Recent Advances in Structured Prediction

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Tutorial at AAAI Conference on Artificial Intelligence (AAAI), 2018

Dedication: Ben Taskar (1977-2013)



- Ben made fundamental contributions to the area of structured prediction
- We dedicate this tutorial to him

Outline of Tutorial

Different frameworks for structured prediction [Jana]

- Cost function learning framework and recent advances
- Control knowledge learning framework (greedy and beam search)
- HC-Search: A Unifying framework

Integrating deep learning and structured prediction [Liping]

- Deep learning ∩ cost function learning
- ▲ Deep learning ∩ control knowledge learning

Multi-task structured prediction [ChaoMa]

- Graphical models approach
- Search based learning and inference architectures

Part 1: Introduction

Introduction

Structured Prediction problems are very common

- Natural language processing
- Computer vision
- Computational biology
- Planning
- Social networks
- **^** ..

Natural Language Processing Examples

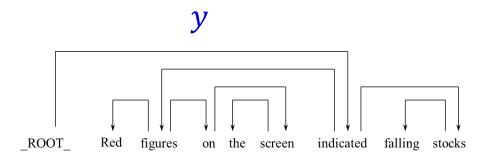
NLP Examples: POS Tagging and Parsing

POS Tagging

x = "The cat ran" $y = \langle article \rangle \langle noun \rangle \langle verb \rangle$

Parsing

x "Red figures on the screen indicated falling stocks"



NLP Examples: Coreference and Translation

Co-reference Resolution

X

"Barack Obama nominated Hillary Clinton as his secretary of state on Monday. He chose her because she had foreign affair experience as a former First Lady." *Y "Barack Obama nominated Hillary Clinton as his secretary of state on Monday. He chose her because she had foreign affair experience as a former First Lady."*

Machine Translation

x = "The man bit the dog"

y = 该男子咬狗

Examples of Bad Prediction



Computer Vision Examples

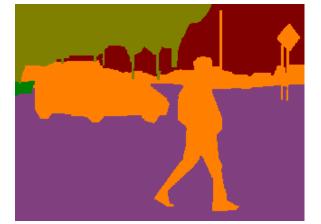
Scene Labeling



Image







Labeling

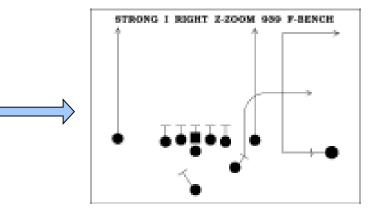
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sky	sky	sky	sky	sky	sky	sky	sky	sky	sky
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rocks	rocks	rocks	rocks	rocks	rocl	ocks	sky	sky	sky
rocks	rocks	rocks	rocks	rocks	rocks	rocks	rocks	water	water
sand	sand	sand water	sand water	water	water	water	water	water	water
sand	sand	water	water	water	water	water	water	water	water
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The OSU Digital Scout Project

Objective: compute semantic interpretations of football video



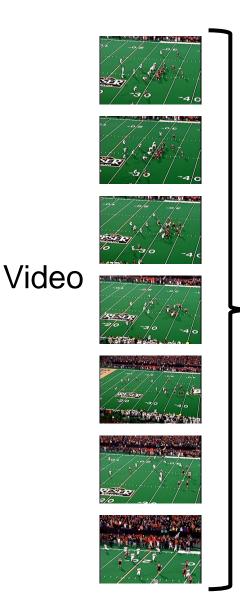
Raw video



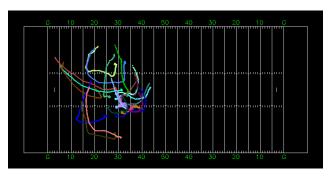
High-level interpretation of play

- Help automate tedious video annotation done by pro/college/HS teams
 - Working with hudl (hudl.com)
- Requires advancing state-of-the-art in computer vision, including:
 - registration, multi-object tracking, event/activity recognition

Multi-Object Tracking in Videos



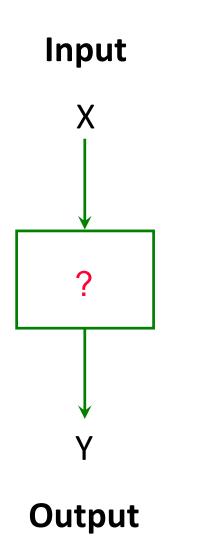
Player Trajectories



Common Theme

- POS tagging, Parsing, Co-reference resolution, detecting parts of biological objects
 - Inputs and outputs are highly structured
- Studied under a sub-field of machine learning called "Structured Prediction"
 - Generalization of standard classification
 - Exponential no. of classes (e.g., all POS tag sequences)

Classification to Structured Prediction





?

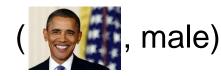
male

Example problem:

X - image of a face

 $Y \in \{male, female\}$

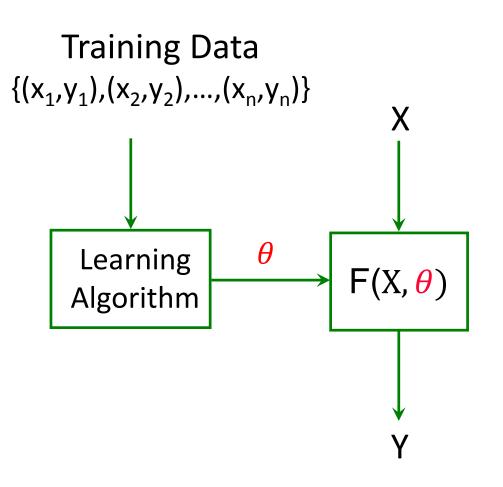
Y



Training Data $\{(x_1, y_1), (x_2, y_2), ..., (x_n, y_n)\}$ Learning Algorithm ? Example problem:

X - image of a face

 $Y \in \{male, female\}$

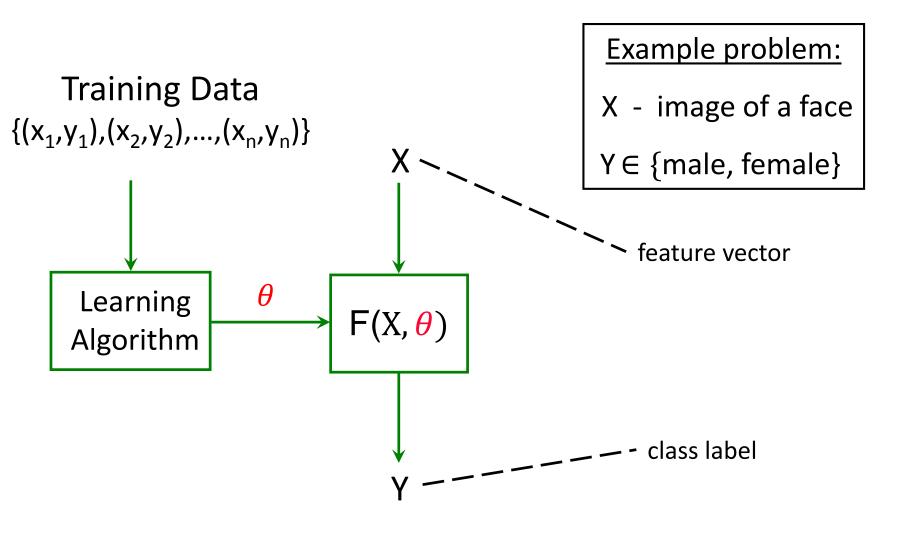


Example problem:

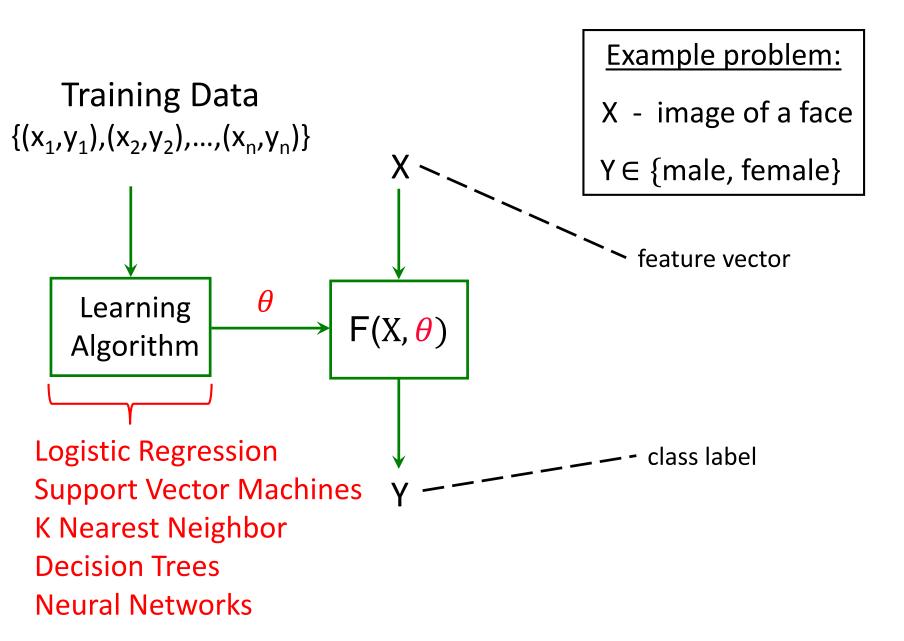
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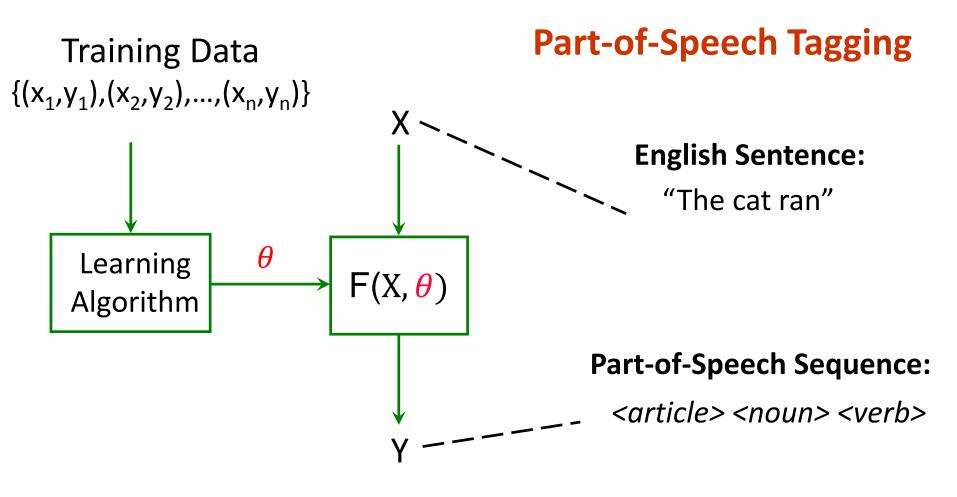
Learning for <u>Simple</u> Outputs



Learning for <u>Simple</u> Outputs



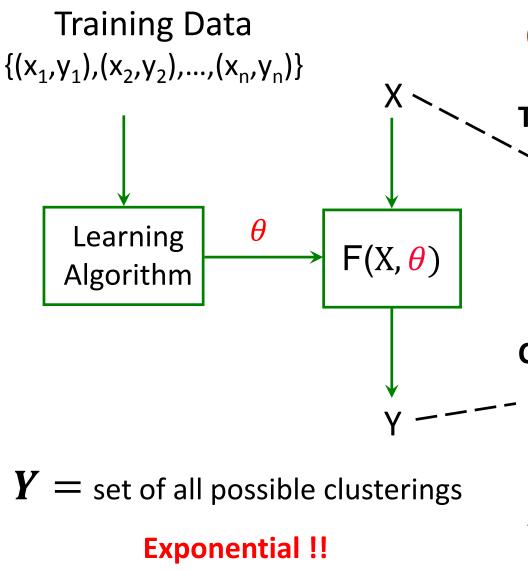
Learning for <u>Structured</u> Outputs



Y = set of all possible POS tag sequences

Exponential !!

Learning for <u>Structured</u> Outputs



Co-reference Resolution

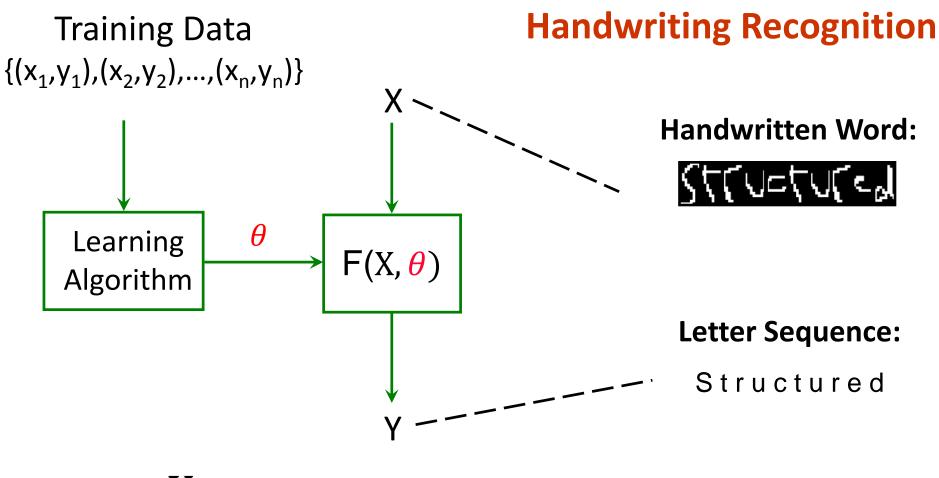
Text with input mentions:

"Barack Obama nominated Hillary Clinton as his secretary of state on Monday. He chose her because she had foreign affair experience as a former First Lady."

Co-reference Output:

"Barack Obama nominated Hillary Clinton as his secretary of state on Monday. He chose her because she had foreign affair experience as a former First Lady."

Learning for <u>Structured</u> Outputs



Y = set of all possible letter sequences

Exponential !!

