{i-1} + 1 + (\text{kernel} - 1) \times j_{i-1}$
 - $j_i = j_{i-1} \times \text{stride}_i$

9 Neural Network on Sequential Data

9.1 Recurrent Neural Network (RNN)

- Sequential Data:** Data where order of elements is essential for capturing patterns & relationships → Each data element depends on previous elements in the sequence (Eg. text, audio, video)
- One-hot Encoding:** Transforms each element in the sequence into unique binary vector, where only position representing element is set to 1 & all other positions set to 0
- RNN:**
 - x_i are inputs, h_i are hidden states, \hat{y}_i are outputs, h_0 is set to 0

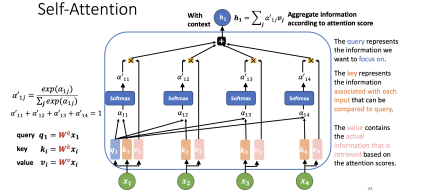
- $h_t = g[h] \left(\left(W[xh] \right)^T x_t + \left(W[h] \right)^T h_{t-1} \right)$
- $\hat{y}_t = g[y] \left(\left(W[yh] \right)^T h_t \right)$
- Deep RNN:** RNN with multiple layers
- Bidirectional RNN:** 2 unidirectional RNN layers chained together in opposite directions & acting on same input → Concatenate together corresponding outputs of 2 underlying unidirectional RNN layers
- Long Short Term Memory (LSTM)**
 - Specialised RNN designed to overcome limitations of traditional RNNs, especially their inability to capture long-range dependencies effectively
 - Key Components of LSTM:** (1): Cell State (memory pipeline that runs through entire LSTM), (2): Forget Gate (decides what information from cell state should be discarded), (3): Input Gate (determines what new info should be added to cell state), (4): Output Gate (decides what next hidden state should be)
 - Procedure in LSTM cell:**
 - Given $g^{[1]}$ is sigmoid activation function, $g^{[2]}$ is tanh activation function, z is input, z_i is input gate weight, z_f is forget gate weight, z_o is output gate weight
 - At input gate: Obtain $a = g^{[1]}(z_i) \times g^{[2]}(z)$
 - At forget gate: Obtain $b = c \times g^{[1]}(z_f)$, where c is from memory state
 - Update memory state $c \leftarrow a + b$
 - At output gate: Obtain $h = g^{[1]}(z_o) \times g^{[2]}(c)$, where h is the next hidden state
 - LSTM over multiple cells:** Previous hidden state $h_{t-1} ||$ Current input x_t → Multiplied with W_i to produce input z_t , and gate weights



- Types of RNN:** (1): One-to-many (Image captioning), (2): Many-to-one (Sentiment analysis), (3): Many-to-many (Video classification with a label for each frame), (4): Encoder-decoder (Language Translation)

9.2 Self-attention

- Motivation:** Unlike RNN which needs to wait for previous time steps, Self-attention model can capture context information without waiting for previous time steps
- Procedure:** To calculate h_i



- Multiply q_i ($i=1$ in this case) with all k_j → Obtain α_{ij}
- Apply soft-max function to all α_{ij} and multiply resulting α_{ij} with v_j
- Sum up all α_{ij} to obtain h_i
- Repeat 1-3 to obtain other h_i values

9.3 Issues with Deep Learning

- Overfitting:** Addressed by dropout (randomly set some activations to 0 during neural network training, not the weights), early stopping (so that $J_{val}(w)$ does not increase)
- Vanishing/Exploding Gradient:** Vanishing (small gradients multiplied again and again until it reaches almost 0), Exploding (Large gradients multiplied again and again until it overflows) → Addressed by non-saturating activation functions (ReLU) or Gradient Clipping (clip gradient within $[\min, \max]$)

10 Unsupervised Learning

10.1 Supervised Learning VS Unsupervised Learning

- Supervised Learning:** Given a set of m input-output pairs (training samples), learn to make a prediction
- Unsupervised Learning:** Learning happens by experiencing data → Given a set of m data points, learn patterns in data

10.2 K-means Clustering

- Centroid:** Let points $x^{(i)}$ for $i = 1, \dots, m_1$ be assigned to cluster 1 → For these points, Cluster Centroid is $\mu_1 = \frac{1}{m_1} \sum_{i=1}^m 1 x^{(i)}$ ($\mu_1, x^{(i)}$ are vectors)
- K-means Algorithm (m data points, K centroids):**
 - Randomly initialise K centroids μ_1, \dots, μ_K
 - Repeat until convergence:

