CS2109S

AY22/23 Sem 2

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01. Introduction

- Agent Anything that can perceive its environment through sensors and acting upon that env. through actuators
- Agent Function Maps from percept histories to actions
- Rational Agent Chooses an action that is expected to maximize its performance measure, given by percept sequence and built-in knowledge
- Autonomous Agent If behavior is determined by its own expereince

Performance Measure of Function

Motivation: For an agent to do the right thing, need a measure of goodness

Defining the Problem: PEAS

- 1. Performance measure
- 2. Environment
- 3. Actuators
- 4. Sensors

Characterizing the Environment

- 1. Fully observable (vs. Partially) Agent's sensors can access complete state of env. all the time
- Deterministic (vs. Stochastic) Next state of env. is determined by current state and action executed by agent
 - Strategic If env. is deterministic except for actions of other agents
- 3. Episodic (vs. Sequential) Agent's experience is divided into atomic episodes, where each episode includes perceiving and an action, and action depends on episode itself
- 4. Static (vs. Dynamic) Env. is unchanged while agent is deciding
- Semi Time does not affect env., but affects performance score
- 5. Discrete (vs. Continuous) Discrete num. of percepts and actions
- 6. Single Agent (vs. Multi-agent) Agent operating by itself in an env.

Implementing Agents (in ascending complexity)

- 1. Simple Reflex Agents Fixed conditional rules
- 2. Model-based Reflex Agents Stores percept history to make decisions about internal model of world with conditional rules. Eg. Roomba
- 3. Goal-based Agents Keep in mind a goal and action aims to achieve it
- 4. Utility-based Agents Find best way to achieve goal
- 5. Learning Agents Learn from previous experiences

Exploitation vs. Exploration

- Exploitation Maximize expected utility using current knowledge of world
- Exploration Learn more about the world to improve future gains. May not always maximize performance measure.

02. Uninformed Search

- Deterministic, fully observable
- Tree Search Can revisit nodes
- Graph Search Tracks visited (Tree Search + Memoization)
- Uninformed Search Uses only information available in problem definition $| \bullet |$ Space: O(bd)

Formulating the Problem

- 1. How to represent state in problem?
- 2. Initial state
- 3. Actions: Successor function
- 4. Goal test
- 5. Path cost
- Abstraction Function Maps abstracted representation to real world state
- Representation Invariant $I(c) = \text{True} \rightarrow \exists a \text{ s.t. } AF(c) = a$

Breadth-first Search

- Idea: Expand shallowest unexpanded node using queue
- Given: b: Branching factor and d: Depth of optimal solution
- Complete: Yes (if tree is finite)
- Time: $O(b^{d+1})$
- Space: $O(b^d)$
- Optimal: Yes (if cost = 1)
- BFS is Uniform-cost Search with same cost

Uniform-cost Search

- Idea: Expand least-cost unexpanded node using priority queue (Dijkstra's)
- Given: C*: Cost of optimal solution
- Complete: Yes (if step cost $\geq \epsilon$ where $\epsilon \geq 0$)
- Time: $O(b^{(C^*/\epsilon)})$ (C^*/ϵ is approx. number of layers)
- Space: $O(b^{(C^*/\epsilon)})$
- Optimal: Yes

Depth-first Search

- Idea: Expand deepest unexpanded node using stack
- Given: m: Maximum depth of tree
- Complete: No (fails with infinite depth or loops)
- Time: $O(b^m)$
- Space: O(bm) (better than BFS)
- Optimal: No

Depth-limited Search

- Motivation: How to handle infinite depth for DFS?
- Idea: DFS with depth limit I where nodes at depth I have no children
- Time: $b^0 + b^1 + ... + b^{(d-1)} + b^d = O(b^d)$

Iterative Deepening Search

- Motivation: How to determine depth limit? We don't.
- Idea: Try different depths for depth-limited search
- BFS pretending to be DFS to save space
- Complete: Yes
- Time: $(d+1)b^0 + db^1 + ... + b^d = O(b^d)$ (More overhead than DLS)