Part 2: Cost Function Learning Framework and Argmin Inference Challenge

Cost Function Learning Approaches: Inspiration

 Generalization of traditional ML approaches to structured outputs

- SVMs \Rightarrow Structured SVM [Tsochantaridis et al., 2004]
- ▲ Logistic Regression ⇒ Conditional Random Fields [Lafferty et al., 2001]
- ▲ Perceptron \Rightarrow Structured Perceptron [Collins 2002]

Cost Function Learning: Approaches

- Most algorithms learn parameters of linear models
 - $\phi(x, y)$ is n-dim feature vector over input-output pairs
 - ▲ w is n-dim parameter vector

$$F(\mathbf{x}) = \arg\min_{y \in Y} w \cdot \boldsymbol{\phi}(x, y)$$

Cost Function Learning: Approaches

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Example: Part-of-Speech Tagging

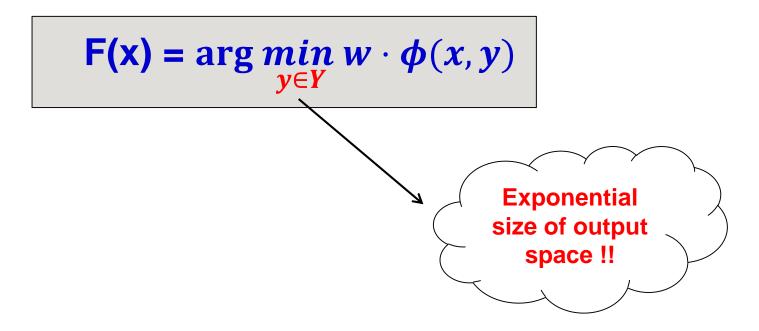
x = "The cat ran" y = <article> <noun> <verb>

 $\phi(x, y)$ may have unary and pairwise features

unary feature: e.g. # of times 'the' is paired with <article>

pairwise feature: e.g. # of times <article> followed by <verb>

Key challenge: "Argmin" Inference



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$$F(\mathbf{x}) = \arg\min_{y \in Y} w \cdot \phi(x, y)$$

• Time complexity of inference depends on the dependency structure of features $\phi(x, y)$

Key challenge: "Argmin" Inference

$$F(\mathbf{x}) = \arg\min_{y \in Y} w \cdot \phi(x, y)$$

- Time complexity of inference depends on the dependency structure of features $\phi(x, y)$
 - NP-Hard in general
 - Efficient ``exact'' inference algorithms exist only for simple features
 - Approximate inference techniques are employed in practice and they work reasonably well

Cost Function Learning: Key Elements

Joint Feature Function

- How to encode a structured input (x) and structured output
 (y) as a fixed set of features \u03c6(x, y)?
- (Loss Augmented) Argmin Inference Solver
 - $F(x) = \arg \min_{v \in Y} w \cdot \phi(x, y)$
 - Viterbi algorithm for sequence labeling
 - CKY algorithm for parsing
 - (Loopy) Belief propagation for Markov Random Fields
 - Sorting for ranking

Optimization algorithm for learning weights

(sub) gradient descent, cutting plane algorithm ...

Cost Function Learning: Generic Template

• Training goal:

Find weights w s.t

For each input x, the cost of the correct structured output y is lower than all wrong structured outputs

repeat

- For every training example (x, y)
- Inference: $\hat{y} = \arg \min_{y \in Y} w \cdot \varphi(x, y)$
- If mistake $y \neq \hat{y}$,

Learning: online or batch weight update

• until convergence or max. iterations

Exponential

size of output

space !!

Expensive Training Process

Main Reason

 repeated calls to "Argmin inference solver" (computationally expensive) on all the training examples

Recent Solutions

- Amortized Inference: Kai-Wei Chang, Shyam Upadhyay, Gourab Kundu, Dan Roth: Structural Learning with Amortized Inference. AAAI 2015
- Decomposed Learning: Rajhans Samdani, Dan Roth: Efficient Decomposed Learning for Structured Prediction. ICML 2012

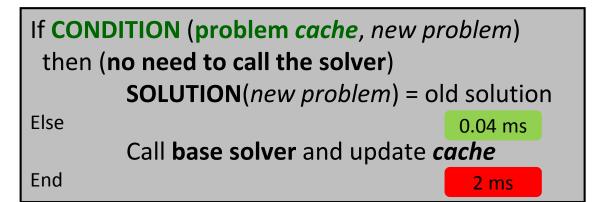
Amortized Inference and Speedup Learning

- We need to solve many inference problems during both training and testing
 - Computationally expensive!

- Can we improve the speed of solving new problems based on past problem-solving experience?
 - Yes, amortized Inference!
 - A Highly related to ``speedup learning'' [Fern, 2010]

Amortized Inference with ILP Formulation

- Inference can be formulated as ILP [Roth and Yih, 2004]
- Imagine that you already solved many inference problems
 - Your algorithmic solution method doesn't matter
- How can we exploit this fact to save inference cost?
 - After solving n inference problems, can we make the (n+1)th one faster?
- Conditions under which the solution of a new problem Q is the same as the one of P (which we already cached)



The Theorem Must Fire a Lot

- Inference formulation provides a new level of abstraction for amortization
- Modulo renaming
 - Dan gave a talk
 - Vinod ate a pizza
 - Heng read a book
- Have same POS tag structure, Parse Tree, Semantic Parse

Pigeon Hole Principle

- Many different instances have to be mapped into identical inference outcomes
- Often, saves 85% of the computation.

Amortized ILP Inference: References

- Vivek Srikumar, Gourab Kundu, Dan Roth: *On Amortizing Inference Cost for Structured Prediction*. **EMNLP** 2012
- Gourab Kundu, Vivek Srikumar, Dan Roth: *Margin-based Decomposed Amortized Inference*. **ACL** 2013
- Kai-Wei Chang, Shyam Upadhyay, Gourab Kundu, Dan Roth: Structural Learning with Amortized Inference. AAAI 2015
- PAC Theory for ILP Inference: The behavior of ILP inference (integrality of relaxed solutions) on training examples generalize to testing examples
 - Ofer Meshi, Mehrdad Mahdavi, Adrian Weller, David Sontag: Train and Test Tightness of LP Relaxations in Structured Prediction. ICML 2016

Decomposed Learning (DecL)

 Key Idea: Inference over a smaller structured output space
 All structured outputs that have a hamming accuracy of k from the ground truth structured output: DecL(k)

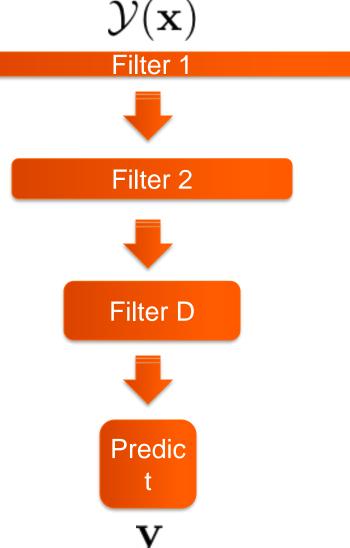
- As k increases, learning approaches standard learning
 - Theoretical guarantees on when DecL will behave similar to standard learning [Samdani and Roth, 2012]

- Special case (k=1):
 - Pseudo-max training [Sontag et al., 2010]

Structured Prediction Cascades [Weiss and Taskar, 2010]

 Accuracy: Minimize the number of errors incurred by each level

 Efficiency: Maximize the number of filtered assignments at each level



Cost Function Learning: "Exact" vs. "Approximate" Inference Solver

- Most theory works for "Exact" Inference
- Theory breaks with "Approximate" Inference
 - Alex Kulesza, Fernando Pereira: Structured Learning with Approximate Inference. NIPS 2007
 - Thomas Finley, Thorsten Joachims: Training structural SVMs when exact inference is intractable. ICML 2008: 304-311

Active Research Topic: Interplay between (approximate) inference and learning

- Veselin Stoyanov, Alexander Ropson, Jason Eisner: Empirical Risk Minimization of Graphical Model Parameters Given Approximate Inference, Decoding, and Model Structure. AISTATS 2011
- Justin Domke: Structured Learning via Logistic Regression. NIPS 2013
- Tamir Hazan, Alexander G. Schwing, Raquel Urtasun: Blending Learning and Inference in Conditional Random Fields. JMLR-2016

Search-based Structured Prediction

 Integrating "Learning" and "Search" two fundamental branches of AI to solve structured prediction problems

• Key Idea:

- Learning "with Inference" vs. Learning "for Inference"
- Select a computationally bounded search architecture for making predictions
- Optimize the parameters of that procedure to produce accurate outputs using training data

Part 3: Control Knowledge Learning Framework: Greedy Methods

Greedy Control Knowledge Learning

Given

- Search space definition
- Training examples (input-output pairs)

Learning Goal

 Learn a policy or classifier to that directly predicts good structured outputs (no inference needed!)

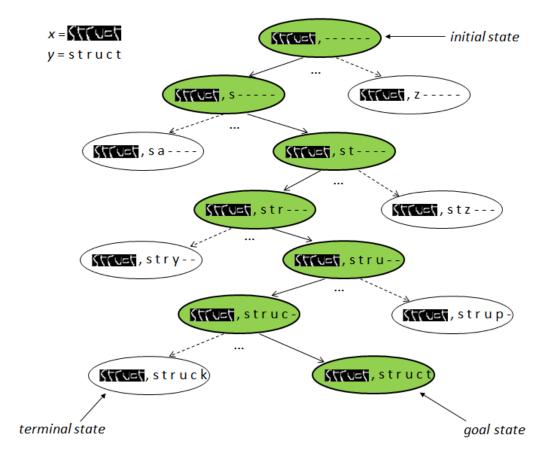
• Key Idea:

- Training examples can be seen as expert demonstrations
- Equivalent to "Imitation Learning" or "Learning from Demonstration"
- Reduction to classifier or rank learning

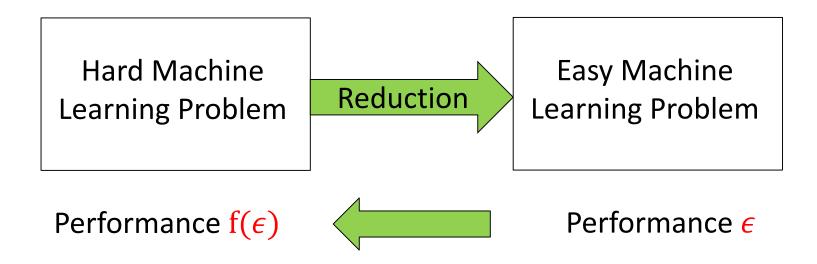
Classifier-based Structured Prediction

- Reduction to classifier learning
 - 26 classes

- IL Algorithms
 - Exact-Imitation
 - SEARN
 - DAgger
 - AggreVaTe
 - LOLS



Aside: Reductions in Machine Learning



- Reduce complex problem to simpler problem(s)
- A better algorithm for simpler problem means a better algorithm for complex problem
- Composability, modularity, ease-of-implementation

Imitation Learning Approach

Expert demonstrations

 each training example (input-output pair) can be seen as a "expert" demonstration for sequential decision-making

Collect classification examples

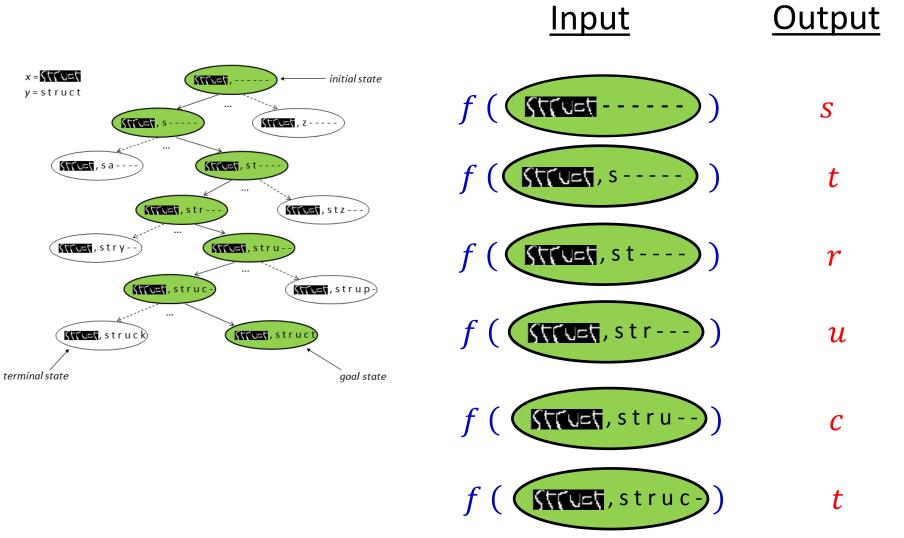
- Generate a multi-class classification example for each of the decisions
- Input: f(n), features of the state n
- Output: y_n , the correct decision at state n

Classifier Learning

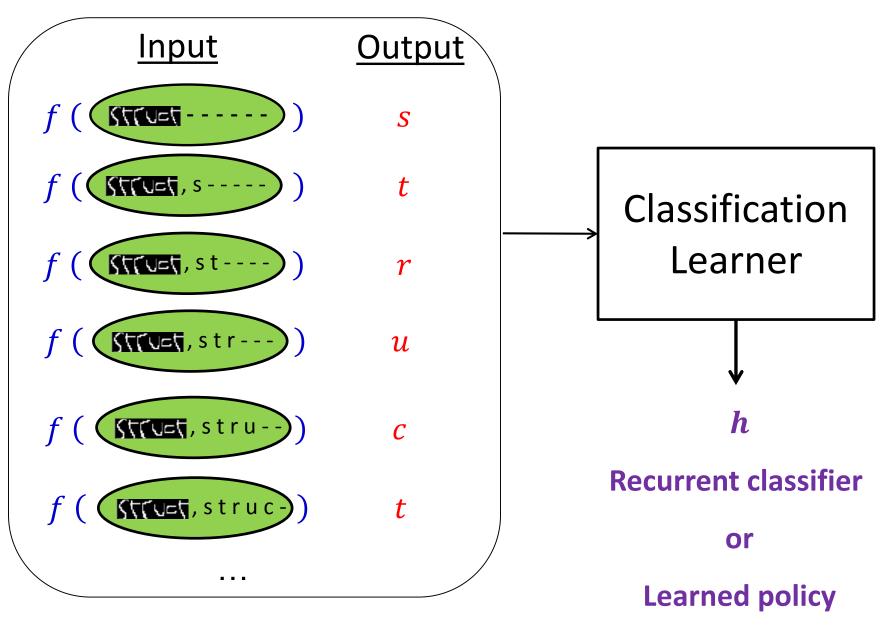
Learn a classifier from all the classification examples

Exact Imitation: Classification examples

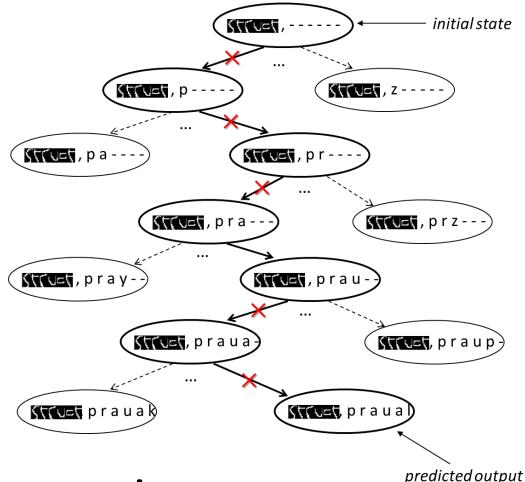
For each training example



Exact Imitation: Classifier Learning



Learned Recurrent Classifier: Illustration



• Error propagation:

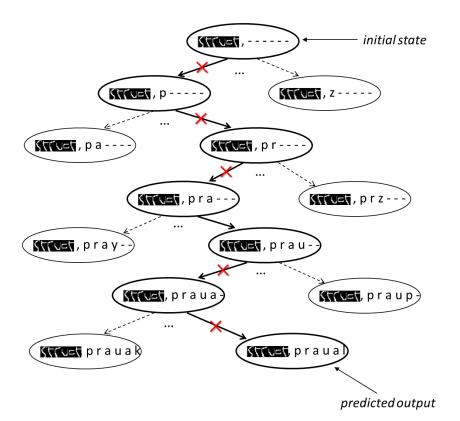
errors in early decisions propagate to down-stream decisions

Recurrent Error

- Can lead to poor global performance
- Early mistakes propagate to downstream decisions: $f(\epsilon) = O(\epsilon T^2)$, where ϵ is the probability of error at each decision and T is the number of decision steps [Kaariainen 2006] [Ross & Bagnell 2010]
- Mismatch between training (IID) and testing (non-IID) distribution
- Is there a way to address error propagation?