- For $i = 1, \dots, m$: $c^{(i)} \leftarrow$ Index of cluster centroid (μ_1, \dots, μ_K) closest to $x^{(i)}$ (Assign data points to centroid)
- For $k = 1, \dots, K$: $\mu_k \leftarrow$ Centroid of data points $x^{(i)}$ assigned to cluster k (Reposition centroid based on data points)
- No more changes in centroid positions → Converged (Can be shown that each step in algorithm never increases loss function)
- Local Optima:** Possible for K-means to reach a local optimum where centroids do not move anymore, but loss might be high
- K-means Loss Function:** Average distance of each sample to its centroid
- K-medoids:** Pick K initial centroids randomly from points in data → Pick data points that is closest to centroids & use them as centroids
- Notes about K-means:**
 - Centroids are usually not located at 1 of the data points
 - K parameter is chosen by the user
 - Multiple restarts of the K-means give different solutions

10.3 Hierarchical Clustering

- Purpose:** In a situation where we cannot decide on a fixed number of clusters, we want a hierarchy of clusters

- Algorithm:**
 - Every data point is in a cluster
 - Loop (until all points are in 1 cluster): Find a pair of cluster that "is nearest", merge them together (NOTE: We have $N' = 2^n$ data points → Hierarchical Clustering algorithm produces a sequence of clusterings → Number of clusters in sequence is $N, N - 1, \dots, 1$ (Basically merge 2 clusters at 1 single time only))
- Variaints (Pick the minimum)**
 - Single Linkage:** Distance between closest elements in 2 clusters
 - Complete Linkage:** Distance between furthest elements in 2 clusters
 - Average Linkage:** Average of distances of all pairs in 2 clusters
 - Centroid Method:** Distance between centroids of 2 clusters
- Analysis:** It doesn't require # of clusters to be pre-defined, handles noise well, works well with non-linearly separable data, can be computationally expensive for large data sets ($O(n^3)$ to merge every cluster, where $O(n^2)$ to calculate distance for every pair & $O(n)$ to find nearest pair)

10.4 Dimensionality Reduction

- Overview:** Many ML problems have data with high dimensional features → Number of samples to learn a hypothesis class increases exponentially with the number of features

- Reduction:** Change basis of vector remove dependence between components, Remove non-important components that do not cause variations in data
 - Reconstruction:** Add non-important components back, Restore basis
- Singular Value Decomposition (SVD):** Take without loss of generality $n > m$, for any $n \times m$ rectangular real-valued matrix X , there exists a factorisation $X = U \Sigma V^T$

$$X = \begin{bmatrix} x_1 & x_2 & \dots & x_m \end{bmatrix} = U \Sigma V^T = \begin{bmatrix} u_1 & u_2 & \dots & u_m \end{bmatrix} \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_m \end{bmatrix} \begin{bmatrix} v_1^T & v_2^T & \dots & v_m^T \end{bmatrix}$$

Combination of basis u_i to form x_i

- U is $n \times m$ and has m orthonormal columns
 - Σ is $m \times m$, diagonal with $\sigma_j \geq 0$ ordered from largest to smallest
 - V is $m \times m$ and has m orthonormal columns and rows
- Dimensionality Reduction via SVD:** Instead of m singular values, we set all singular values except the first r to 0 → Resulting matrix is the "best" approximation with new basis size of r to the original matrix
 - Transforms from $n \times m = n \times m, m \times m, m \times m$ to $n \times m = n \times r, r \times r, r \times m$, where $r < m$

$$X = \begin{bmatrix} x_1 & x_2 & \dots & x_m \end{bmatrix} = U \Sigma V^T = \begin{bmatrix} u_1 & u_2 & \dots & u_m \end{bmatrix} \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_m \end{bmatrix} \begin{bmatrix} v_1^T & v_2^T & \dots & v_m^T \end{bmatrix}$$

"Measures" of "face templates" to make each individual face

- Reduction & Reconstruction via SVD:**
 - Data Matrix ($n \times m$): $X = U \Sigma V^T \approx \tilde{U} \tilde{\Sigma} \tilde{V}^T$
 - Reduced Data ($r \times m$): $Z = \tilde{U}^T X$
 - Reconstructed Data ($n \times m$): $\tilde{X} = \tilde{U} Z$
- r-SVD:** defines an encoder-decoder structure for reduction and reconstruction of high-dimensional data
- Principal Component Analysis (PCA):** Captures components that max the statistical variations of the data
 - Given the data matrix $X = (x^{(1)}, \dots, x^{(m)})$, where $x^{(i)}$ is the i^{th} row of X
 - Compute mean over samples: $\bar{x} = \frac{1}{m} \sum_{i=1}^m x^{(i)}$
 - Compute mean-centred data: $\hat{x}^{(i)} = x^{(i)} - \bar{x}$
 - Define data matrix $\tilde{X} = (\hat{x}^{(1)}, \dots, \hat{x}^{(m)})$
 - Create covariance matrix of data: $Cov(X) = \frac{1}{m} \tilde{X} \tilde{X}^T$
 - Compute SVD on $Cov(X)$ to obtain the U matrix
 - Reduce to r components to obtain \tilde{U} (choose minimum r s.t. $\frac{\sum_{i=1}^r \sigma_i^2}{\sum_{i=1}^m \sigma_i^2} \geq 0.99$, where $\geq 99\%$ of variance in data is retained)