Summary

	BFS	Uniform Cost	DFS	DLS	IDS
Complete	Yes	Yes	No	No	Yes
Time	$O(b^d)$	$O(b^{C^*/\epsilon})$	$O(b^m)$	$O(b^l)$	$O(b^d)$
Space	$O(b^d)$	$O(b^{C^*/\epsilon})$	O(bm)	O(bl)	O(bd)
Optimal	Yes	Yes	No	No	No

Bidirectional Search

- Idea: Search both forwards from initial state and backwards from goal state. Stop when searches meet.
- Time: $O(2b^{d/2})$
- Operators must be reversible
- Can have many goal states
- How to check if node intersects with other half?

03. Informed Search

Heuristic

- Heuristic Estimated cost from n to goal
- Admissible h(n) is admissible if, for every node n, $h(n) < h^*(n)$ where h^* is the true cost
- if h is admissible, then A* using tree search is optimal
- Consistent h(n) is consistent if, for every node n and every successor n'of n generated by action a, $h(n) \le c(n, a, n') + h(n')$
- Triangle inequality
- If h is consistent, f(n) is non-decreasing along any path (f(n') > f(n))
- If h is consistent, then h is admissible
- if h is admissible, then A* using graph search is optimal

Dominance

- If $h_2(n) \geq h_1(n)$ for all n, then h_2 dominates h_1
- If h_2 dominates h_1 and both are admissible, then h_2 is better for search

How to invent admissible heuristic?

- Set fewer restrictions on actions
- E.g. Number of misplaced tiles, Total manhattan distance

Best-first Search

- Idea: Expand most desirable node using priority queue
- Evaluation Function: f(n) = h(n)
- Complete: No. Possible to be stuck in loop
- Time and space: $O(b^m)$
- Optimal: No

A* Search

- Idea: Take note of cost so far and heuristic
- Evaluation Function: f(n) = g(n) + h(n) where g(n) is cost to reach n
- Complete: Yes, unless non-increasing, since cost is factored in
- Time and space: Same as BFS
- Optimal: Yes, depending on the heuristic

Iterative Deepening A* Search (IDA*)

- Motivation: How can we save space?
- ullet Idea: Have a cutoff for f and remember the best f that exceeds cutoff
- Similar to IDS. Linear space complexity.
- Optimal and complete

Simplified Memory A* Search (SMA*)

- Motivation: How can we save space?
- Idea: Do normal A*. If memory is full, drop node with worst f.
- Lose completeness

Local Search

- Motivation: What if the goal state is the solution? The path is irrelevant.
- Idea: Keep single current state and try improving it
- Formulating the problem:
 - 1. Initial state
 - 2. Actions: Successor function
 - 3. Good heuristic
 - 4. Goal test

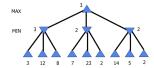
Hill-climbing

- Idea: Generate successors from current and pick the best using heuristic
- What if stuck into local minima?
- Introduce randomness
- Simulated Annealing Search Allow some bad moves and gradually decrease frequency
- Why only keep 1 best state?
- Beam Search Perform k hill-climbing searches in parallel
- How to generate successors?
- Genetic Algorithms Successsor is generated by combining 2 parent states

04. Adversarial Search

- Assumption: Opponents reacts rationally
- Formulating the problem:
- Initial state
- Successor function
- Terminal test
- Utility function: Measures how good the move is for a player

Minimax



- Idea: Choose move that yields highest minimax value using DFS
- Complete: Yes (if tree is finite)
- Time: $O(b^m)$
- Space: O(bm)
- Optimal: Yes (against an optimal opponent)

Alpha-Beta Pruning

- Motivation: How to save time for Minimax?
- Idea: By tracking max. and min. values so far, can prune some paths that we would never choose
 - 1. α contains max. and β contains min.
 - 2. Initially, $\alpha = -\infty$ and $\beta = \infty$
 - 3. When going down, copy α and β
 - 4. Prune if $\alpha \geq \beta$
 - 5. When going up, depending on MIN/MAX level, update α or β
- ullet With perfect ordering, time complexity: $O(b^{m/2})$. Doubles search depth.