Addressing Error Propagation

- <u>Rough Idea:</u> Iteratively observe current policy and augment training data to better represent important states
- Several variations on this idea [Fern et al., 2006], [Daume et al., 2009], [Xu & Fern 2010], [Ross & Bagnell 2010], [Ross et al. 2011, 2014], [Chang et al., 2015]



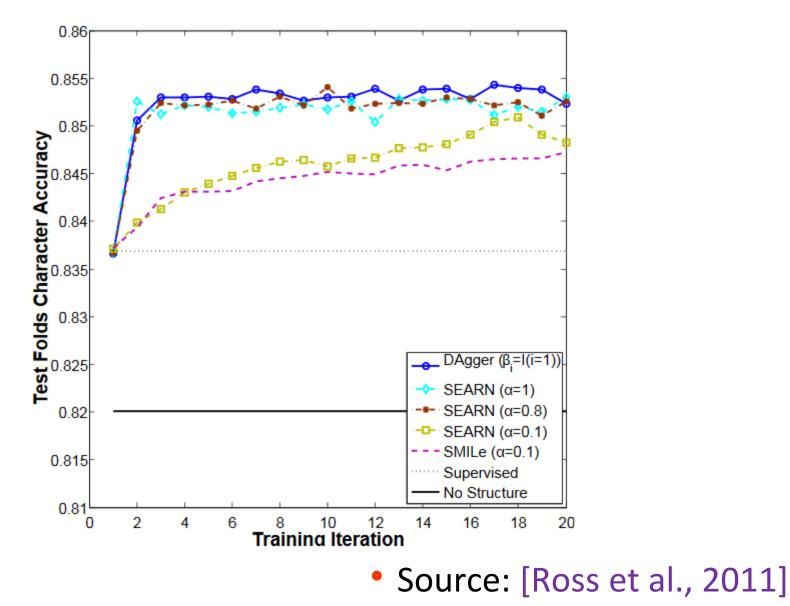
- Generate trajectories using current policy (or some variant)
- Collect additional classification examples using optimal policy (via ground-truth output)

DAgger Algorithm [Ross et al., 2011]

- Collect initial training set D of N trajectories from reference policy π^*
- Repeat until done
 - $\pi \leftarrow \text{LearnClassifier}(D)$
 - \clubsuit Collect set of states S that occur along N trajectories of π
 - For each state $s \in S$
 - $D \leftarrow D \cup \{(s, \pi^*(s))\}$ // add state labeled by expert or reference policy
- Return π

Each iteration increases the amount of training data (data aggregation)

DAgger for Handwriting Recognition



Easy-First Approach: Big Picture

Drawbacks of classifier-based structured prediction

- Need to define an ordering over the output variables (e.g., leftto-right in sequence labeling)
- Which order is good? How do you find one?
- Some decisions are hard to make if you pre-define a fixed order over the output variables

• Easy-First Approach: Key Idea

- Make easy decisions first to constrain the harder decisions
- Learns to dynamically order the decisions
- Analogous to constraint satisfaction algorithms

Easy-First Learning as Imitation Learning

- Imitation learning with a non-deterministic oracle policy
 multiple good decisions (actions) at a state
- Ties are broken with the learned policy (scoring function)
- NLP researchers employ imitation learning ideas and call them "training with exploration"
 - Miguel Ballesteros, Yoav Goldberg, Chris Dyer, Noah A. Smith: Training with Exploration Improves a Greedy Stack-LSTM Parser. CoRR abs/1603.03793 (2016)
- Imitation learning ideas are also employed in training recurrent neural networks (RNNs) under the name (ask advalated equality of)
 - "scheduled sampling"
 - Samy Bengio, Oriol Vinyals, Navdeep Jaitly, Noam Shazeer: Scheduled Sampling for Sequence Prediction with Recurrent Neural Networks. NIPS 2015

Part 4: Control Knowledge Learning: Beam Search Methods

Beam Search Framework

• Given

- Search space definition (ordered or unordered)
- Training examples (input-output pairs)
- Beam width B (>1)

Learning Goal

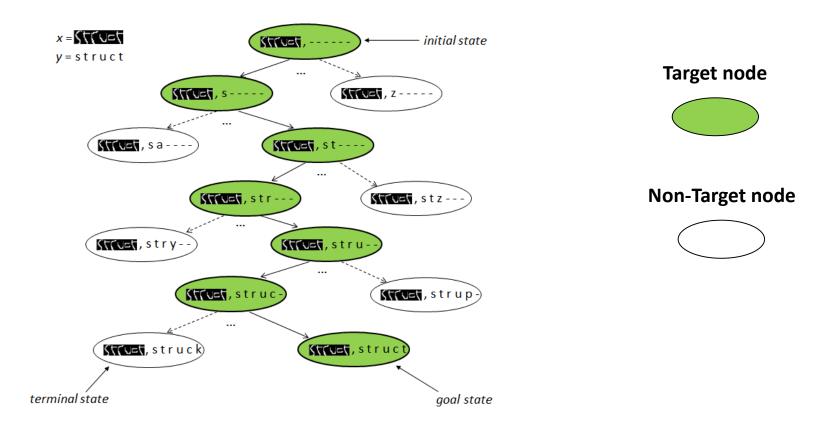
Learn a heuristic function to quickly guide the search to the correct "complete" output

• Key Idea:

- Structured prediction as a search problem in the space of partial outputs
- Training examples define target paths from initial state to the goal state (correct structured output)

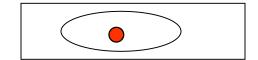
Beam Search Framework: Key Elements

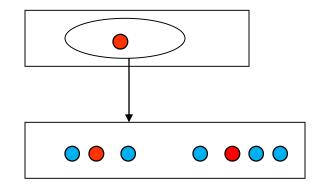
• 1) Search space; 2) Search procedure; 3) Heuristic function

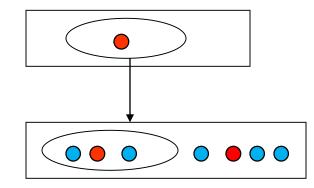


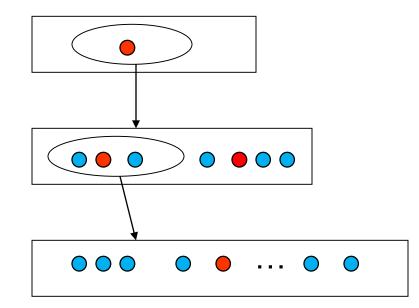
Represent heuristic function as a linear function

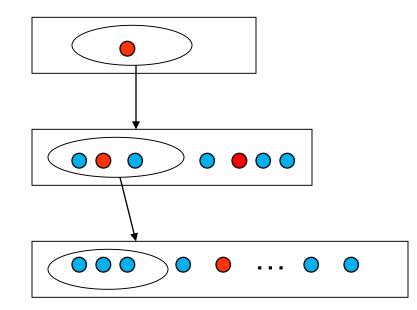
• $H(n) = w \cdot \psi(n)$, where $\psi(n)$ stands for features of node n











Beam Search Framework: Inference

 Input: learned weights w; beam width B; structured input x

repeat

- Perform search with heuristic $H(n) = w \cdot \psi(n)$
- until reaching a terminal state
- Output: the complete output y corresponding to the terminal state

Beam Search Framework: Generic Learning Template

Three design choices

- How to define the notion of "search error"?
- How to "update the weights" of heuristic function when a search error is encountered?
- A How to "update the beam" after weight update?

Beam Search Framework: Learning Instantiations

Early update

[Collins and Roark, 2004]

• Max-violation update [Huang et al., 2012]

Learning as Search Optimization (LaSO)

[Daume et al., 2005], [Xu et al., 2009]

Beam Search Framework: LaSO

• Search error: NO target node in the beam

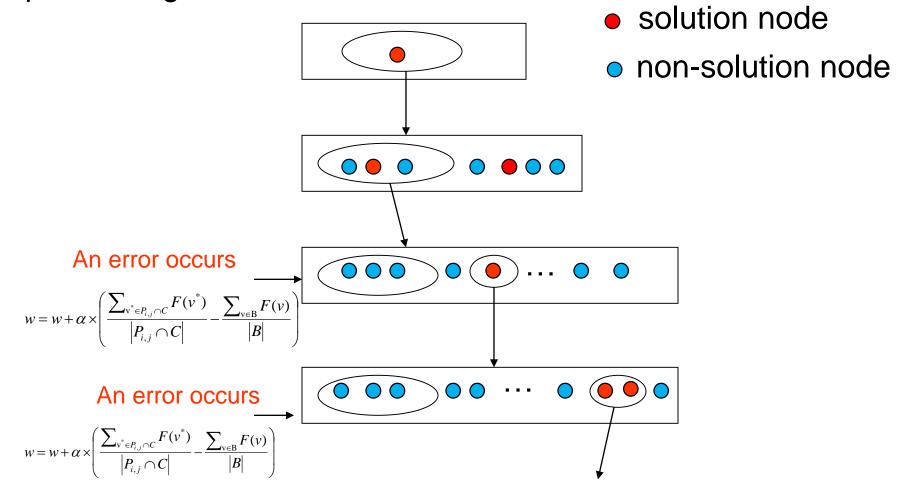
We cannot reach the goal node (correct structured output)

• Weight update: perceptron update

- $w_{new} = w_{old} + \alpha \cdot (\psi_{avg}(target) \psi_{avg}(non target))$
- $\psi_{avg}(target)$ = Average features of all target nodes in the candidate set
- $\psi_{avg}(non target)$ = Average features of all non-target nodes in the candidate set
- Intuition: increase the score of target nodes and decrease the score of the non-target nodes
- Beam update: reset beam with target nodes in the candidate set

LaSO Training: Illustration

Basic Idea: repeatedly conduct search on training examples update weights when error occurs



Beam Search Framework: LaSO

repeat

• For every training example (x, y)

- Perform search with current heuristic (weights)
- If search error, update weights
- Reset beam with target nodes in the candidate set
- Continue search
- until convergence or max. iterations

LaSO Convergence Results

 Under certain assumptions, LaSO-BR converges to a weight vector that solves all training examples in a finite number of iterations

Interesting convergence result

- Mistake bound depends on the beam width
- Formalizes the intuition that learning becomes easier as we increase the beam width (increase the amount of search)
- First formal result of this kind

Part 5: HC-Search: A Unifying Framework for Cost Function and Control Knowledge Learning

Outline of HC-Search Framework

Introduction

- Unifying view and high-level overview
- Learning Algorithms
 - Heuristic learning
 - Cost function learning
- Search Space Design
- Engineering Methodology for applying HC-Search
- Relation to Alternate Methods

Outline of HC-Search Framework

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- Unifying view and high-level overview
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HC-Search: A Unifying View

Cost Function Learning Approaches

Don't learn search control knowledge

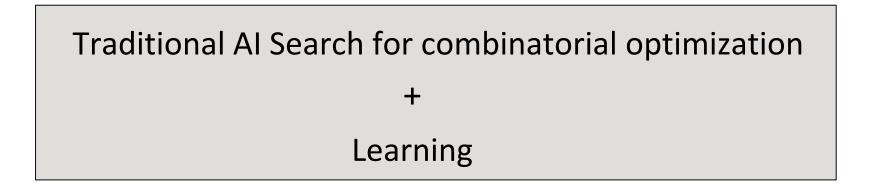
Control Knowledge Learning Approaches

Don't learn cost functions

HC-Search Learning Framework

- Unifies the above two frameworks and has many advantages
- Without H, degenerates to cost function learning
- Without C, degenerates to control knowledge learning
- Supports learning to improve both speed and accuracy of structured prediction

HC-Search framework: Inspiration



HC-Search Framework

HC-Search Framework: Overview

• Key Idea:

- Generate high-quality candidate outputs by conducting a time-bounded search guided by a learned heuristic *H*
- Score the candidate outputs using a learned cost function C to select the least cost output as prediction

Heuristic Learning

- can be done in primitive space (e.g., IJCAI'16 paper on incremental parsing)
- OR complete output space

IJCAI'16 paper on computing M-Best Modes via Heuristic Search

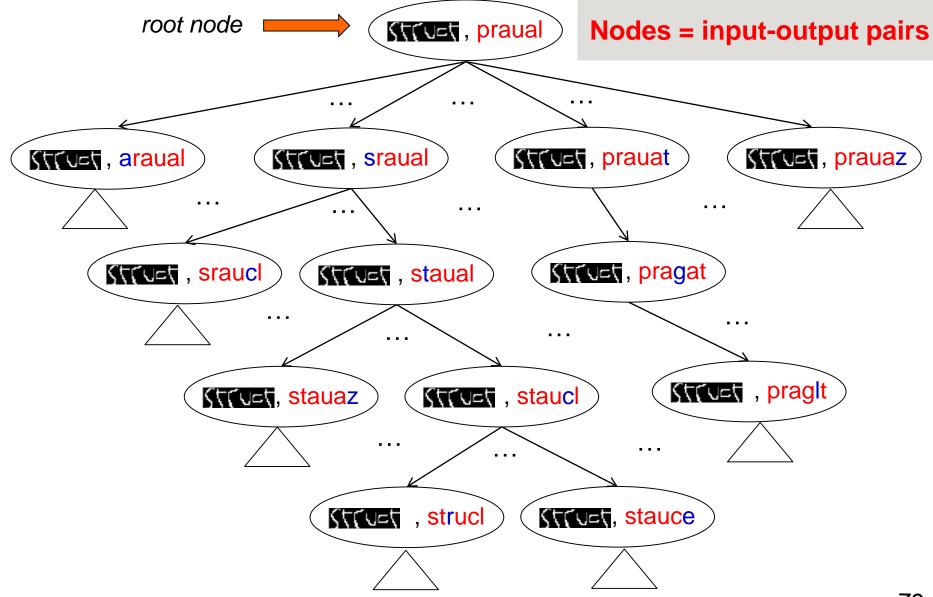
HC-Search framework: Overview

Our approach:

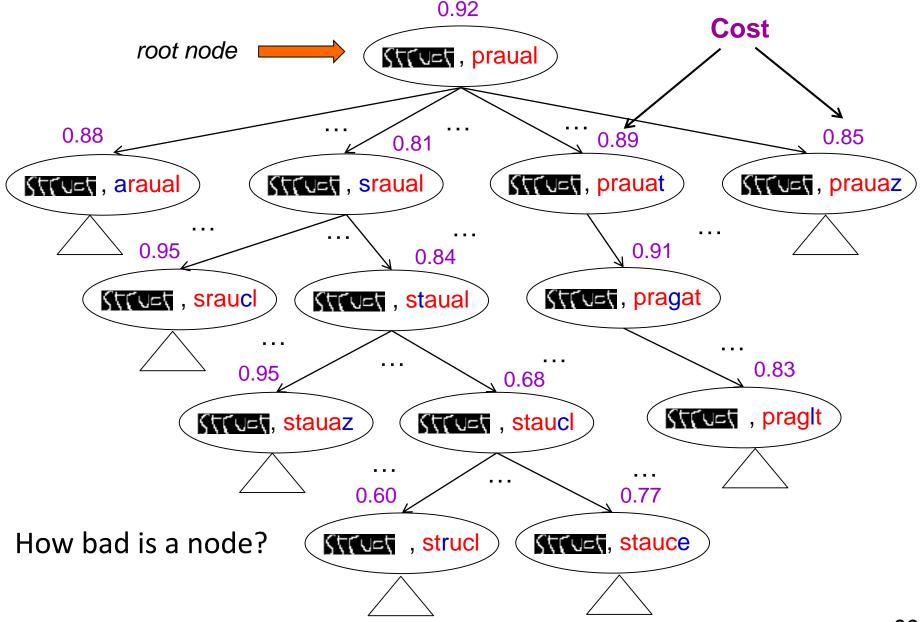
 Structured Prediction as a search process in the combinatorial space of outputs

