

10-418/10-618 Machine Learning for Structured Data



Machine Learning Department School of Computer Science Carnegie Mellon University

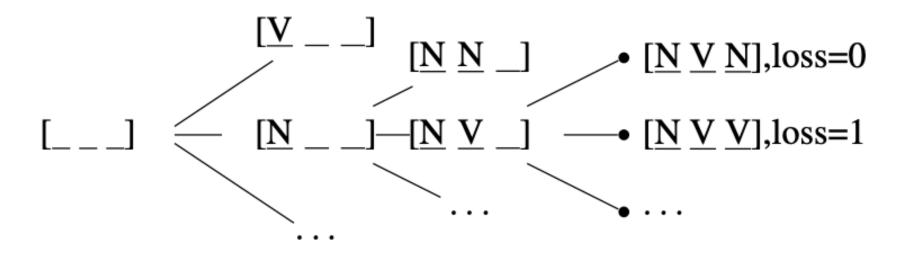
Learning to Search (Part III)

Matt Gormley Lecture 6 Sep. 18, 2022

STRUCTURED PREDICTION AS SEARCH

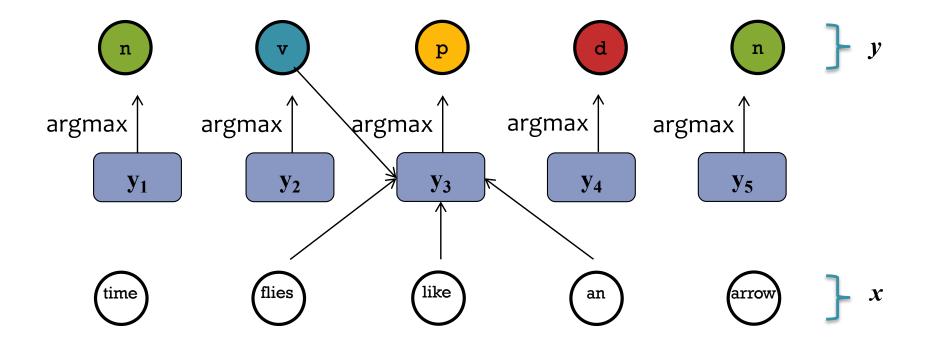
Structured Prediction as Search

- Key idea: convert your structured prediction problem to a search problem!
- **Example:** for POS tagging, each node in the search space corresponds to a partial tag sequence



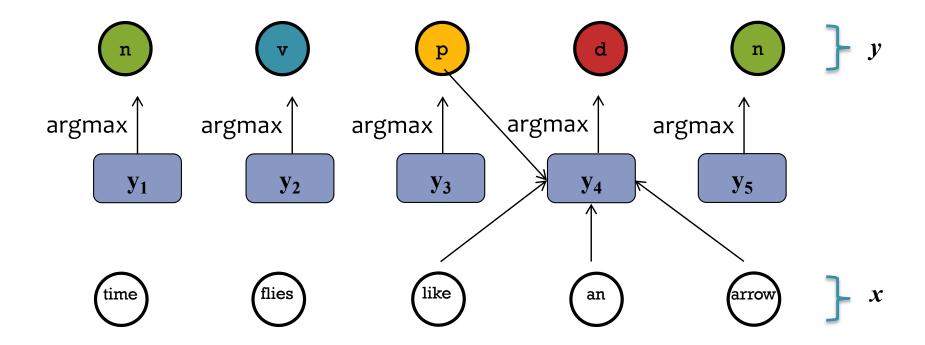
Basic Neural Network

- Suppose we wish to predict the tags greedily left to right
- Simple neural network looks at the previous word, the previous tag **prediction**, the current word, and the next word
- From these it builds a probability distribution over output tags
- Then it selects the argmax



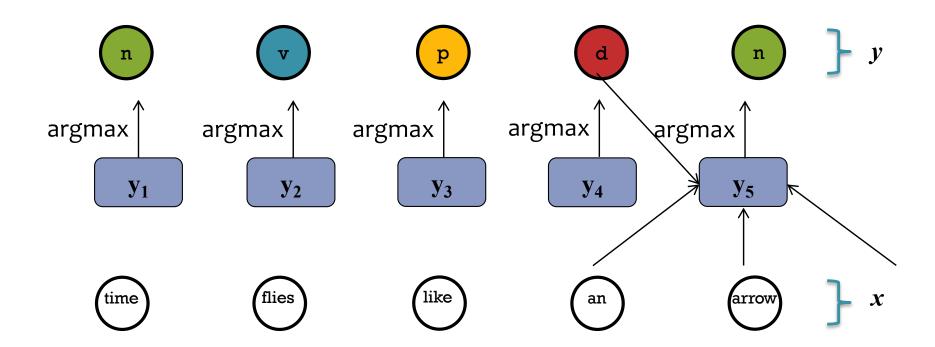
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 prediction, the current word, and the next word
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Learning to Search

Whiteboard:

- Problem Setting
- Ex: POS Tagging
- Other Solutions:
 - Completely Independent Predictions
 - Sharing Parameters / Multi-task Learning
 - Graphical Models
- Today's Solution: Structured Prediction to Search
 - Search spaces
 - Cost functions
 - Policies

EXPOSURE BIAS

The Exposure Bias Problem

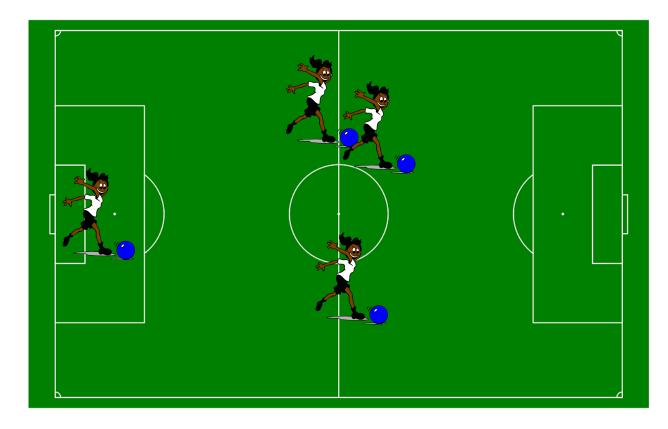
Imagine you join (for the first time ever) a intramural soccer team.

Position, 1st practice: midfielder

Position, 2nd practice: midfielder

Position, 3rd practice: midfielder

• **Position, 1st game**: goalie



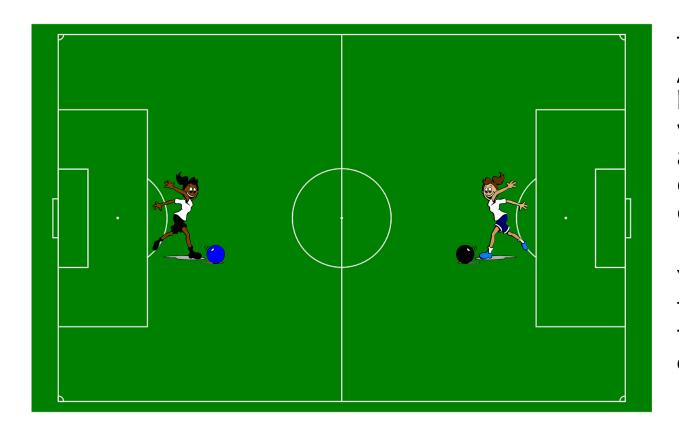
This could end badly! After all, you've never had any training on what to do as a goalie.