Resource Limits

- ullet In reality, search space for games can be very large. α - β pruning also not fast enough.
- Solution: Limit depth (Only see a finite moves ahead) and determine best move using evaluation function to estimate desirability of position (Heuristic)
- Other hacks:
- **Transpoisitions** Memoize equivalent states
- Pre-computation of opening/closing moves

05. Introduction to Machine Learning

A machine learns if it improves performance P on task T based on experience E. Where T must be fixed, P must be measurable, E must exist

Types of Feedback

- Supervised Correct answer given for each example
- Regression Predict results within continuous output
- Classification Predict results in discrete output
- Unsupervised No answers given
- Weakly supervised Answer given, but not precise
- Reinforcement Occasional rewards given

Decision Trees

- DT can express any function of input attributes, if data is consistent
- Goal: Make DT compact. How?

Information Theory

- Idea: Choose attribute that splits examples into subsets that are ideally 'all positive' or 'all negative'
- Entropy Measure of randomness in set of data

$$I(P(v_1), ..., P(v_n)) = -\sum_{i=1}^{n} P(v_i) \log_2 P(v_i)$$

ullet For data with p positive examples and n negative examples:



$$I(\frac{p}{p+n}, \frac{n}{p+n}) =$$

$$-\frac{p}{p+n} \log_2 \frac{p}{p+n}$$

$$-\frac{n}{p+n} \log_2 \frac{n}{p+n}$$

- Information Gain (IG) Reduction in entropy from attribute test
- Goal: Choose attribute with largest information gain
- Intuition: IG = Entropy of this node Entropy of children nodes
- Given chosen attribute A with v distinct values:

$$\begin{aligned} \text{remainder}(A) &= \sum_{i=1}^v \frac{p_i + n_i}{p+n} I(\frac{p_i}{p_i + n_i}, \frac{n_i}{p_i + n_i}) \\ &IG(A) = I(\frac{p}{p+n}, \frac{n}{p+n}) - \text{remainder}(A) \end{aligned}$$

- Decision Tree Learning Recursively choose attributes with highest IG
- IG is not the only way. Can use whatever objective function that achieves the criteria we want.

Performance Measurement

- Correctness Correct if $\hat{y} = y$
- Accuracy $\frac{1}{m}\sum_{j=1}^{m}(\hat{y_j}=y_j)$
- Confusion Matrix:

		Actual Label		
		+ve	-ve	
Predicted Label	+ve	TP True Positive	FP False Positive	
	-ve	FN False Negative	TN True Negative	

- Accuracy = $\frac{TP+TN}{TP+FN+FP+TN}$
- **Precision** $\frac{TP}{TP+FP}$ How precise are positive predictions?
- Recall $\frac{TP}{TP+FN}$ How many actual positives are predicted?
- F1 Score $\frac{2}{1/P+1/R}$ Harmonic mean of precision and recall
- Type I Error: FP, Type II Error: FN
- FP Rate = $\frac{FP}{FP+TN}$ TP Rate = $\frac{TP}{TP+FN}$

Pruning

- Motivation: DT overfits to training set, but performs poorly on test set
- Occam's Razor: Simple hypothesis preferred
- Pruning Ignores outliers, which reduces overfitting
- \bullet Idea: Go with the majority of T/Fs
- E.g. Min-sample, Max-depth

06. Linear Regression

Notation

- ullet m= Number of training examples
- \bullet n =Number of features
- $x_i^{(i)} = \text{Input feature } j \text{ of } i \text{th training example}$
- y =Output variables