- Key Ingredients:
 - Define a search space over structured outputs
 - Learn a cost function C to score potential outputs
 - Use a search algorithm to find low cost outputs
 - Learn a heuristic function H to make search efficient

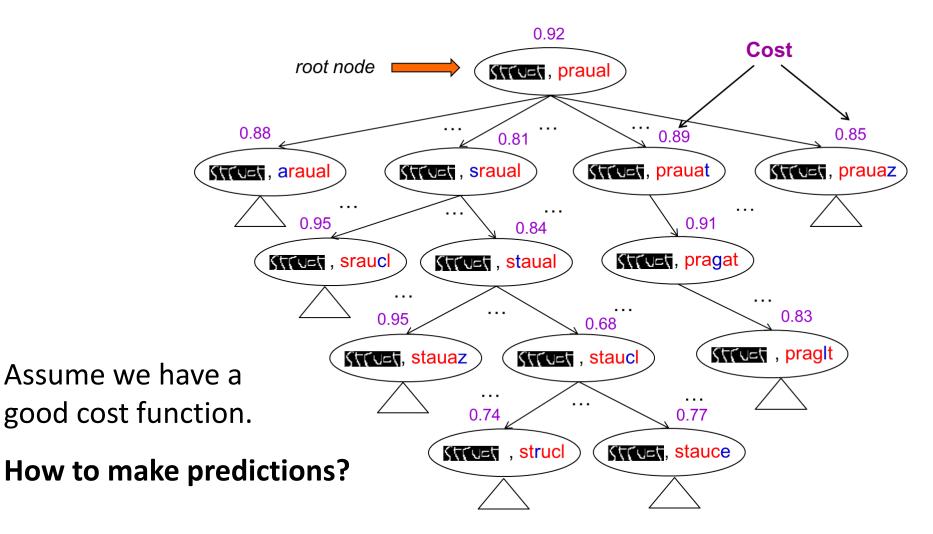
HC-Search Illustration: Search Space

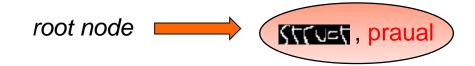


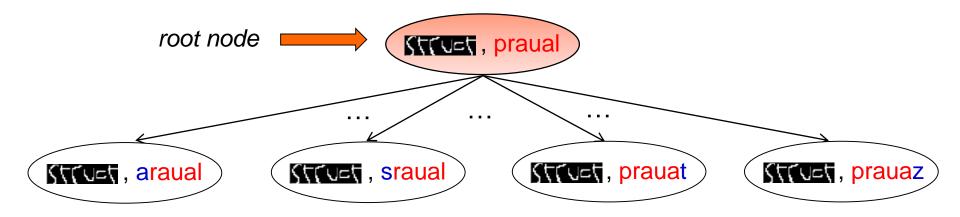
HC-Search Illustration: Cost Function

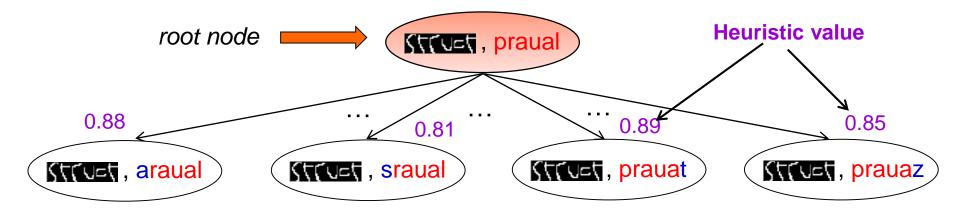


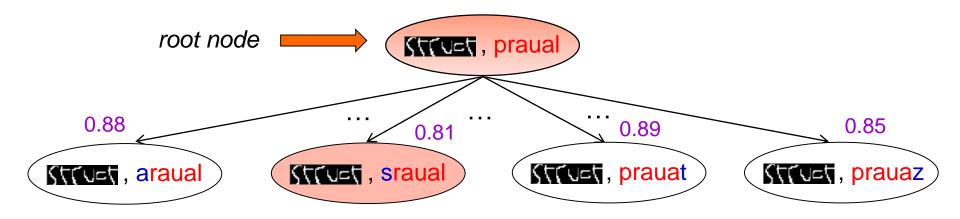
HC-Search Illustration: Making Predictions