Your training is **biased** to the parts of the field that you were **exposed** to (midfield).

The Exposure Bias Problem

To really make this analogy work, we should adjust it slightly:

- 1st, 2nd, 3rd, practice: your coach assigns each of you to mimic the exact steps of a specific player in the 1986 world cup final; every practice each of you make the same maneuvers every time
- 1st game: you play a real team, that makes creative autonomous decisions, you are forced to be creative as well



This could end badly!
After all, you've never had any training on what to do when you are exposed to the outcomes of your own decisions!

Your training is **biased** to the 1986 behaviors to which you were **exposed**.

The Exposure Bias Problem

Consider two (related) explanations for why maximum likelihood training (aka. fully supervised imitation learning) is a poor choice for a seq2seq model.

Mismatched Test-Time Inference Algorithm

MLE training assumes that at test time we will do exact inference to find the highest probability output string (e.g. for an HMM, using the Viterbi algorithm)

However, in general, exact inference over the space of exponentially many output strings is intractable for a seq2seq model (e.g. unlike an HMM, seq2seq makes no Markov assumption)

beam search

Exposure Bias

At training time, MLE trains to generate the next token conditioned on the ground truth prefix sequence.

At test time, the model generates the next token conditioned on model's prefix sequence (obtained by greedy decoding or sampling).

So the model is exposed to only real prefixes at training time, and is therefore biased towards proper behavior only on those ground truth prefixes.

LEARNING TO SEARCH

Imitation Learning

Algorithm 1: Supervised Imitation Learning (for structured prediction)

```
def trainSupervised(\pi^*, E, x_{1:S}, y_{1:T}):
      initialize policy \pi_{\theta}
      for i in 1... N:
             for t in 1... T:
                   observe state s_t = (y_{1:t}, x_{1:S})
                    take action a_t = y_{t+1} = \pi^*(s_t)
                    \boldsymbol{\tau}^{(i)} = \boldsymbol{\tau}^{(i)} + [(s_t, a_t)]
             for (s_t, a_t) in \tau^{(i)}:
                   update policy \pi_{\theta} with
                   one step of SGD on
                   example (s_t, a_t)
      repeat for E epochs
```

return π_{Θ}

 $\begin{aligned} \textbf{def} \ \text{predict}(\pi_{\theta}) &: \\ \textbf{for t in 1... T:} \\ observe \ state \ s_{t} = (y_{1:t}, x_{1:S}) \\ take \ action \ a_{t} = \hat{y}_{t+1} = \pi_{\theta}(s_{t}) \\ incur \ loss \ \ell_{t} = loss(y_{1:t}, \hat{y}_{1:t}) \end{aligned}$

The state is the full input sequence and the partial output sequence, up to step t

The action is the next output token we predict at step t+1

This is equivalent to accumulating the gradient of the full computation graph for input X_{1/5}

Imitation Learning

Algorithm 2: DAgger for Imitation Learning (for structured prediction)

```
def trainDAgger(\pi^*, E, \beta = [\beta_1, ..., \beta_N], x_{1:S}, y_{1:T}):
       initialize policy \pi_{\Theta}
       for i in 1... N:
             \pi_i = \beta_i \pi^* + (1 - \beta_i) \pi_{\theta}
               for t in 1... T:
                      observe state s_t \neq (y_{1:t}, x_{1:S})
                      sample action \hat{a}_t = \hat{y}_{t+1} \sim \pi_i(s_t)
                      store action a_t = y_{t+1} = \pi^*(s_t)
                       \boldsymbol{\tau}^{(i)} = \boldsymbol{\tau}^{(i)} + [(s_t, a_t)]
              for (s_t, a_t) in \tau^{(i)}:
                      update policy \pi_{\theta} with
                      one step of SGD on
                      example (s_t, a_t)
```

Now the prediction for the next time step \hat{y}_{t+1} comes from the the model policy.+ oracle policy.

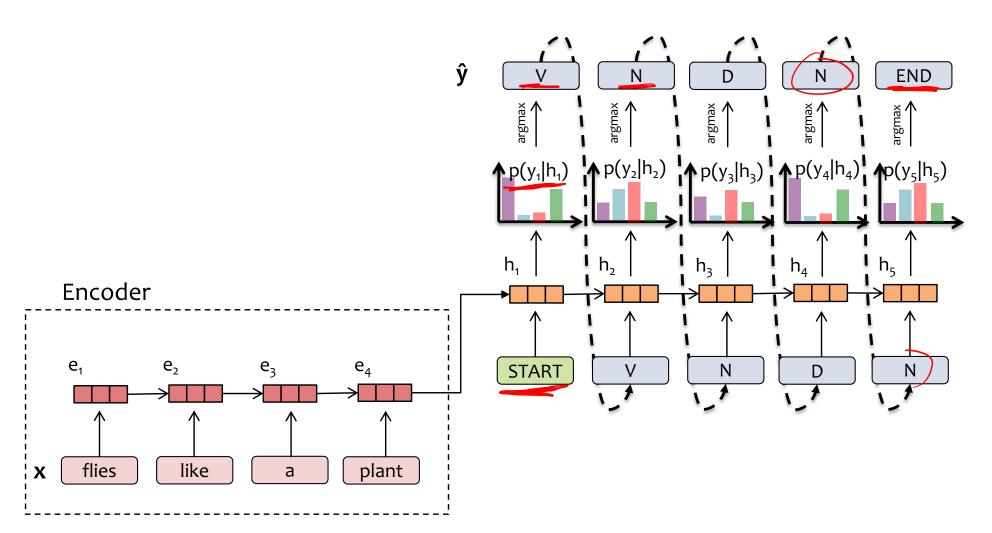
This will typically be fed back into the model.