Hypothesis

$$h_w(x): w_0 + w_1 x$$

Cost Function (Square Error Function)

$$J(w_0, w_1) = \frac{1}{2m} \sum_{i=1}^{m} (h_w(x^{(i)}) - y^{(i)})^2$$

- Goal: Minimize cost function. Thus, hypothesis is close to training samples
- Why squared error? Convenience, since we need to differentiate later

Gradient Descent

- Start at some (w_0, w_1) . Pick nearby point that reduces $J(w_0, w_1)$.
- Algorithm: Repeat until convergence:

$$w_j := w_j - \alpha \frac{dJ(w_0, w_1, \dots)}{dw_j}$$

- All updates done at end
- How to do $\frac{dJ(w_0,w_1)}{dw_i}$? Partial derivative: Hold everything else constant
- $\frac{dJ(w_0, w_1)}{dw_i} = \frac{d}{dw_i} (\frac{1}{2m} \sum_{i=1}^m (w_0 + w_1 x^{(i)} y^{(i)})^2)$
- $\frac{dJ(w_0, w_1)}{dw_0} = \frac{1}{m} \sum_{i=1}^m (w_0 + w_1 x^{(i)} y^{(i)})$ (Note: Chain rule)
- $\bullet \frac{dJ(w_0, w_1)}{dw_i} = \frac{1}{m} \sum_{i=1}^m (w_0 + w_1 x^{(i)} y^{(i)}) x^{(i)}$
- Time complexity: O(kmn) where k is number of iterations

Learning Rate

- If α too small, then descent is too slow. If α too big, then might overshoot.
- Given constant α , descent will grow smaller as we approach minimum

Variants of Gradient Descent

- Batch gradient descent: Consider all training examples when updating
- Stochastic gradient descent: Consider 1 random data point at a time (Cheaper and more randomness)
- Mini-batch gradient descent

Using Matrices

• Given:
$$w = \begin{pmatrix} w_0 \\ \vdots \\ w_n \end{pmatrix}$$
 and $x = \begin{pmatrix} x_0 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} 1 \\ \vdots \\ x_n \end{pmatrix}$

 \bullet $h_w(x): w^T x$

Feature Scaling

- Motivation: Gradient descent does not work well if features have different
- Mean Normalization $x_i \leftarrow \frac{x_i \mu_i}{\sigma_i}$

Normal Equation

$$w = (X^T X)^{-1} X^T Y$$

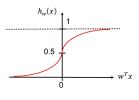
- ullet No need to choose lpha and feature scaling
- X^TX needs to be invertible
- Time complexity: $O(n^3)$. Slow if n is big

07. Logistic Regression

- Motivation: Classification with continuous input values.
- Idea: Come up with a decision boundary to seperate data points. $h_w(x_1, x_2) = 1$, if $w_0 + w_1x_1 + w_2x_2 > 0$, or 0, otherwise

Sigmoid Function

• Motivation: Step function is discontinuous and not differentiable



$$h_w(x) = g(w^T x)$$

$$g(z) = \frac{1}{1+e}$$

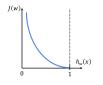
Hypothesis

$$h_w(x): \frac{1}{1+e^{-w^T x}}$$

• Interpretation: Estimated probability that y=1 given input x

Cost Function

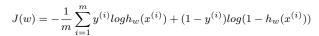
- Problem: Least square error gives non-convex cost function, which is bad for G.D.
- Solution: Use log



- If y = 1, let cost be $-log(h_w(x))$
- $h_w(x) \to 0, J(w) \to \infty$
- $h_w(x) \to 1, J(w) \to 0$



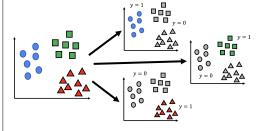
- If y = 0, let cost be -log(1 -
- $h_{av}(x) \rightarrow 0, J(w) \rightarrow 0$
- $h_w(x) \to 1, J(w) \to \infty$



Gradient Descent

- Same algorithm as linear regression
- ullet $rac{dJ(w)}{dw_i}=rac{1}{m}\sum_{i=1}^m(h_w(x^{(i)})-y^{(i)})x_n^{(i)}$ (Same as linear regression)