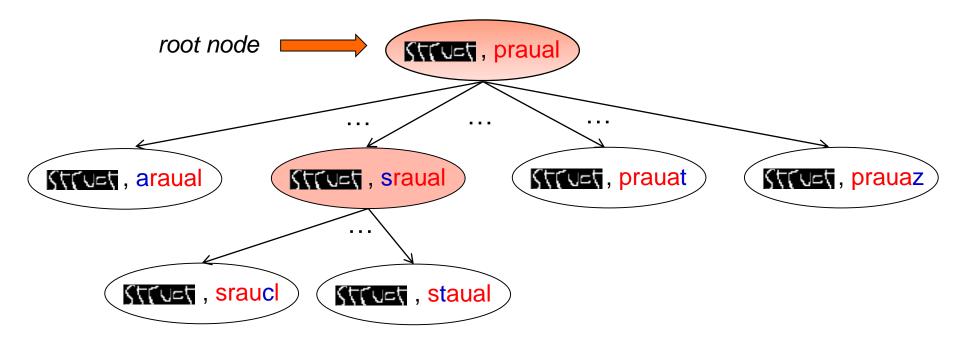


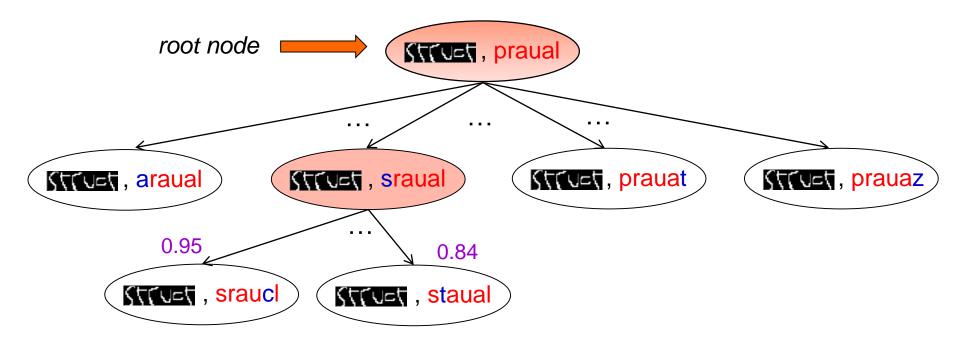


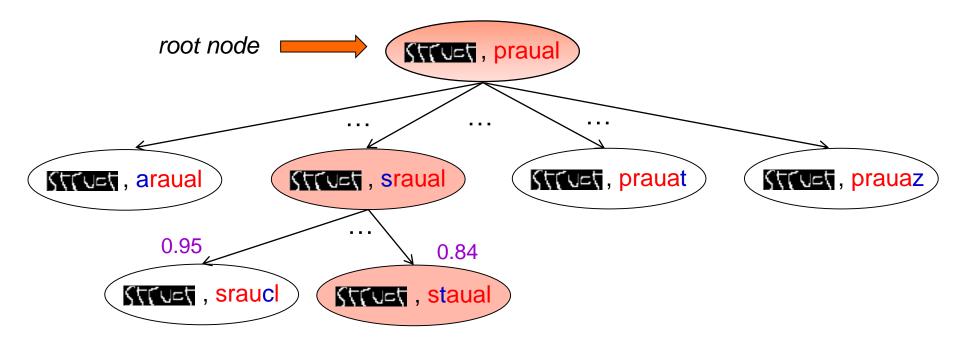


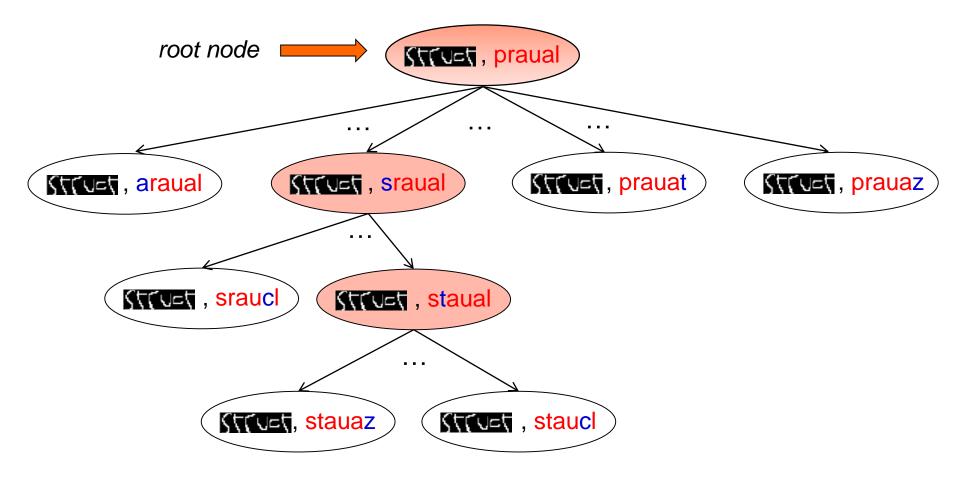


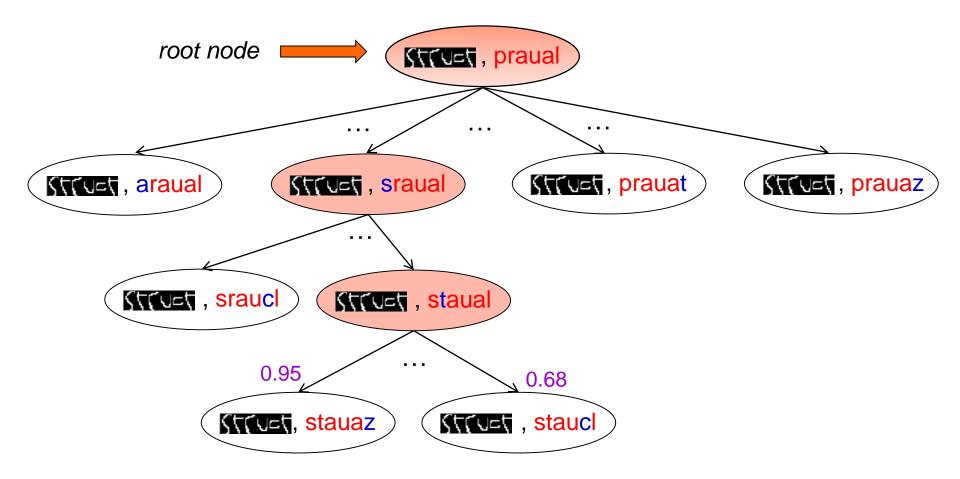


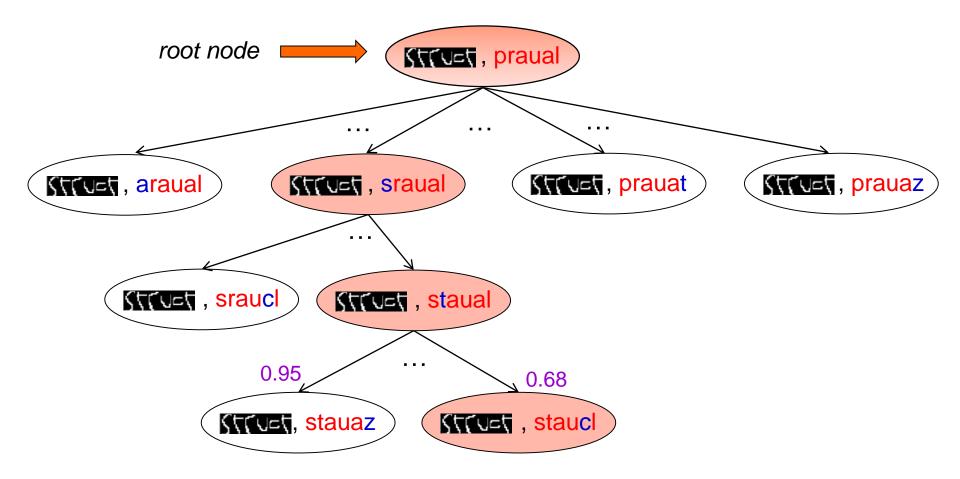


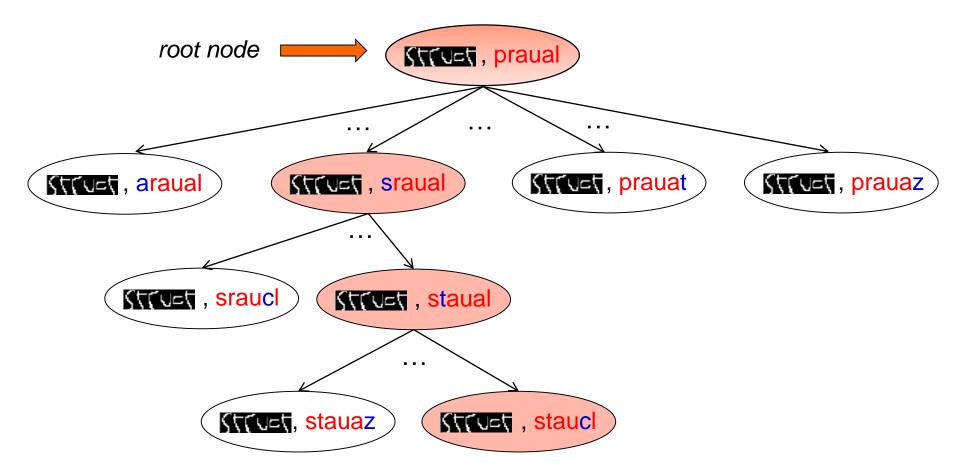


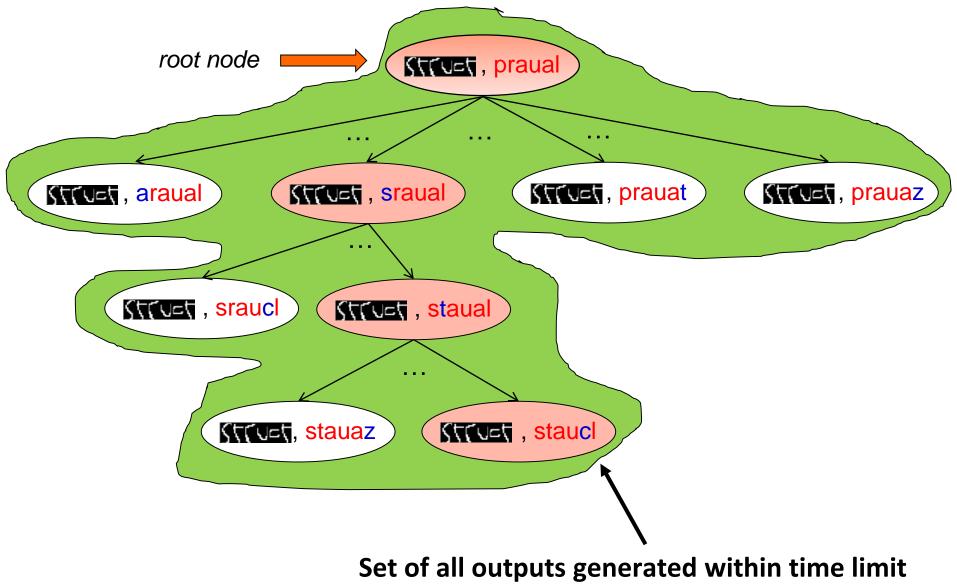


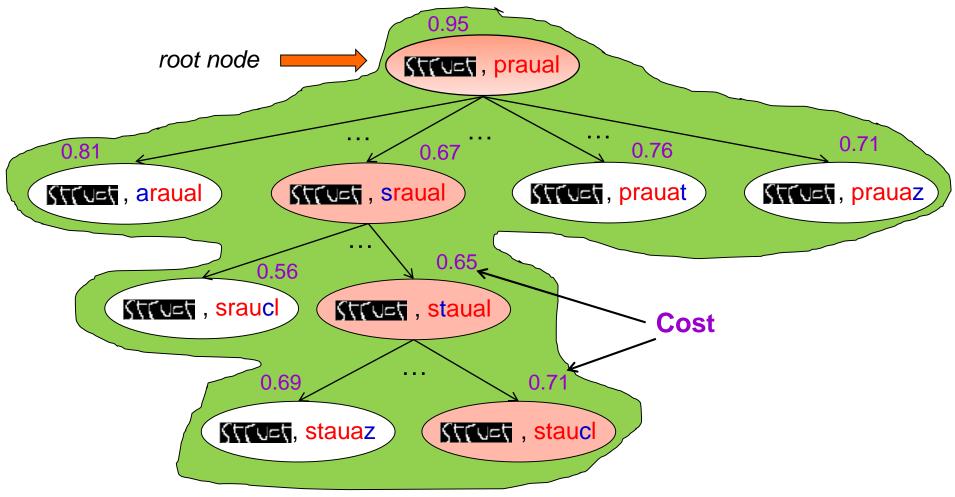


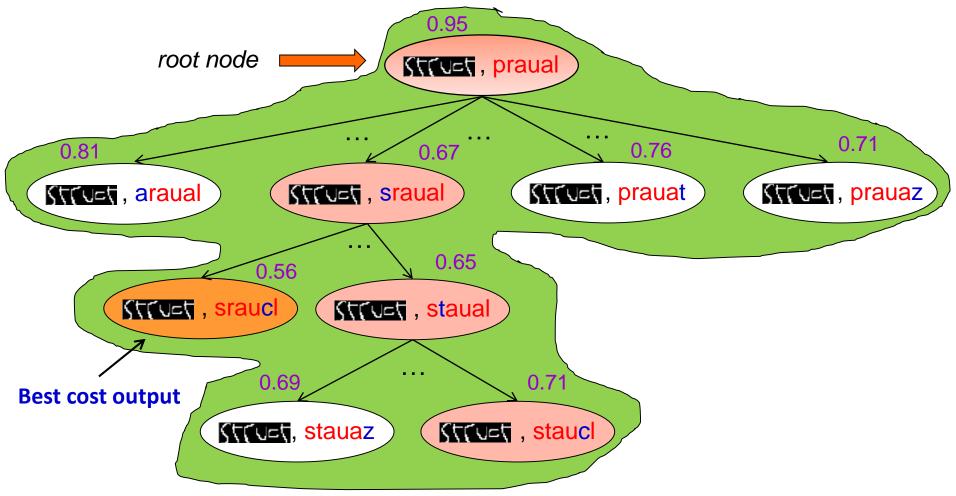


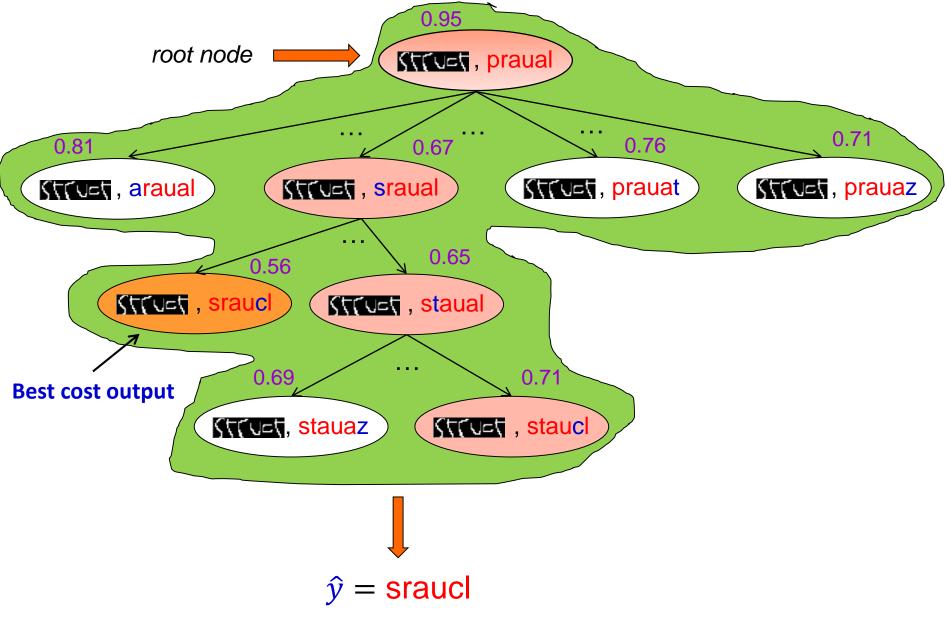












HC-Search: Properties

- Anytime predictions
 - Stop the search at any point and return the best cost output
- Minimal restrictions on the complexity of heuristic and cost functions
 - Only needs to be evaluated on complete input-output pairs
 - Can use higher-order features with negligible overhead
- Can optimize non-decomposable loss functions
 - e.g., F1 score
- Error Analysis: Heuristic error + Cost function error
 - engineering methodology guided by the error decomposition

HC-Search: Key Learning Challenges

• Search Space Design:

How can we automatically define high-quality search spaces ?

• Heuristic Learning:

How can we learn a heuristic function to guide the search to generate high-quality outputs ?

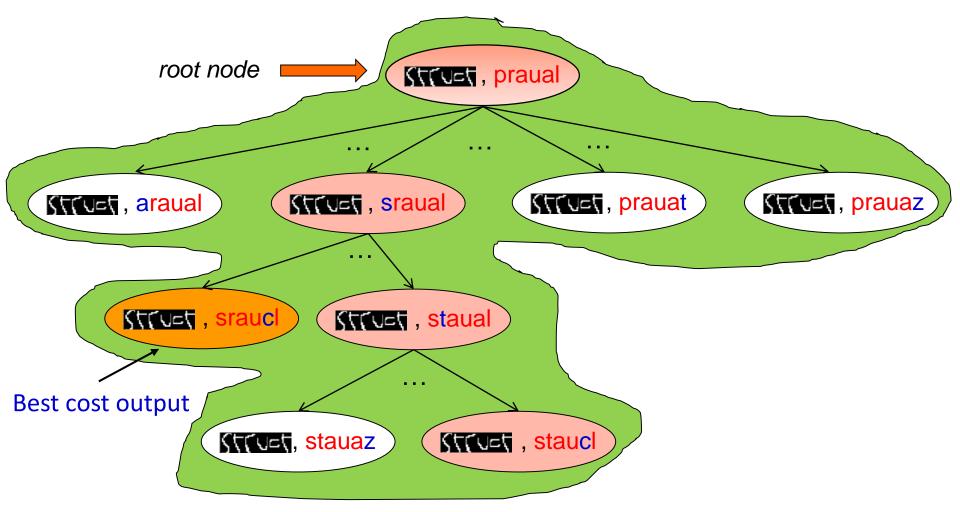
Cost Function Learning:

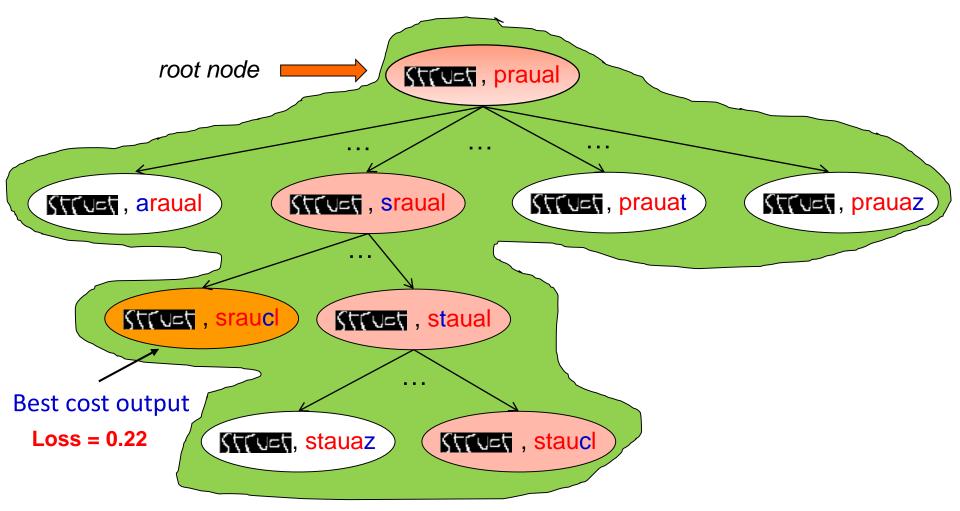
How can we learn a cost function to score the outputs generated by the heuristic function ?

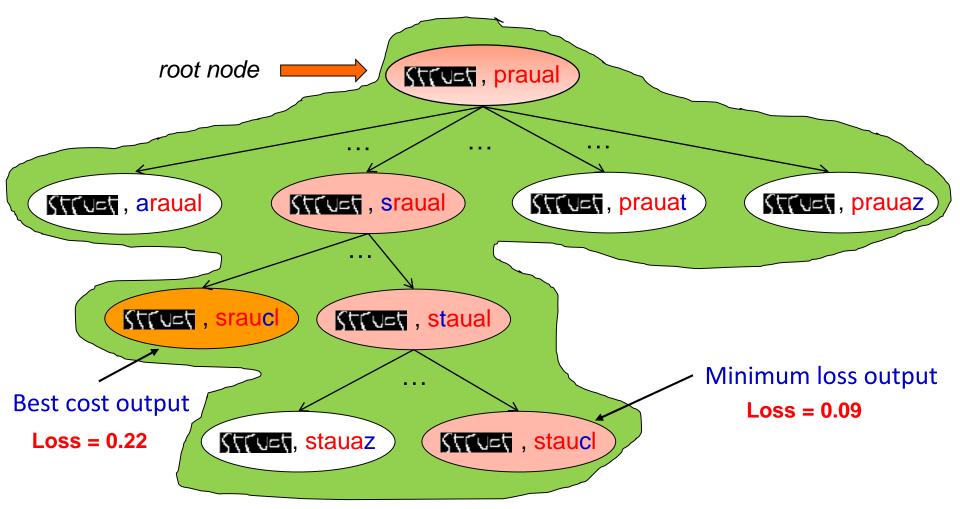
Outline of HC-Search Framework

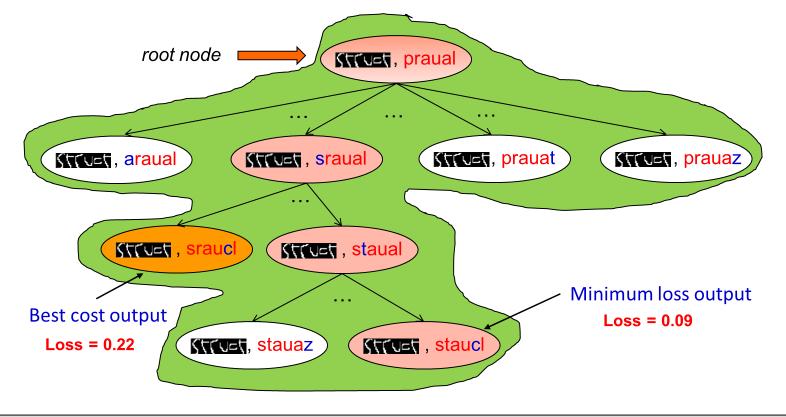
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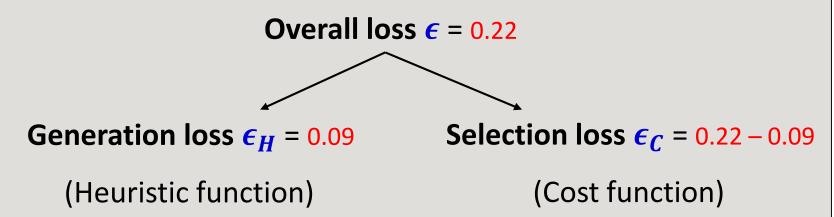
- Unifying view and high-level overview
- Learning Algorithms
 - Heuristic learning
 - Cost function learning
- Search Space Design
- Engineering Methodology for applying HC-Search
- Relation to Alternate Methods