We still train by updating on the expert policy's prediction of y_{t+1}

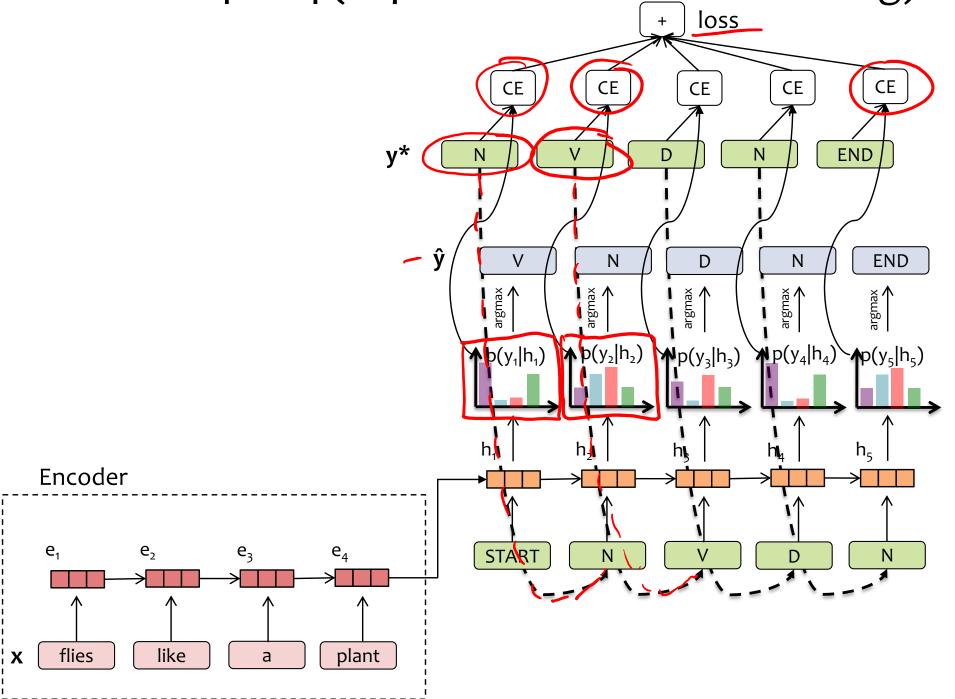
- this is the output of the dynamic oracle

repeat for E epochs **return** π_{θ}

Decoding for seq2seq (test time)



MLE for seq2seq (supervised imitation learning)

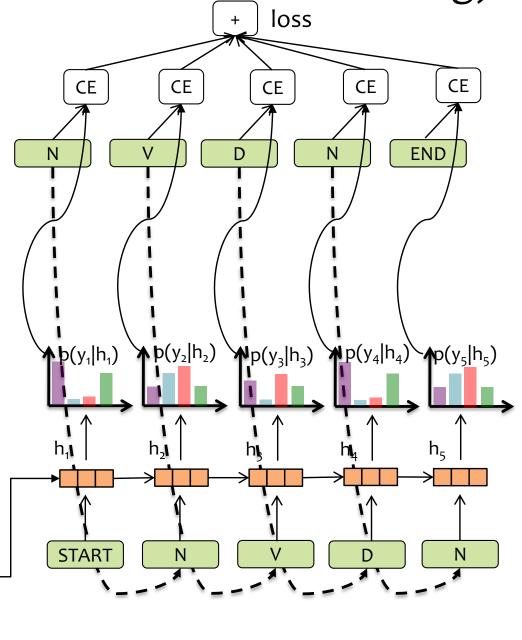


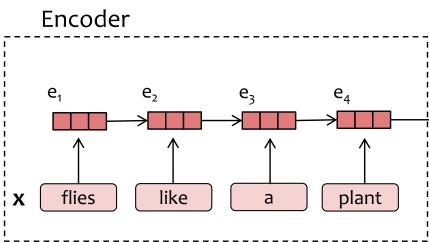
MLE for seq2seq (supervised imitation learning)

y*

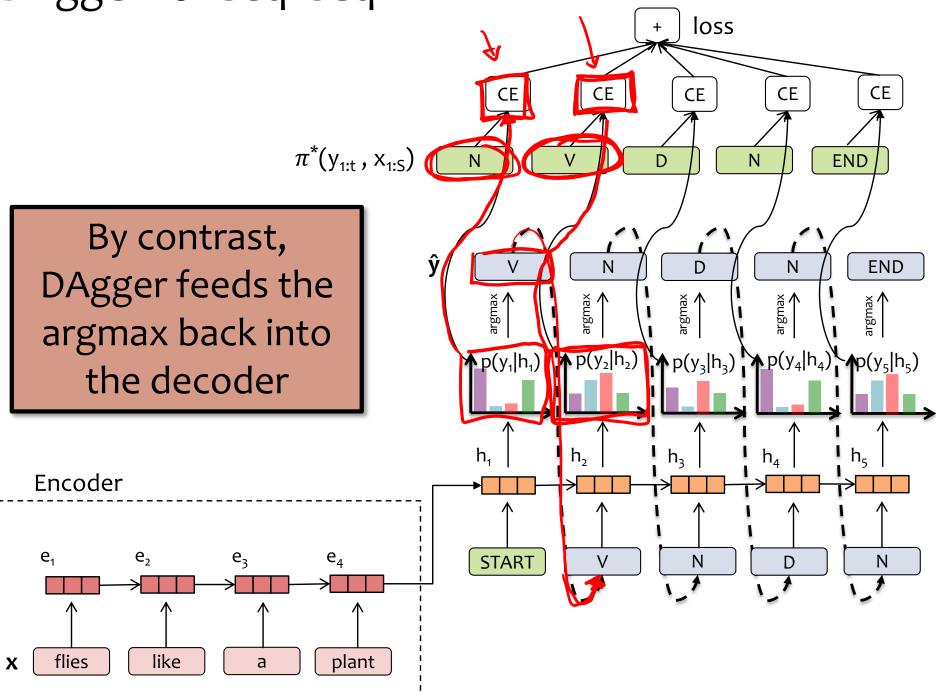
MLE computes, for each time step, the crossentropy between the ground truth y_t and the model's softmax $p(\cdot|h_t)$

At training time, it ignores the predictions (i.e. argmax)





DAgger for seq2seq



DAgger for seq2seq loss CE CE CE CE CE $\pi^*(y_{1:t}, x_{1:S})$ **END** Recall: Dagger feeds in a mixture of the **END** model policy and the $h p(y_2|h_2) h_p(y_3|h_3)$ $\mathbf{A} p(y_4|h_4) \mathbf{A} p(y_5|h_5)$ oracle policy Encoder e₁ START