Multi-class Classification



- 1. Train binary classifier $h_w^{(i)}(x)$ for each class i to predict y=i
- 2. For each input x, pick class i is greatest (i.e. $\max_i h_w^{(i)}(x)$)

08. Model Evaluation and Selection

Linear Regression

$$J_{\mathsf{test}}(w) = \frac{1}{2m_{\mathsf{test}}} \sum_{i=1}^{m_{\mathsf{test}}} (h_w(x_{\mathsf{test}}^{(i)}) - y_{\mathsf{test}}^{(i)})^2$$

Logistic Regression

$$\operatorname{error}(h_w(x), y) = \begin{cases} 1 & \text{if misclassification} \\ 0 & \text{otherwise} \end{cases}$$

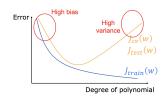
$$\text{Test Error} = \frac{1}{m_{\text{test}}} \sum_{i=1}^{m_{\text{test}}} \operatorname{error}(h_w(x_{\text{test}}^{(i)}), y_{\text{test}}^{(i)})$$

Model Selection

- How to choose model? (i.e. x^2 , x^3 , etc. for hypothesis)
 - 1. Split data into 3 sets: Training set, validation set, and test set
 - 2. Train each model using training set
 - 3. Compute $J_{cv}(w)$ for each model and pick model with lowest $J_{cv}(w)$
 - 4. Use $J_{\text{test}}(w)$ to estimate performance on unseen samples

Bias and Variance

- High bias Underfit, High variance Overfit
- As degree of polynomial increases:



Impact of m: High Bias

Impact of m: High Variance

 $J_{train}(w)$

• Observation: If overfit, more train-

- ing samples does not help • How do we address overfitting?
- Reduce number of features
- Regularization Keep all features, but reduce corresponding weights

09. Regularization

- Idea: Include w inside J(w) to minimize weights and get simpler hypothesis
- What if λ is too large? Weights tend to 0, resulting in straight line

 $J_{cv}(w)$

- How to choose λ ? Use validation set
- Small λ : $J_{\text{train}}(w)$ low and $J_{cv}(w)$ high (Overfit)
- Large λ : $J_{\text{train}}(w)$ high and $J_{cv}(w)$ high (Underfit)

Linear Regression with Regularization

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

$$w_n := w_n - \frac{\alpha}{m} \sum_{i=1}^m ((h_w(x^{(i)}) - y^{(i)}) x_n^{(i)}) - \frac{\alpha \lambda}{m} w_n$$

Logistic Regression with Regularization

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

$$w_n := w_n - \frac{\alpha}{m} \sum_{i=1}^m ((h_w(x^{(i)}) - y^{(i)}) x_n^{(i)}) - \frac{\alpha \lambda}{m} w_n$$

$$\boldsymbol{w} = (\boldsymbol{X}^T\boldsymbol{X} + \lambda \boldsymbol{I})^{-1}\boldsymbol{X}^T\boldsymbol{Y}$$
 where \boldsymbol{I} 's first column is 0

 $\bullet X^T X$ can be non-invertible

10. Support Vector Machine

• Idea: Maximize margin between positive and negative samples

Decision Rule

$$w \cdot x \ge c \to \mathsf{Positive}; w \cdot x < c \to \mathsf{Negative}$$

- Dot product: $u \cdot v = u^T v = p||v||$ (By law of cosine)
- \bullet Intuition: Decision boundary \bot Weight vector. $w\cdot x=p||w||.$ Sample a is on decision boundary if $w\cdot a=c$
- ullet Constraints: Let b=-c
- $w \cdot x + b > 1$ if y = 1
- $w \cdot x + b < -1$ if y = 0
- Combined: Let $\hat{y}^{(i)}=1$ or -1 for pos. and neg. samples respectively. $\hat{y}^{(i)}(w\cdot x^{(i)}+b)>1$
- If x is inside margin, then $w \cdot x + b = 1$ or -1 respectively
- Why add these constraints? Mathematical convenience for hinge loss