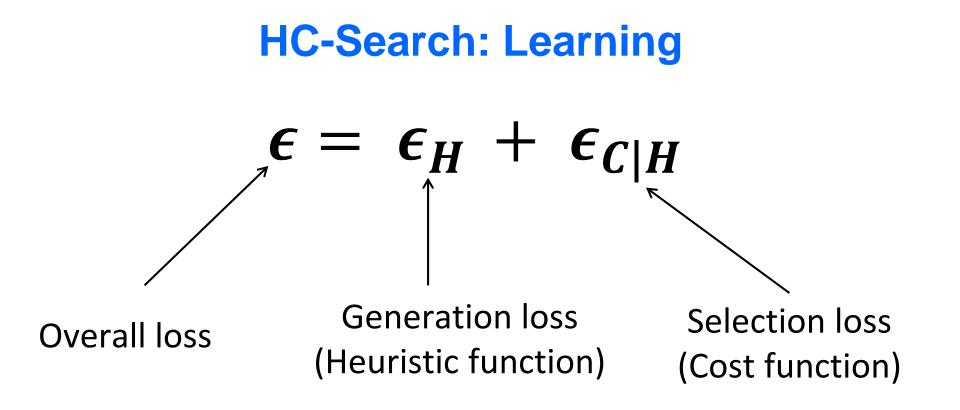




$$C(x, y) = w_{c} \cdot \phi_{H}(x, y)$$

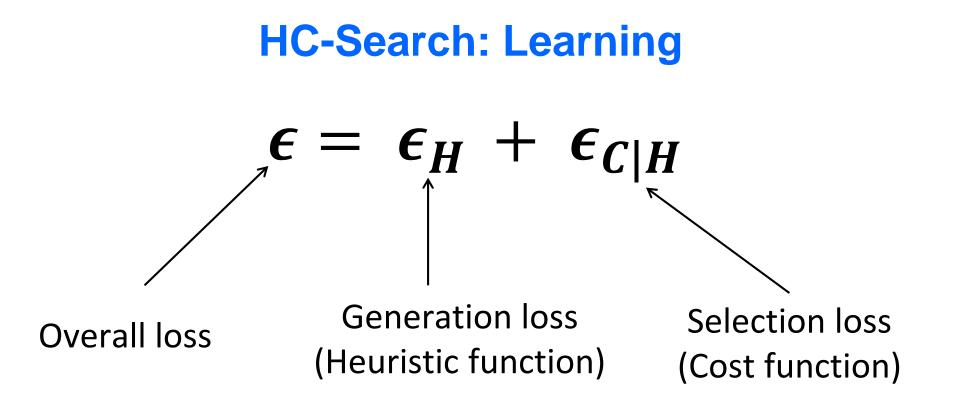
$$H(x, y) = w_{H} \cdot \phi_{C}(x, y)$$

$$C(x, y) = \psi_{H} \cdot \phi_{C}(x, y$$



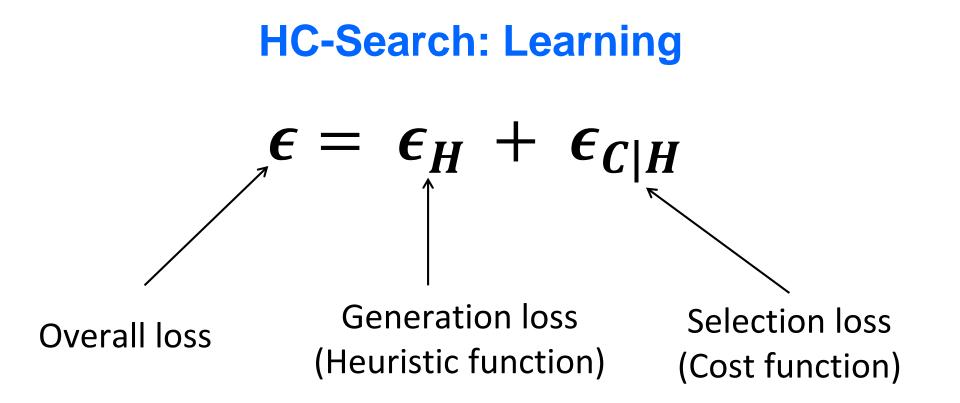
 Key idea: Greedy stage-wise minimization guided by the loss decomposition

Doppa, J.R., Fern, A., Tadepalli, P. HC-Search: A Learning Framework for Search-based Structured Prediction. Journal of Artificial Intelligence Research (JAIR) 2014.



 Key idea: Greedy stage-wise minimization guided by the loss decomposition

• Step 1: $\hat{H} = \arg \min_{H \in H} \epsilon_H$ (heuristic training)



 Key idea: Greedy stage-wise minimization guided by the loss decomposition

- Step 1: $\widehat{H} = \arg \min_{H \in H} \epsilon_H$ (heuristic training)
- Step 2: $\hat{C} = \arg \min_{C \in C} \epsilon_{C|\hat{H}}$ (cost function training)

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HC-Search: Heuristic learning

• Learning Objective:

 Guide the search quickly towards high-quality (low loss) outputs

HC-Search: Heuristic Learning

• Given a search procedure (e.g., greedy search)

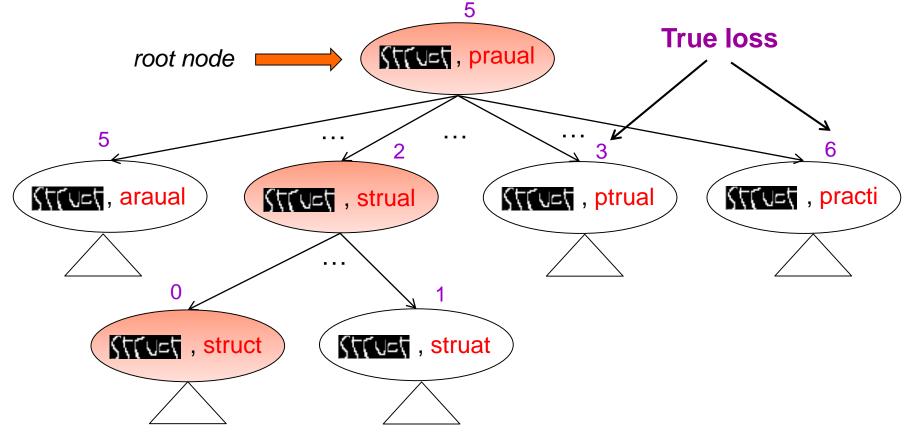
• Key idea: Imitation of true loss function

 Conduct searches on training example using the true loss function as a heuristic

(generally is a good way to produce good outputs)

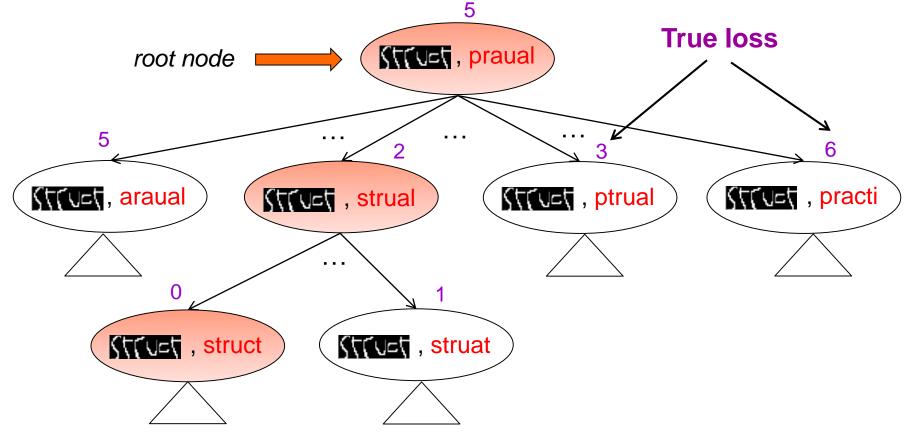
 Learn a heuristic function that tries to imitate the observed search behavior

Greedy Search: Imitation with true loss



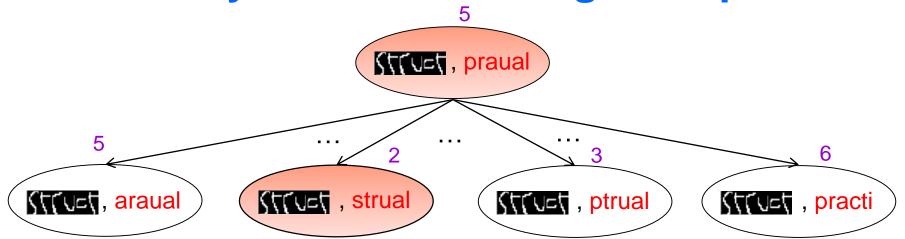


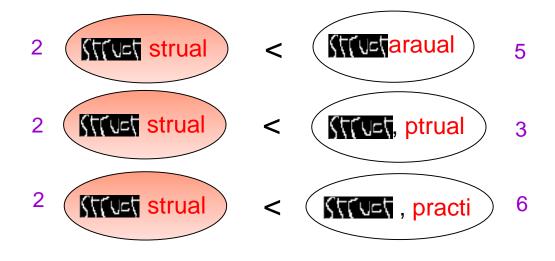
Greedy Search: Imitation with true loss



Generation loss $\epsilon_{H^*} = 0$

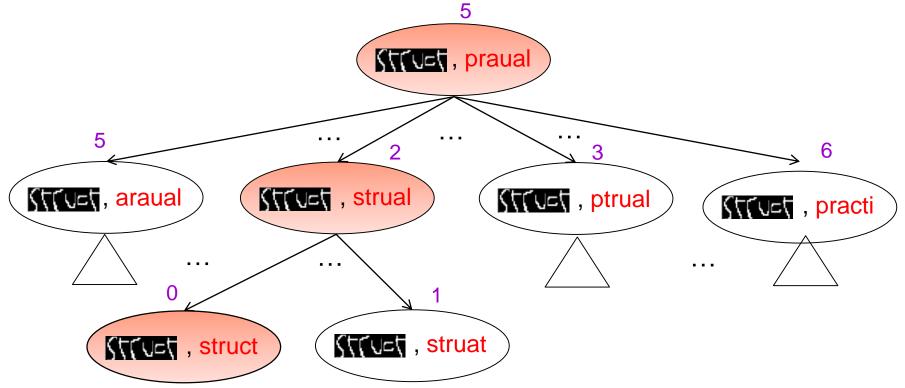
Greedy Search: Ranking examples



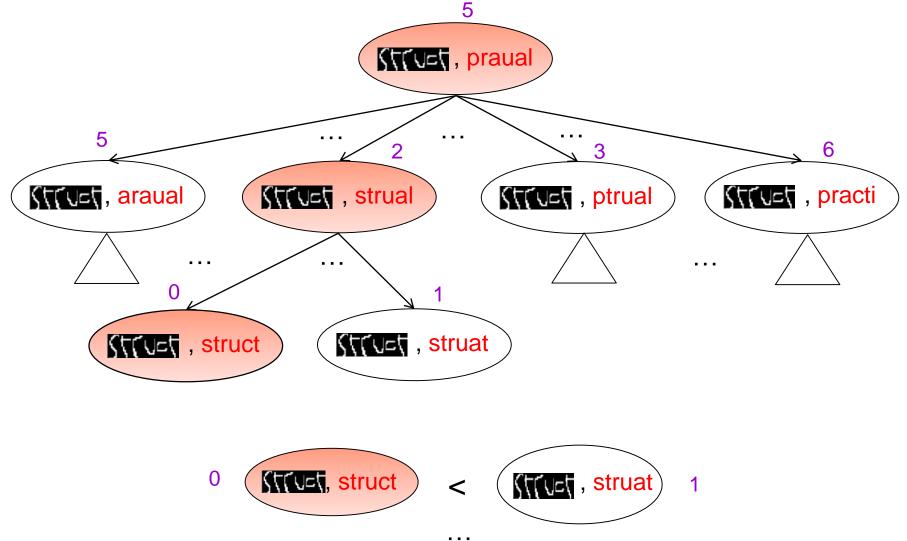


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Greedy Search: Ranking examples

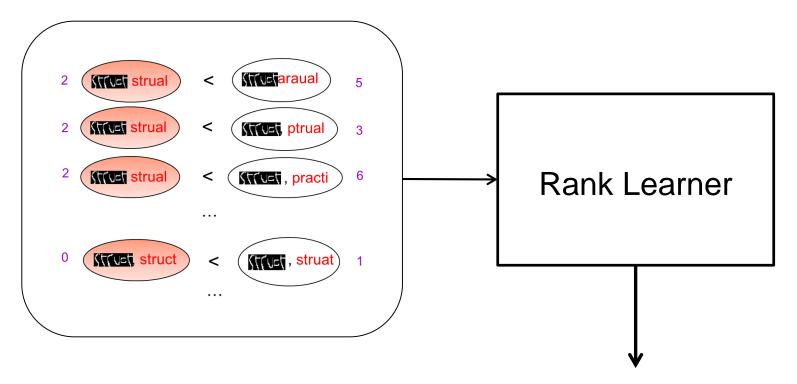


Greedy Search: Ranking examples



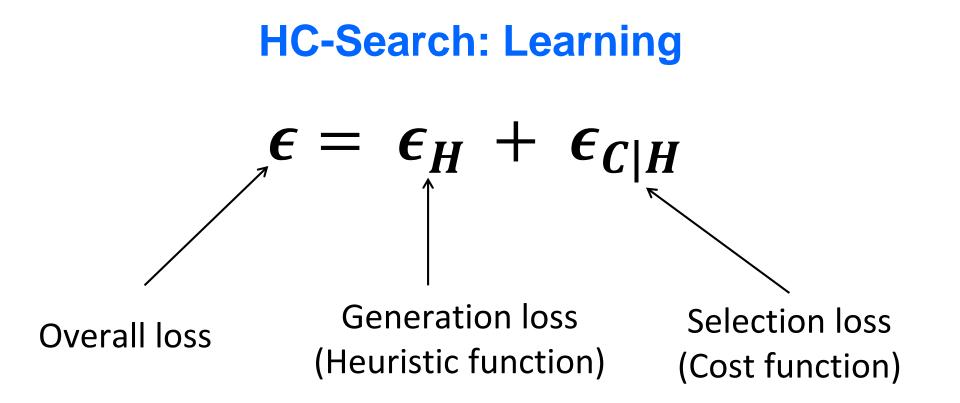
HC-Search: Heuristic Function Learning

Ranking examples



Heuristic function \widehat{H}

Can prove generalization bounds on learned heuristic [Doppa et al., 2012]



 Key idea: Greedy stage-wise minimization guided by the loss decomposition

- Step 1: $\widehat{H} = \arg \min_{H \in H} \epsilon_H$ (heuristic training)
- Step 2: $\hat{C} = \arg \min_{C \in C} \epsilon_{C|\hat{H}}$ (cost function training)

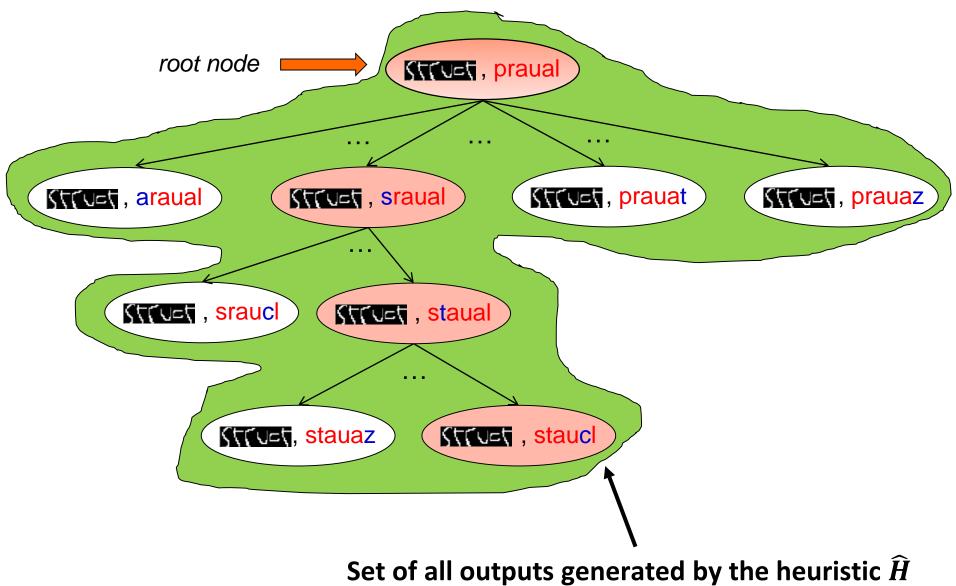
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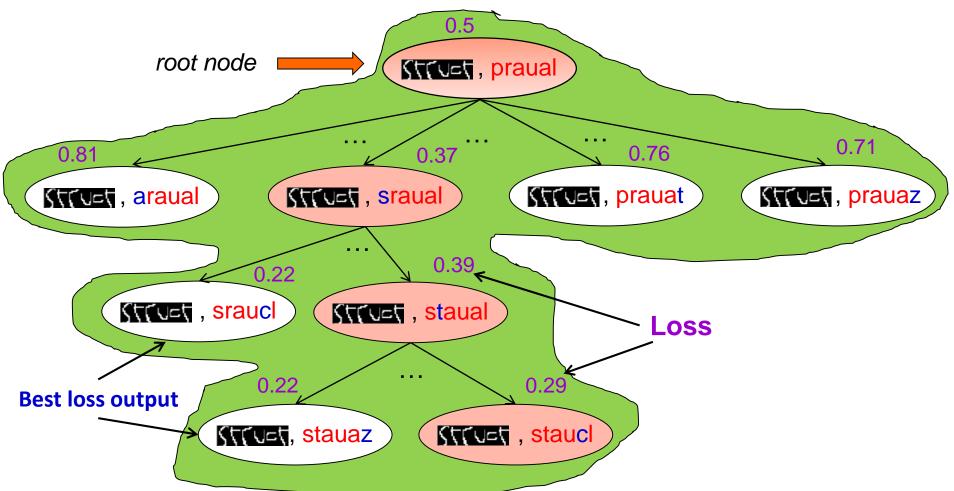
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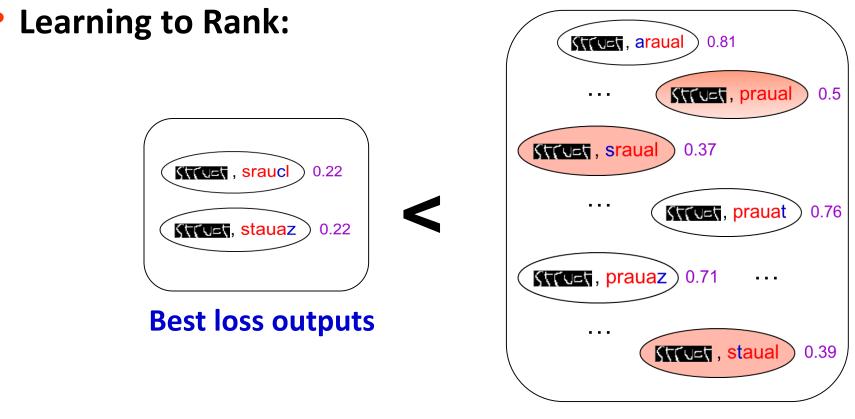
• Learning Objective:

 Correctly score the outputs generated by the heuristic as per their losses





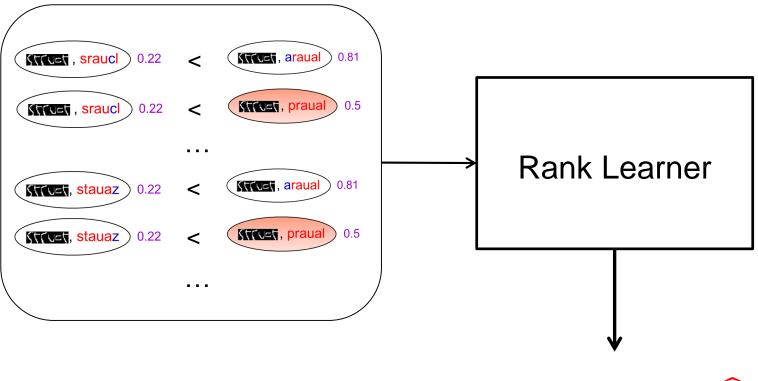
• Key Idea: Learn to rank the outputs generated by the learned heuristic function \widehat{H} as per their losses



Non-best loss outputs

Create a ranking example between every pair of outputs (y_{best}, y) such that: C(x, y_{best}) < C(x, y)

Ranking examples



Cost function \widehat{C}

Can borrow generalization bounds from rank-learning literature [Agarwal and Roth, 2005 & Agarwal and Niyogi, 2009]

Outline of HC-Search Framework

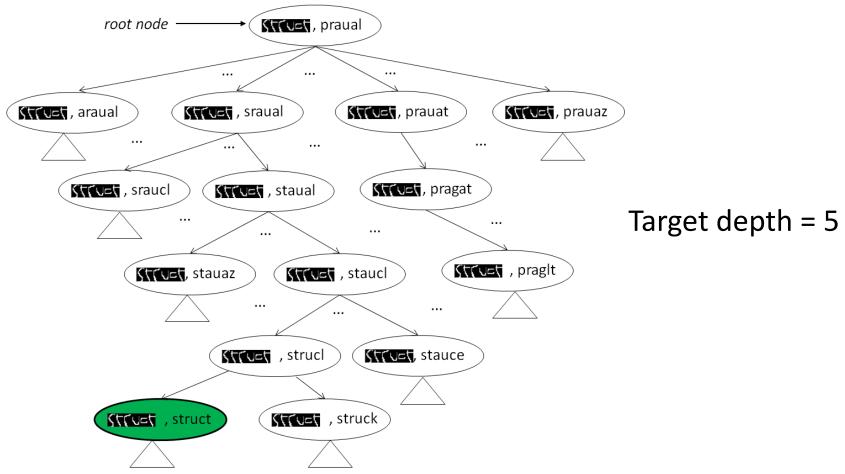
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HC-Search: Search Space Design

• Objective:

High-quality outputs can be located at small depth



HC-Search: Search Space Design

• Objective:

High-quality outputs can be located at small depth

• Solution #1:

Flipbit Search Space [JMLR, 2014]

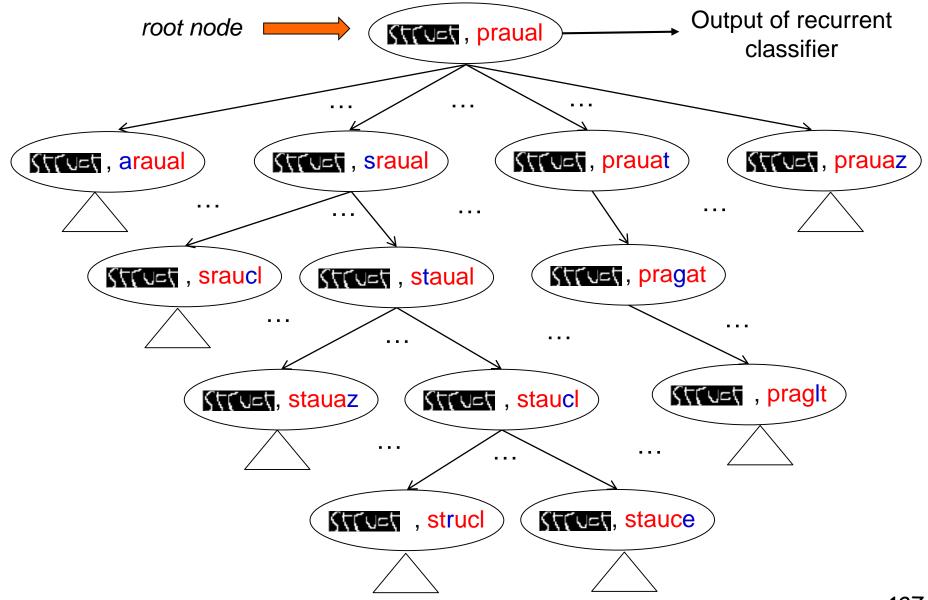
Solution #2:

- Limited Discrepancy Search (LDS) Space [JMLR, 2014]
- Defined in terms of a greedy predictor or policy

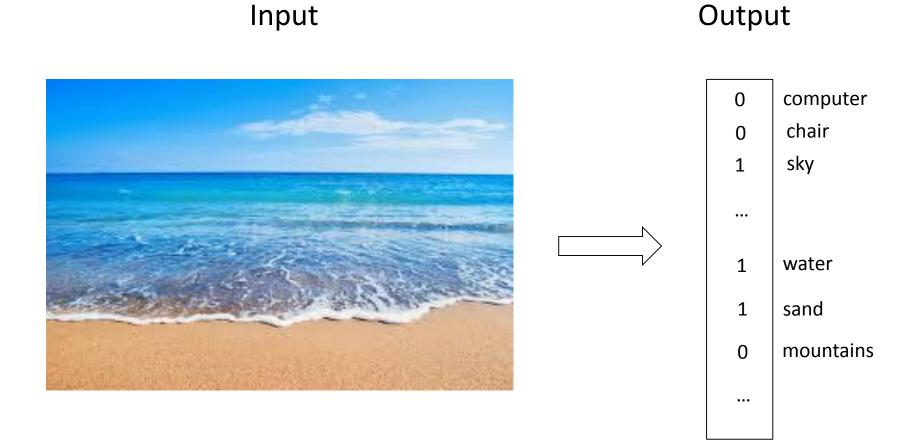
Solution #3:

Segmentation Search Space for computer vision tasks [CVPR, 2015]

Flip-bit Search Space



Multi-Label Prediction: Problem



Multi-Label Prediction: Problem

- Commonly arises in various domains
 - Biology predict functional classes of a protein/gene
 - Text predict email tags or document classes



Multi-Label Prediction

Benchmark data

Dataset	Domain	#TR	#TS	#F	#L	<i>E</i> [<i>d</i>]
Scene	image	1211	1196	294	6	1.07
Emotions	music	391	202	72	6	1.86
Medical	text	333	645	1449	45	1.24
Genbase	biology	463	199	1185	27	1.25
Yeast	biology	1500	917	103	14	4.23
Enron	text	1123	579	1001	53	3.37
LLog	text	876	584	1004	75	1.18
Slashdot	text	2269	1513	1079	22	2.15

Multi-Label Prediction

Benchmark data

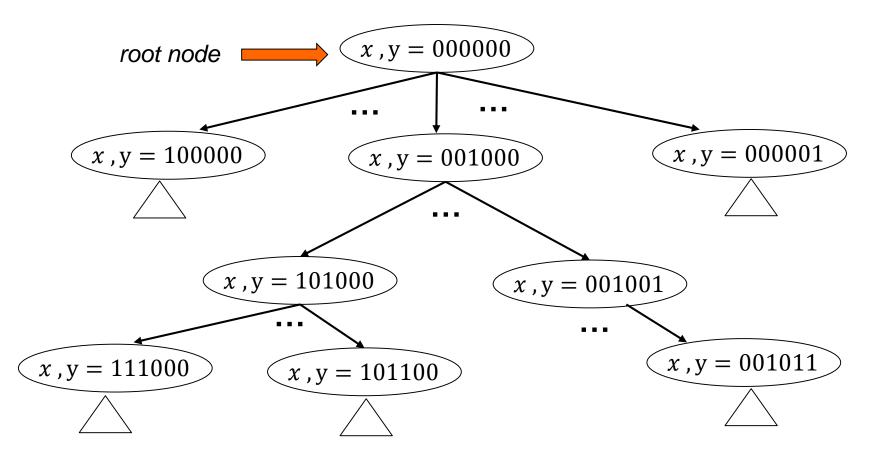
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Slashdot	text	2269	1513	1079	1	2.15		

Label vectors are highly sparse

Multi-Label Prediction via HC-Search

• HC-Search

Exploit the sparsity property (Null vector + flip bits)



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Engineering Methodology

Select a time-bounded search architecture

- High-quality search space (e.g., LDS space or its variant)
- Search procedure
- Time bound
- Effectiveness can be measured by performing LL-Search (loss function as both heuristic and cost function)

Training and Debugging

- Overall error = generation error (heuristic) + selection error (cost function)
- Take necessary steps to improve the appropriate error guided by the decomposition

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HC-Search vs. CRF/SSVM

- Inference in CRF/SSVM
 - Cost function needs to score exponential no. of outputs

$$F(x) = \arg \min_{y \in Y(x)} C(x, y)$$

- Inference in HC-Search
 - Cost function needs to score only the outputs generated by the search procedure guided by heuristic *H*

$$F(x) = \arg \min_{y \in Y_H(x)} C(x, y)$$

HC-Search vs. Re-Ranking Algorithms

Re-Ranking Approaches

k-best list from a generative model

Michael Collins: *Ranking Algorithms for Named Entity Extraction: Boosting and the Voted Perceptron*. ACL 2002: 489-496

Diverse M-best modes of a probabilistic model

Payman Yadollahpour, Dhruv Batra, Gregory Shakhnarovich: Discriminative Re-ranking of Diverse Segmentations. CVPR 2013: 1923-1930

No guarantees on the quality of generated candidate set

• HC-Search

- Candidate set is generated via generic search in high-quality search spaces guided by the learned heuristic
- Minimal restrictions on the representation of heuristic
- PAC guarantees on the quality of candidate set

HC-Search: A "Divide-and-Conquer" Solution

- HC-Search is a "Divide-and-Conquer" solution with procedural knowledge injected into it
 - All components have clearly pre-defined roles
 - Every component is contributing towards the overall goal by making the role of other components easier

HC-Search: A "Divide-and-Conquer" Solution

- Every component is contributing towards the overall goal by making the role of other components easier
 - LDS space leverages greedy classifiers to reduce the target depth to make the heuristic learning easier
 - Heuristic tries to make the cost function learning easier by generating high-quality outputs with as little search as possible

Advances in cost function learning

Amortized inference and learning with ILP:

Vivek Srikumar, Gourab Kundu, Dan Roth: On Amortizing Inference Cost for Structured Prediction. EMNLP 2012 Gourab Kundu, Vivek Srikumar, Dan Roth: Margin-based Decomposed Amortized Inference. ACL 2013 Kai-Wei Chang, Shyam Upadhyay, Gourab Kundu, Dan Roth: Structural Learning with Amortized Inference. AAAI 2015

PAC theory for ILP inference:

Ofer Meshi, Mehrdad Mahdavi, Adrian Weller, David Sontag: Train and Test Tightness of LP Relaxations in Structured Prediction. ICML 2016

Decomposed learning:

Rajhans Samdani, Dan Roth: Efficient Decomposed Learning for Structured Prediction. ICML 2012

Structured prediction cascades:

David J. Weiss, Benjamin Taskar: Structured Prediction Cascades. AISTATS 2010: 916-923

Classifier-based structured Prediction

Recurrent classifier:

Thomas G. Dietterich, Hermann Hild, Ghulum Bakiri: A Comparison of ID3 and Backpropagation for English Textto-Speech Mapping. Machine Learning 18(1): 51-80 (1995)

PAC Results and Error Propagation:

Roni Khardon: Learning to Take Actions. Machine Learning 35(1): 57-90 (1999)

Alan Fern, Sung Wook Yoon, Robert Givan: Approximate Policy Iteration with a Policy Language Bias: Solving Relational Markov Decision Processes. J. Artif. Intell. Res. (JAIR) 25: 75-118 (2006)

Umar Syed, Robert E. Schapire: A Reduction from Apprenticeship Learning to Classification. NIPS 2010

Stéphane Ross, Drew Bagnell: Efficient Reductions for Imitation Learning. AISTATS 2010: 661-668

Advanced Imitation Learning Algorithms:

SEARN: Hal Daumé III, John Langford, Daniel Marcu: Search-based structured prediction. Machine Learning 75(3): 297-325 (2009)

DAgger: Stéphane Ross, Geoffrey J. Gordon, Drew Bagnell: A Reduction of Imitation Learning and Structured Prediction to No-Regret Online Learning. AISTATS 2011: 627-635

AggreVaTe: Stéphane Ross, J. Andrew Bagnell: Reinforcement and Imitation Learning via Interactive No-Regret Learning. CoRR abs/1406.5979 (2014)