flies

like

plant

a

 $\pi_i = \beta_i \pi^* + (1 - \beta_i) \pi_{\theta}$

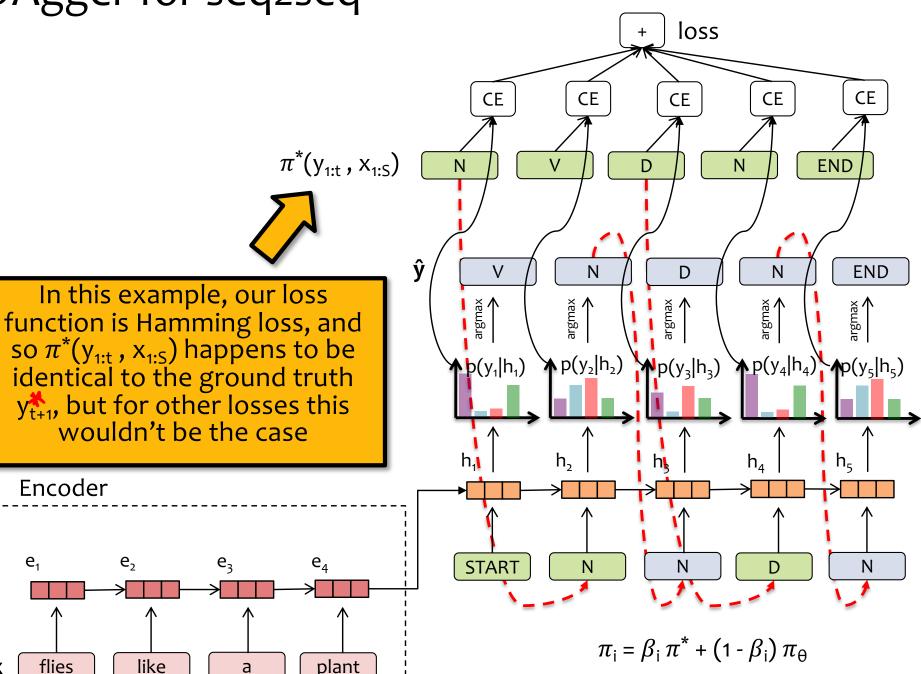
DAgger for seq2seq

Encoder

flies

like

 e_1



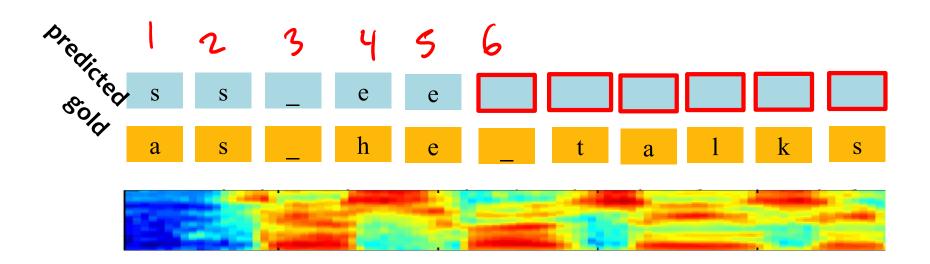
aka. Expert Policies for structured prediction problems

DYNAMIC ORACLES

Dynamic Oracles

Definition: a dynamic oracle is a function that answers this question:

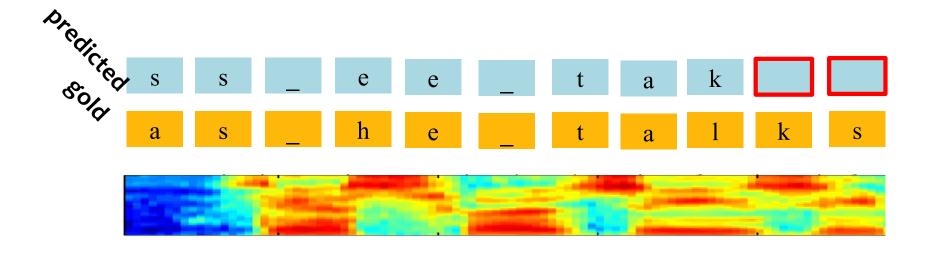
Given a partial output sequence, what is the completion that minimizes loss w.r.t the gold output?



Dynamic Oracles

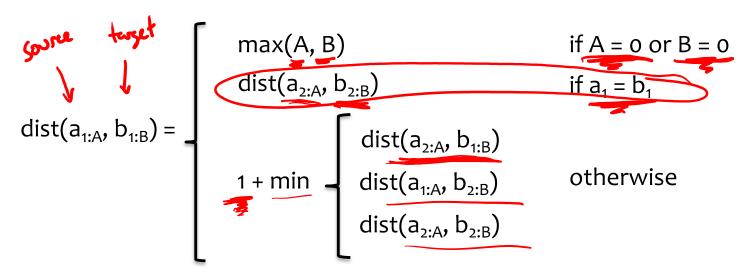
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Background: Levenshtein Distance

- Given: two strings, a source string and a target string
- **Definition**: Levenshtein distance (aka. edit distance) is the smallest <u>number of insertions</u>, <u>deletions</u>, <u>and substitutions</u> to transform the source string into the target string
- Example Transformations:
 - learning → learning (insertion of 'r')
 - reading → leading (substitution of 'r' for 'l')
 - learning → earning (deletion of 'l')
- Recursive Definition: (but not quite how it's implemented)



Background: Levenshtein Distance

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- Recursive Definition: (but not quite how it's implemented)

$$dist(a_{1:A}, b_{1:B}) = \begin{cases} max(A, B) & \text{if } A = 0 \text{ or } B = 0 \\ \\ dist(a_{2:A}, b_{1:B}) + 1 \\ \\ dist(a_{1:A}, b_{2:B}) + 1 \\ \\ dist(a_{2:A}, b_{2:B}) + 1 \end{cases} \text{ otherwise}$$

Background: Levenshtein Distance

 Algorithm: use dynamic programming; store the distance of every pair of substrings in table so that we don't recompute any distances

```
for i = 0...A: table[i][0] = i
for j = 0...B: table [0][j] = j
for i = 1...A:
   for j = 1...B:
      sub = 1
      else:
         sub = 0
      table[i][j] = min(table[i-1, j] + 1,
                         table[i, j-1] + 1,
                         table[i-1, j-1] + sub)
```

return table CAZEBI

Algorithm:

- 1. Build edit distance table from current prefix, $a_{1:A}$, and ground truth, $b_{1:B}$
- 2. Let M denote the set of column indices that are minima in the last row
- 3. The optimal next characters for the last row are $M' = [b_{m+1}]$ for m in M

				ba					
		OCD Targets	min. dist.						
		S	U	N	D	Α	Υ		
	0	S	0						
S	1								

A:ID

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			OCD Targets	min. dist.					
		S	U	N	D	Α	Υ		
	0	1	2	3	4	5	6	S	0
S	1	0							

- 1. Build edit distance table from current prefix, $a_{1:A}$, and ground truth, $b_{1:B}$
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		OCD Targets	min. dist.						
		S							
	0	1	2	3	4	5	6	S	0
S	1	0	1						

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		OCD Targets	min. dist.						
	S U N D A Y								
	0	1	2	3	4	5	6	S	0
S	1	0	1	2					

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		OCD Targets	min. dist.						
	S U N D A Y								
	0	1	2	3	4	5	6	S	0
S	1	0	1	2	3				

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		OCD Targets	min. dist.						
	S U N D A Y								
	0	1	2	3	4	5	6	S	0
S	1	0	1	2	3	4			

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		Ed	it Dista	nce Tal	ole	5	6	OCD Targets	min. dist.
		S	(0)	N	D	А	Υ		
	0	_ 1	2	3	4	5	6	S	0
S	1	0	1	2	3	4	5		

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		OCD Targets	min. dist.						
	0	1	2	3	4	5	6	S	0
S	1	0	1	2	3	4	5	U	