Margin

$$\mathsf{Margin}\;\mathsf{width} = \frac{2}{||w||}$$

- Let x^+ and x^- be closest positive and negative samples
- Margin width $=(x^+-x^-)\cdot \frac{w}{||w||}$ (i.e. Length of projection of x^+-x^- on weight vector) $=\frac{1-b+1+b}{||w||}$ (since x^+ and x^- are inside margin) $=\frac{2}{||w||}$

Objective Function for Hard-Margin

$$\min \frac{1}{2} ||w||^2$$
 s.t. $\hat{y}^{(i)}(w \cdot x + b \ge 1)$

- 1. Maximize margin: $\max \frac{2}{||w||} = \min ||w|| = \min \frac{1}{2} ||w||^2$
- 2. Classify correctly
- Hard-Margin No samples inside margin
- Before, we assume hard margin. What if there exists outliers that causes SVM to overfit?

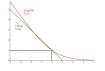
Objective Function for Soft-Margin

$$h_w(x) = \begin{cases} 1 & \text{if } w^T x \ge 0 \\ 0 & \text{otherwise} \end{cases}$$

- Slack Variable (ξ) Loss of misclassified point
- ullet Goal: Maximize margin and allow misclassification by tweaking C
- i.e. $\min(\frac{1}{2}||w||^2 + C\sum_i \xi^{(i)})$ s.t. $\forall i, \xi^{(i)} \geq 0$ and $\hat{y}^{(i)}(w \cdot x^+b) \geq 1 \xi^{(i)} \rightarrow J(w) = C\sum_i \max(0, 1 \hat{y}^{(i)}(w^Tx^{(i)})) + \frac{1}{2}\sum_{i=1}^n w_i^2$

• Hard-margin: Must follow constraint. Soft-margin: Constraint is flexible with slack variable, so can define cost function to minimize.

$$J(w) = C \sum_{i}^{m} y^{(i)} \mathsf{cost}_1(w^T x^{(i)}) + (1 - y^{(i)}) \mathsf{cost}_0(w^T x^{(i)}) + \frac{1}{2} \sum_{i=1}^{n} w_i^2$$



- Hinge Loss
- $\bullet \cot_1(z) = \max(0, 1 z)$
- $\bullet \cot_0(z) = \max(0, 1+z)$

Kernel

- Motivation: What if data is not linearly separable?
- Idea: Map features to higher dimensions (i.e. $\phi(x)$). High dim. is slow.
- Kernel Function Dot product between two points in transformed dim.

$$K(u, v) = \phi(u) \cdot \phi(v)$$

- Property: Getting K(u,v) does not need $\phi(u)$ and $\phi(v)$
- Linear Kernel $K(u, v) = u \cdot v$
- Polynomial Kernel $K(u, v) = (u \cdot v)^d$
- \bullet Gaussian Kernel $K(u,v)=e^{-||u-v||^2/2\sigma^2}$ (Note: $\phi(u)$ can map to infinite dimensions)

Kernel Trick

- By manipulating SVM objective func. and decision rule, $x^{(i)} \cdot x^{(j)}$ emerges
- If we map features (i.e. $\phi(x)$), can replace above term with kernel (K(u,v))
- Trick: No need to compute transformed features explicitly

Similarity Features

- Idea: Compute new features based on proximity to landmarks
- Given example x. $f_i = sim(x, l^{(i)}) = K(x, l^{(i)})$ where K is gaussian kernel
- Transformed x: $f = [f_0, f_1, \dots, f_m]^T$. Plug into obj. function.
- Do feature scaling, else similarity value may be dominated by some features
- \bullet Small σ leads to overfitting. Large σ leads to underfitting.
- Not all similarity functions get valid kernels. Need to satisfy Mercer's Thm.