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		OCD Targets	min. dist.						
		S							
	0	1	2	3	4	5	6	S	0
S	1	0	1	2	3	4	5	U	0

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		Ed	it Dista ~	nce Tal	ole			OCD Targets	min. dist.
		S	U	N	D	Α	Υ		
	0	1	2	3	4	5	6	S	0
S	1	0	1	2	3	4	5	U	0
Α	2	1	_1	2	3	3	4		1
	(1 = 2	1,27		M' =	ر ه	, b.	37 = 7 	

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		OCD Targets	min. dist.						
	0	1	2	3	4	5	6	S	0
S	1	0	1	2	3	4	5	U	0
A	2		1	2	3	3	4	U,N	1
UN									
ND									

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		OCD Targets	min. dist.						
		S							
	0	1	2	3	4	5	6	S	0
S	1	0	1	2	3	4	5	U	0
Α	2	1	1	2	3	3	4	U,N	1
Т	3	2	2	2	3	4	4	U,N,D	2

- 1. Build edit distance table from current prefix, $a_{1:A}$, and ground truth, $b_{1:B}$
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		OCD Targets	min. dist.						
	0	0 1 2		3	4	5	6	S	0
S	1	0	1	2	3	4	5	U	0
Α	2	1	1	2	3	3	4	U,N	1
Т	3	2 2		2	3	4	4	U,N,D	2
R	4 3 3			3	3	4	5	U,N,D,A	3

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		OCD Targets	min. dist.						
		S	U						
	0	1	2	3	4	5	6	S	0
S	1	0	0 1		3	4	5	U	0
Α	2	1	1	2	3	3 4	4	U,N	1 2
Т	3	2	2	2	3		4 4	U,N,D	
R	4	3	3	3	3	4 5		U,N,D,A	3
A	5	4	4	4	4	3	4	Y	3

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		OCD Targets	min. dist.						
		S	U	N					
	0	1	2	3	4	5	6	S	0
S	1	0	1	2	3	4	5	U	0
Α	2	1	1	2	3	3	4	U,N	1
Т	3	2	2	2 2 3		4	4	U,N,D	2
R	4	3	3	3	3	4	5	U,N,D,A	3
Α	5	4	4	4	4	3	4	Υ	3
P 6 5 5 5 4								Y,	4

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		OCD Targets	min. dist.						
		S	U						
	0	1	2	3	4	5	6	S	0
S	1	0	0 1 2 1 1 2		3	4	5	U	0
Α	2	1			3	3	4	U,N	1
Т	3	2	2	2	3	4	4	U,N,D	2
R	4	3	3	3	3	4	5	U,N,D,A	3
Α	5	4	4 4		4	3	4	Υ	3
Р	6	5 5		5	5	4	4	Y,	4
Υ	7	6	6	6	6	5	4		4

Dynamic Oracles

Definition: a dynamic oracle is a function that answers this question:

Given a partial output sequence, what is the completion that minimizes loss w.r.t the gold output?

Depending on your loss function, there **may or may not** exist an efficient dynamic oracle.

For example, these metrics readily admit an efficient dynamic oracle:

- CER for phoneme recognition
- chunking F1 for named entity
- labeled attachment score for arc-eager dependency parsing

But it's unlikely that there exists an efficient dynamic oracle for:

- BLEU for machine translation
- ROUGE for summarization

TEACHER FORCING, SCHEDULED SAMPLING, & OCD

Algorithms for Seq2Seq

Here we consider three algorithms that are closely related to DAgger and appropriate for training a seq2seq model:

- Teacher Forcing
- 2. Scheduled Sampling
- 3. Optimal Completion Distillation

Teacher Forcing

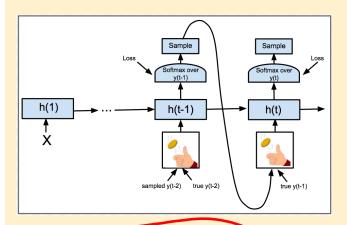
Another name for **supervised imitation learning** when it is applied to training RNNLM/seq2seq models is **teaching forcing**. This is equivalent to **maximum likelihood estimation** if cross-entropy is the loss function.

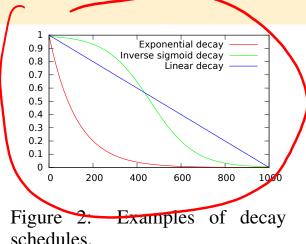
The name 'teacher forcing' was coined by Williams & Zipser (1989) A Learning Algorithm for Continually Running Fully Recurrent Neural Networks.

The only difference between training an RNNLM or seq2seq model is whether the decoder conditions on the output of an encoder or not.

- 1. at training time, feed the **ground truth** from the **previous** time step in as the decoder input for the **next** time step
- 2. at each timestep **minimize cross entropy** (or some other loss) of the **ground truth** for that time step

Scheduled Sampling





The Scheduled Sampling (SS) algorithm is another learning technique for seq2seq models, introduced by Bengio et al. (2015) Scheduled Sampling for Sequence Prediction with Recurrent Neural Networks.

Algorithm:

- at training time, flip a weighted coin to decide whether to feed the model's prediction or the ground truth from the previous time step as the decoder input for the next time step
- 2. at each timestep **minimize cross entropy** (or some other loss) of the **ground truth** for that time step
- **gradually decrease the probability of** feeding in the **ground truth** with each iteration of training

Comments:

- SS is just like Teacher Forcing except that with some probability we feed in the model's prediction from the previous time step.
- SS has the same motivation as DAgger: addressing the problem of exposure bias (i.e. making the states visited at training time similar to those that will be visited at test time)
- SS is not DAgger because it only relies on the ground truth sequence, not a dynamic oracle
- SS does not come with any theoretical gaurantees (DAgger does)

Optimal Completion Distillation

Optimal Completion Distillation (OCD) was introduced in Sabour et al. (2019) Optimal Completion Distillation for Sequence Learning.

Algorithm:

- at training time, feed the model's prediction from the previous time step as the decoder input for the next time step
- at each timestep minimize cross entropy (or some loss) of the ground truth for that time step dynamic occle (expet policy 1714)

Comments:

Optimal Completion Distillation (OCD) is a special of the DAgger metaalgorithm to speech recognition in which:

- the loss function at each time-step is the KL Divergence between the softmax output from the model and a uniform distribution over the dynamic oracle completions
- the dynamic oracle is a dynamic programming algorithm (similar to edit distance) for character error rate (CER)

Optimal Completion Distillation

Optimal Completion Distillation (OCD) was introduced in Sabour et al. (2019) Optimal Completion Distillation for Sequence Learning.

Algorithm:

- 1. at training time, feed the model's prediction from the previous time step as the decoder input for the nextime step
- 2. at each timestep minimize cross ent y (or some loss) of the ground truth for that time step

In the original OCD paper, they **only** feed in model predictions.

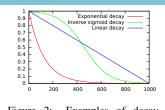
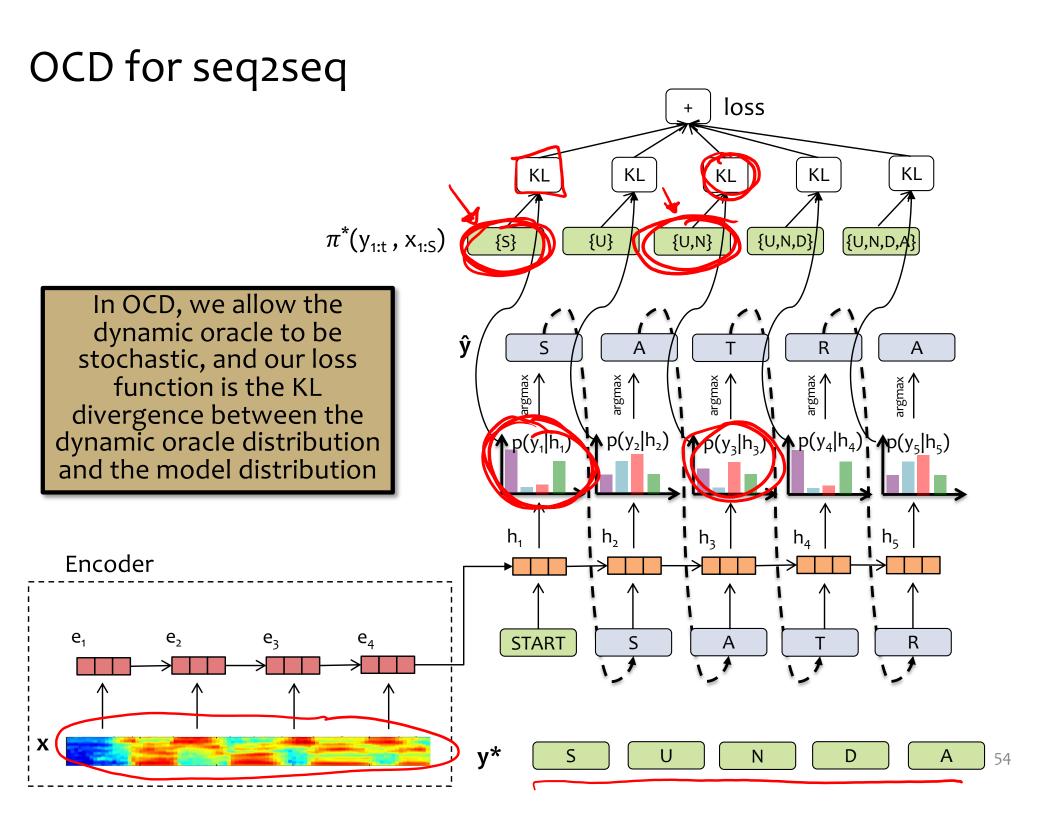


Figure 2: Examples of decay schedules.

However, because OCD is a special case of DAgger, we can generalize OCD to use a beta schedule that gives a mixture of the oracle policy with the model policy, and feed in a sample from the mixture policy to the decoder.



OCD (with DAgger's mixture) for seq2seq loss KL KLKL KL KL $\pi^*(y_{1:t}, x_{1:S})$ {U,N} {U,N,D} {S} $\{U,N,D,A\}$ {U} If we use a mixture of model and oracle policy, the stochasticity also affects the decoder $p(y_2|h_2) p(y_3|h_3)$ $\mathbf{A} p(y_4|h_4) \mathbf{A} p(y_5|h_5)$ inputs h₁ Encoder e₁ e_2 **START y***

Imitation Learning vs. RL

- Q: What is the difference between imitation learning and reinforcement learning?
- A: There are lots of differences but they all stem from one fundamental difference:

Imitation learning assumes that it has access to an **oracle policy** π^* , reinforcement learning does not.

Interesting contrast: Q-Learning vs. DAgger.

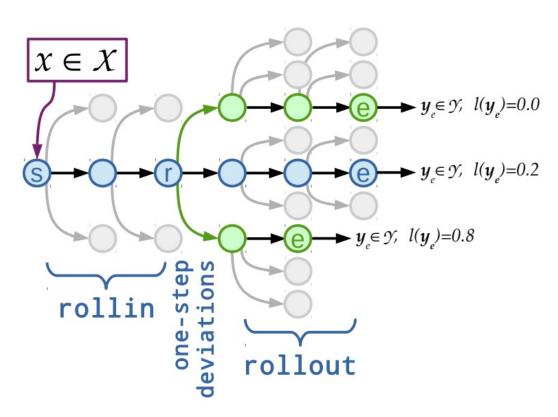
- both have some notion of explore/exploit (very loose analogy)
- but Q-learning's exploration is random, and its exploitation relies on the model's policy
- whereas DAgger exploration uses the model's policy, and its exploitation follows the oracle

COMPARISON OF LEARNERS

Comparison of Learners

Learning to Search Terminology

- roll-in: how we got to the current state
- one-step deviations: immediate neighbors in the search space under consideration
- roll-out: completions of deviations (might be optimal, might not)
- The learner considers each of the one-step deviations and (typically) chooses the one with lowest loss



Comparison of Learners

	Learner	Roll-in	Target	Objective (per time step)		
	MLE	ground truth y*	ground truth y*	cross-entropy of ground truth		
	Scheduled Sampling	mixture of mode predictions \hat{y} and ground truth y^*	ground truth y*	cross-entropy of ground truth		
8	Dagger	mixture of expert policy π^* and model policy $\hat{\pi}$	expert policy π^*	cross-entropy of dynamic oracle completion		
	OCD (special case of DAgger for CER)	model policy $\hat{\pi}$ = model predictions \hat{y}	expert policy π^*	KL Divergence between uniform distribution over set of dynamic oracle completions and model's softmax		
•	Policy Gradient (RL)	model policy $\hat{\pi}$ = model predictions \hat{y}	model policy $\hat{\pi}$	increase score of sequences with high reward $R(\hat{y})$		

Comparison of Learners

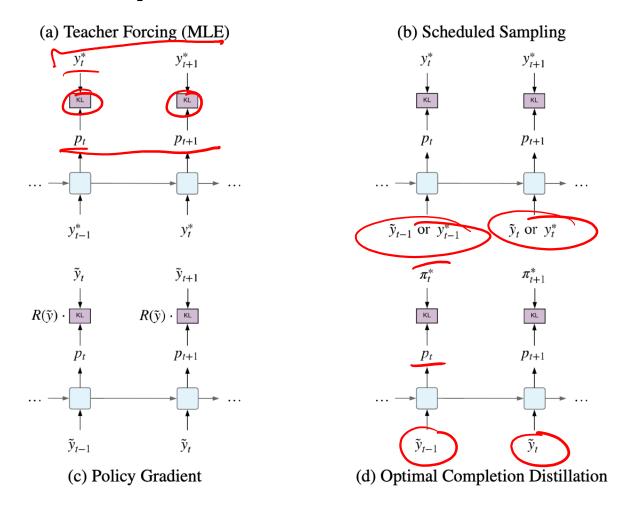
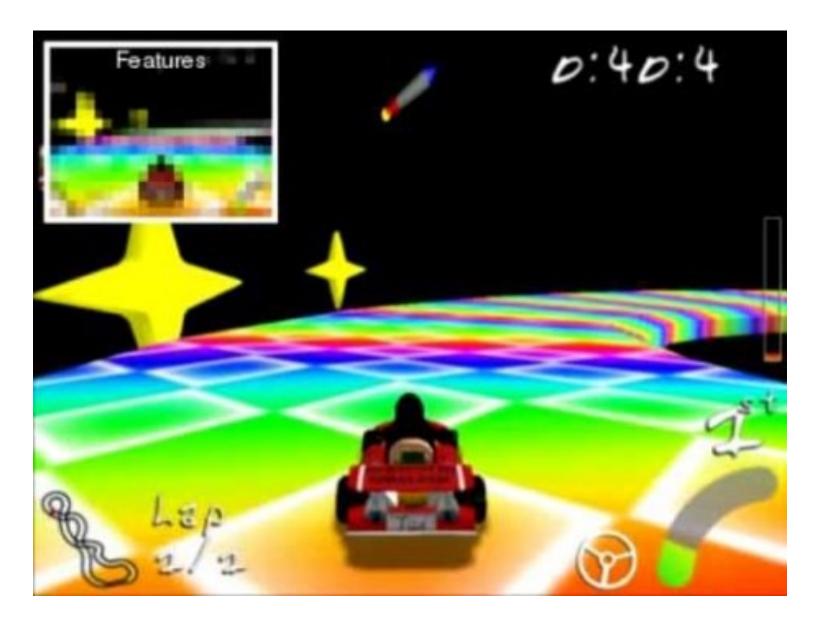


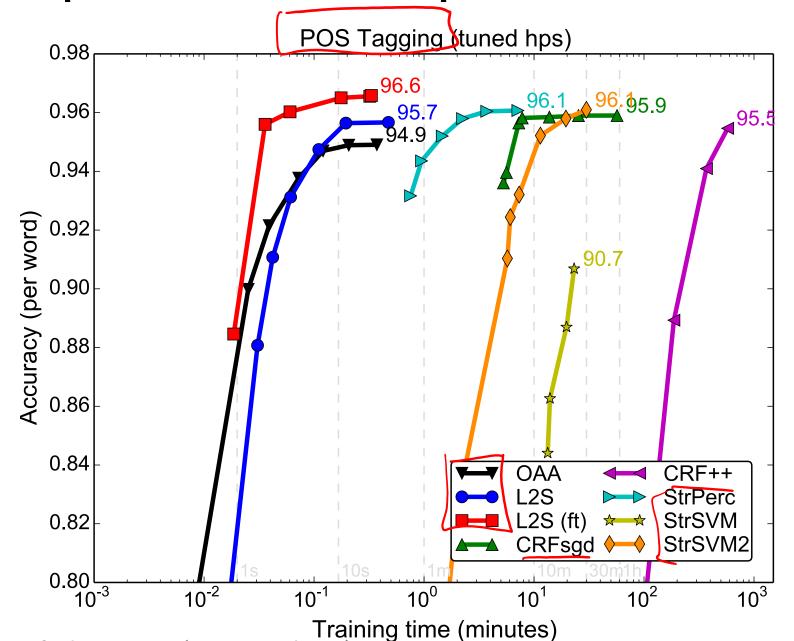
Figure B.1: Illustration of different training strategies for autoregressive sequence models. (a) Teacher Forcing: the model conditions on correct prefixes and is taught to predict the next ground truth token. (b) Scheduled Sampling: the model conditions on tokens either from ground truth or drawn from the model and is taught to predict the next ground truth token regardless. (c) Policy Gradient: the model conditions on prefixes drawn from the model and is encouraged to reinforce sequences with a large sequence reward $R(\tilde{y})$. (d) Optimal Completion Distillation: the model conditions on prefixes drawn from the model and is taught to predict an optimal completion policy π^* specific to the prefix.

LEARNING TO SEARCH: EMPIRICAL RESULTS

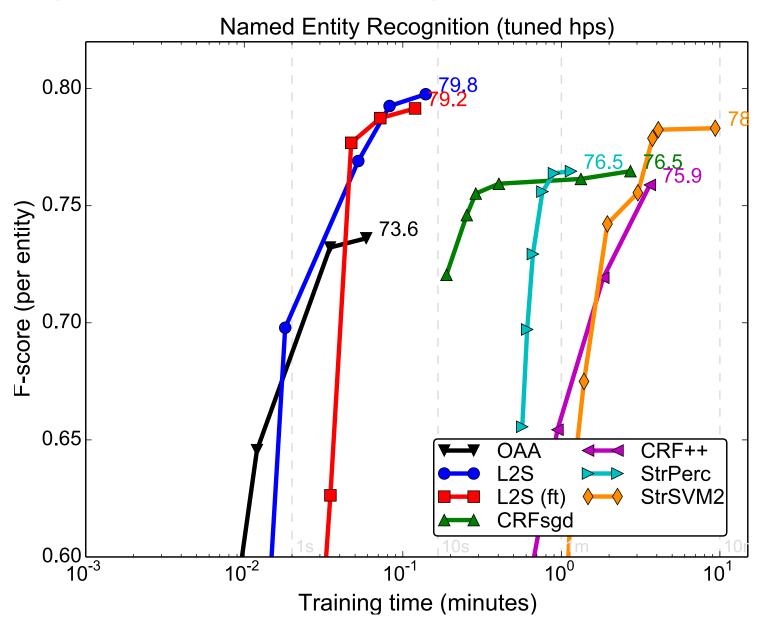
Dagger for Mario Tux Cart



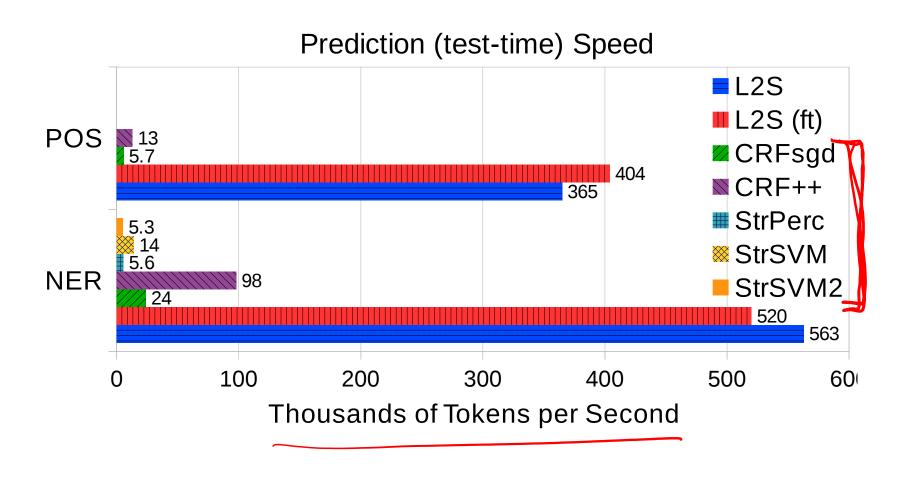
Experiments: Vowpal Wabbit L2S



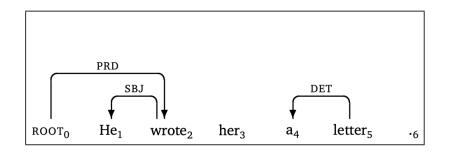
Experiments: Vowpal Wabbit L2S



Experiments: Vowpal Wabbit L2S



Results: Dynamic Oracle for Dependency Parsing



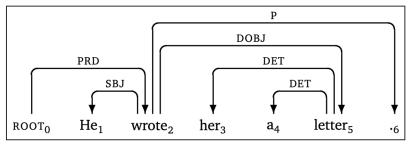


Figure 3: Dependency graphs with loss 3 (left) and loss 1 (right)

	$\sqrt{}$									
	ARA	BAS	CAT	CHI	CZE	ENG	GRE	HUN	ITA	TUR
			<u>Unlabel</u> e	d Attach	ment Sco	ores				
Static	80.60	74.10	91.21	84.13	78.00	86.24	79.16	77.75	84.11	79.02
Dynamic-ambiguity	80.72	74.90	91.09	83.62	78.38	86.83	79.48	76.17	84.52	78.97
Dynamic-explore	83.06	76.10	92.01	84.65	79.54	88.81	80.66	77.10	84.77	78.84
			Labeled	l Attachn	nent Scor	res				
Static	71.04	64.42	85.96	79.75	69.49	84.90	70.94	68.10	79.93	68.80
Dynamic-ambiguity	71.06	65.18	85.73	79.24	69.39	85.56	71.88	66.99	80.63	68.58
Dynamic-explore	73.54	66.77	86.60	80.74	71.32	87.60	73.83	68.23	81.02	68.76

Table 2: Results on the CoNLL 2007 data sets

Results: Dynamic Oracle for Dependency Parsing

Training with a dynamic oracle (Dynamic-ambiguity & Dynamic-explore) consistently outperforms training to produce the ground truth (Static), across many different languages.

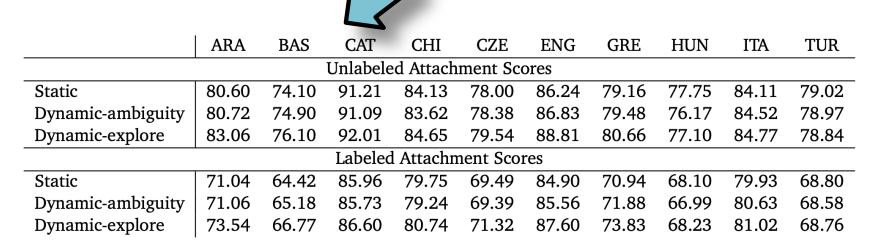


Table 2: Results on the CoNLL 2007 data sets

DAGGER: THEORETICAL RESULTS

DAgger Policy During Training

 DAgger assumes that we follow a stochastic policy that flips a weighted coin (with weight β_i at timestep i) to decide between the oracle policy and the model's policy

$$\pi_i = \beta_i \pi^* + (1 - \beta_i) \hat{\pi}_i$$

We require that (β₁, β₂, β₃, ...) is chosen to be a sequence such that:

$$\overline{\beta}_N = \frac{1}{N} \sum_{i=1}^N \beta_i \to 0 \quad \text{as} \quad N \to \infty.$$



DAgger Theoretical Results

- The theory mirrors the intuition that Exposure Bias is bad
- The Supervised Approach to Imitation performs **not-so-well** even on the oracle (training time) distribution over states (i.e. quadratically number of mistakes grows quadratically in task horizon T and classification cost ϵ)
- DAgger yields an algorithm that performs well on the test-time distribution over states (i.e. number of mistakes grows linearly in task horizon T and classification cost ϵ)

$$J(\pi) = \sum_{t=1}^{T} \mathbb{E}_{s \sim d_{\pi}^{t}} [C_{\pi}(s)]$$

Algo #1: Supervised Approach to Imitation

Theorem 2.1. (Ross and Bagnell, 2010) Let
$$\mathbb{E}_{s \sim d_{\pi^*}}[\ell(s,\pi)] = \epsilon$$
, then $J(\pi) \leq J(\pi^*) + T^2 \epsilon$.

Algo #2: DAgger

Theorem 3.2. For DAGGER, if N is $\tilde{O}(uT)$ there exists a policy $\hat{\pi} \in \hat{\pi}_{1:N}$ s.t. $J(\hat{\pi}) \leq J(\pi^*) + uT\epsilon_N + O(1)$.

$$\epsilon_N = \min_{\pi \in \Pi} \frac{1}{N} \sum_{i=1}^N \mathbb{E}_{s \sim d_{\pi_i}} [\ell(s, \pi)]$$

DAgger Theoretical Results

 The proof of the results for DAgger relies on a reduction to no-regret online learning

From Ross et al. (2011) "A Reduction of Imitation Learning and Structured Prediction to No-Regret Online Learning"...

sarial fashion over time. A no-regret algorithm is an algorithm that produces a sequence of policies $\pi_1, \pi_2, \dots, \pi_N$ such that the average regret with respect to the best policy in hindsight goes to 0 as N goes to ∞ :

$$\frac{1}{N} \sum_{i=1}^{N} \ell_i(\pi_i) - \min_{\pi \in \Pi} \frac{1}{N} \sum_{i=1}^{N} \ell_i(\pi) \le \gamma_N$$
 (3)

for $\lim_{N\to\infty}\gamma_N=0$. Many no-regret algorithms guarantee that γ_N is $\tilde{O}(\frac{1}{N})$ (e.g. when ℓ is strongly convex) (Hazan et al., 2006; Kakade and Shalev-Shwartz, 2008; Kakade and Tewari, 2009).

• The key idea is to choose the loss function to be that of the loss on the distribution over states given by the current policy chosen by the online learner $\boxed{\ell_i(\pi) = \mathbb{E}_{s \sim d_{\pi_s}}[\ell(s,\pi)]}$

Learning 2 Search

Some key challenges:

- performance depends heavily on search order,
 but have to pick this by hand
- expert policy is critical, but what if it's too difficult to design one
- not always easy to make efficient on a GPU

Learning Objectives

Structured Prediction as Search

You should be able to...

- Reduce a structured prediction problem to a search problem
- 2. Implement Dagger, a learning to search algorithm
- 3. (If you already know RL...) Contrast imitation learning with reinforcement learning
- 4. Explain the reduction of structured prediction to no-regret online learning
- 5. Contrast various learning2search algorithms based on their properties