LOLS: Kai-Wei Chang, Akshay Krishnamurthy, Alekh Agarwal, Hal Daumé III, John Langford: Learning to Search Better than Your Teacher. ICML 2015: 2058-2066

Yuehua Xu, Alan Fern, Sung Wook Yoon: Iterative Learning of Weighted Rule Sets for Greedy Search. ICAPS 2010: 201-208

Alan Fern, Sung Wook Yoon, Robert Givan: Approximate Policy Iteration with a Policy Language Bias: Solving Relational Markov Decision Processes. J. Artif. Intell. Res. (JAIR) 25: 75-118 (2006) 141

• Easy-first approach for structured Prediction

Yoav Goldberg, Michael Elhadad: An Efficient Algorithm for Easy-First Non-Directional Dependency Parsing. HLT-NAACL 2010

Karthik Raghunathan, Heeyoung Lee, Sudarshan Rangarajan, Nate Chambers, Mihai Surdeanu, Dan Jurafsky, Christopher D. Manning: A Multi-Pass Sieve for Coreference Resolution. EMNLP 2010

Lev-Arie Ratinov, Dan Roth: Learning-based Multi-Sieve Co-reference Resolution with Knowledge. EMNLP-CoNLL 2012

Veselin Stoyanov, Jason Eisner: Easy-first Coreference Resolution. COLING 2012

Jun Xie, Chao Ma, Janardhan Rao Doppa, Prashanth Mannem, Xiaoli Z. Fern, Thomas G. Dietterich, Prasad Tadepalli: Learning Greedy Policies for the Easy-First Framework. AAAI 2015

Learning Beam search heuristics for structured prediction

Michael Collins, Brian Roark: Incremental Parsing with the Perceptron Algorithm. ACL 2004

Hal Daumé III, Daniel Marcu: Learning as search optimization: approximate large margin methods for structured prediction. ICML 2005

Yuehua Xu, Alan Fern, Sung Wook Yoon: Learning Linear Ranking Functions for Beam Search with Application to Planning. Journal of Machine Learning Research 10: 1571-1610 (2009)

Liang Huang, Suphan Fayong, Yang Guo: Structured Perceptron with Inexact Search. HLT-NAACL 2012

• HC-Search Framework for structured Prediction

Janardhan Rao Doppa, Alan Fern, Prasad Tadepalli: HC-Search: A Learning Framework for Search-based Structured Prediction. J. Artif. Intell. Res. (JAIR) 50: 369-407 (2014)

Janardhan Rao Doppa, Alan Fern, Prasad Tadepalli: Structured prediction via output space search. Journal of Machine Learning Research 15(1): 1317-1350 (2014)

Janardhan Rao Doppa, Jun Yu, Chao Ma, Alan Fern, Prasad Tadepalli: HC-Search for Multi-Label Prediction: An Empirical Study. AAAI 2014

Michael Lam, Janardhan Rao Doppa, Sinisa Todorovic, Thomas G. Dietterich: HC-Search for structured prediction in computer vision. CVPR 2015

Part 6: Integrating Deep Learning and Structured Prediction

Liping Liu

Tufts University

Motivation

Deep models as non-linear functions

- mapping from the input to the output
- non-linear
- need fast training
- How about replacing functions with deep models?
 - potential function for CRF
 - search function for search based predicting models
 - attention model for structured prediction

Motivation

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Conditional Random Field (CRF)

• The basic form

•
$$P(y \mid x; w) = \frac{1}{Z(w)} \exp(\sum_k w_k \cdot \phi_k(x, y))$$

partition function $Z(w) = \sum_{y \in \mathcal{Y}} \exp(\sum_k w_k \cdot \phi_k(x, y))$

▲ The function $\phi_k(x, y) = \phi_k(x, y_{i_k})$ often defines the potential of a single label or a pair of labels

CRF extensions with Deep models

- Deep structured models [Chen et al. ICML 2015]
 - ▲ Replace linear potential $w_k \phi_k(\cdot)$ with a deep function $f_k(x, y; w)$ to extract information from complex object x
- Structured Prediction Energy Network (SPEN) [Belanger et al. ICML 2016, 2017]

• Replace $\sum_{k} w_{k} \cdot \phi_{k}(x, y)$ with a deep function F(x, y; w), so $P(y \mid x; w) = \frac{1}{Z(x,w)} \exp(F(x, y; w))$

- Deep Value Network (DVN) [Gygli et al. ICML 2017]
 - Learn a deep model v(x, y; w) to fit the negative loss (DVN)

Deep Structured Models

- Deep structured models [Chen et al. ICML 2015]
 - The potential F(x, y; w) is decomposable by nodes or node pairs,

$$F(x,y;w) = \sum_k f_k(x,y_{i_k};w)$$

• $f_k(x, y; w)$ is still a single or a pairwise potential

 DSM approximates the partition function with loopy belief propagation

$$\log Z(x,w) = \max_{p} E_p[F(x,y_{i_k};w)] + H[p]$$

(Treat *w* as a constant here)

• Approximate marginal of dist p by local beliefs

Structured Prediction Energy Network

• SPEN [Belanger et al. ICML 2016, 2017] allows high order label interactions through non-linear transformation of label vectors $\min F(x) = s t + x \in \{0, 1\}^L$

 $\min_{y} E_{x}(y) \quad s.t. \ y \in \{0, 1\}^{L}$

- Training in the same way as structured SVM
 - Minimize the hinge loss

 $\min_{w} \max_{y} \left[\Delta(y_i, y) - E_{x_i}(y) + E_{x_i}(y_i) \right]_+$

 Inner optimization problem is solved by LP relaxation, relaxing the space of discrete labels to a continuous one

Deep Value Networks (DVN)

- DVN [Gygli et al. ICML 2017] fit negative loss values
 - Train a network $v(x, y; \theta)$ such that $v(x, y; \theta) \approx -loss(y, y^*)$
- Trained with samples (x, y', -loss(y', y*)), with y' being
 - Training label y*
 - Inference result $\hat{y} = \arg \max v(x, y; \theta)$
 - Random samples
 - Adversarial samples
- Inference is done by optimization of y in the continuous space

Motivation

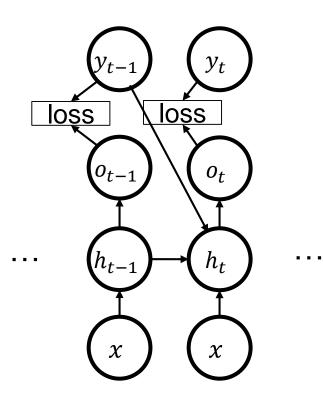
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RNN for Structured Prediction

- RNN can output predictions with structures
 - Input x, y_{t-1}

• Output y_t at time t



RNN for Structured Prediction

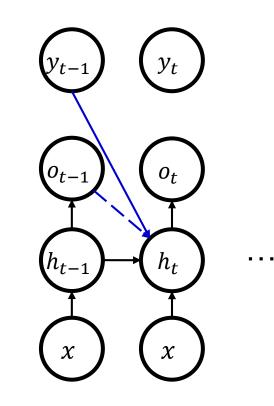
- RNN can output predictions with structures
 - Input x, y_{t-1}
 - Output y_t at time t
- Considerations for structured prediction
 - How to avoid exposure bias (i.e. teacher forcing makes training and testing different)?
 - How to include loss function in training?

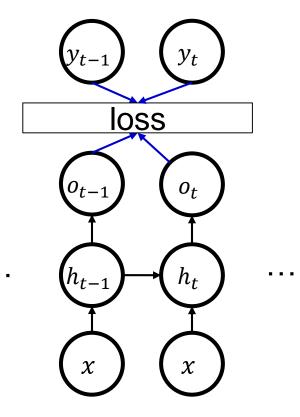
RNN for Structured Prediction

Two issues

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- Exposure bias (teacher enforcing)
- Loss-evaluation mismatch





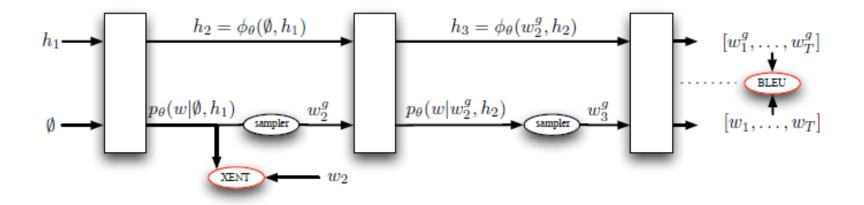
Structured Prediction as an RL Problem

Formulation as reinforcement learning

- (x, o_{t-1}, h_t) as a state
- Negative loss as reward
 - Reward is given at the last step
 - Zero reward for intermediate steps
- Output y_t at each step as action
- RNN as a policy
- Tackle two issues together
 - Minimize loss by maximize reward
 - Learning naturally corrects exposure bias

Training RNN with policy gradient

- Learn RNN with MIXER [Ranzato, ICLR 2016]
 - First time steps are trained by maximize likelihood
 - The last few steps are trained by REINFORCE
 - REINFORCE is a one policy gradient algorithm
 - Use a single sample from RNN to estimated expected reward



Actor-Critic Algorithm for RNN Learning

- An actor-critic algorithm for sequence prediction [Bahdanau et al. ICLR 2017]
 - Actor: $RNN(\theta)$
 - Critic: another network to estimated Q function
- Learning Procedure

Update actor/RNN with gradient,

$$\frac{dV}{d\theta} = E_{y \sim RNN(\theta)} \left[\sum_{t} \sum_{y'_t} \frac{d \ p(y'_t | y_{t-1}, h_t)}{d\theta} \widehat{Q}(y'_t, y_{1:t-1})) \right]$$

• Update critic/estimation of \hat{Q}

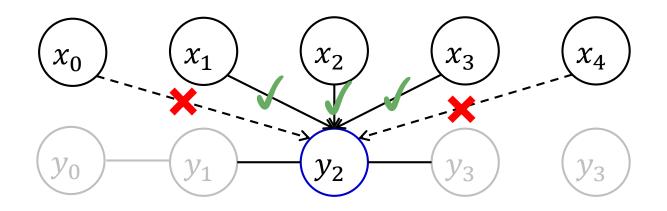
Motivation

Deep models as non-linear functions

- mapping from the input to the output
- non-linear
- need fast training
- How about replacing functions with deep models?
 - potential function for CRF
 - search function for search based predicting models
 - attention model for structured prediction

Structure design of structured prediction

- A single label does not need all inputs
- Let the model to decide which to use



Attention Model

- Attention model for image captioning [Xu et al. ICML 2015]
 - RNN model for image captioning
 - Output: a sequence of words
 - Input: feature vectors extracted from selected image locations at different time steps



A woman is throwing a <u>frisbee</u> in a park. Image is from the paper [Xu et al., ICML 2015]

Structured Attention Model

- Assume attention sequence has structures
 - Define attention sequence as CRF

 $p(attention z \mid output y_t, input x) = softmax(\theta_c(z_c))$

- End-to-end training
 - Gradient calculation is propagated through the inference procedure

Structured Prediction with Deep Models – the Trend

- Less hand crafted model design
 - Function design
 - Structure design
- More Utilization of existing network structures
 - Need to consider the propagation of gradients

Structured Prediction with Deep Models – Summary

- Large data amount calls for flexible models that support fast training (*aka* deep models)
- Batch training and stochastic gradient are important ingredients – as in other deep learning models
- Slow inference methods become less favored
- Disclaimer:
 - Only a small portion of the recent literature is covered here due to time limit.
 - Many more papers worth reading.

Important References

Classifier-based structured Prediction

CRF & Deep models :

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Rémi Leblond, Jean-Baptiste Alayrac, Anton Osokin, and Simon Lacoste-Julien. SEARNN: Training RNNs with global-local losses. ICML Workshop (2017).

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Sam Wiseman and Alexander M. Rush. Sequence-to-Sequence Learning as Beam-Search Optimization. EMNLP (2016).

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Classifier-based structured Prediction

Attention models:

Kelvin Xu, Jimmy Ba, Ryan Kiros, Kyunghyun Cho, Aaron Courville, Ruslan Salakhutdinov, Richard Zemel, and Yoshua Bengio. Show, Attend and Tell: Neural Image Caption Generation with Visual Attention. ICML (2015). Yoon Kim, Carl Denton, Luong Hoang and Alexander M. Rush. Structured Attention Networks. ICLR (2017). Kyunghyun Cho, Aaron Courville, and Yoshua Bengio. Describing Multimedia Content using Attention-based Encoder-Decoder Networks. In IEEE Transactions on Multimedia, 2015.

Jan Chorowski, Dzmitry Bahdanau, Dmitriy Serdyuk, Kyunghyun Cho, and Yoshua Bengio. Attention-Based Models for Speech Recognition. In Proceedings of NIPS, 2015.

Multi-Task Structured Prediction

Chao Ma

Oregon State University

Tutorial at Association for the Advancement of Artificial Intelligence (AAAI), 2018

Entity Analysis in Language Processing

Many NLP tasks process mentions of entities – things, people, organizations, etc.

- Named Entity Recognition
- Coreference Resolution
- Entity Linking
- Semantic Role Labeling
- Entity Relation Extraction

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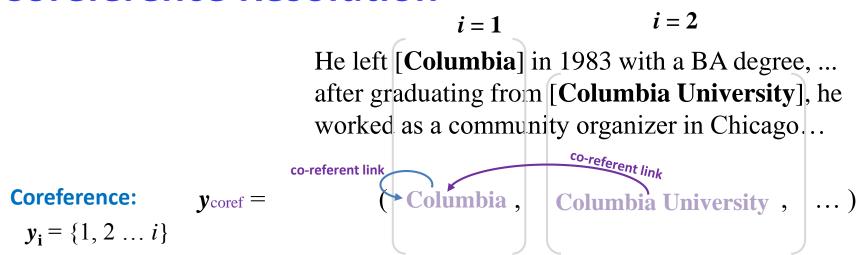


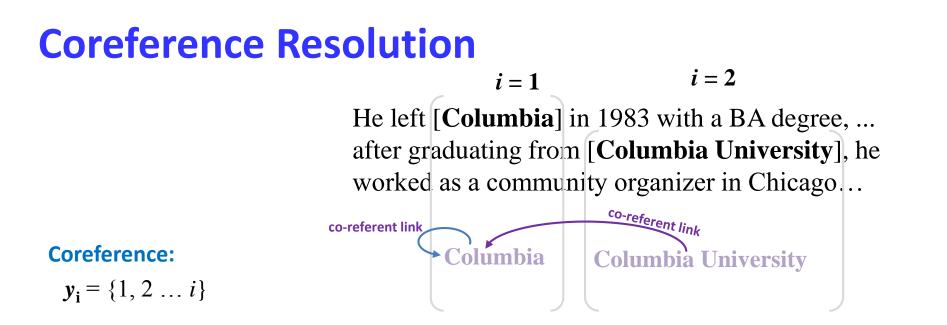
Coreference Resolution

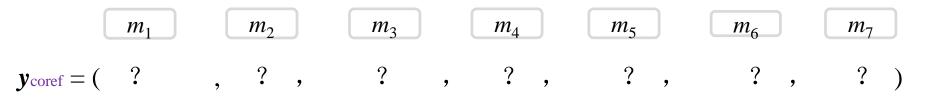
i = 1 *i* = 2

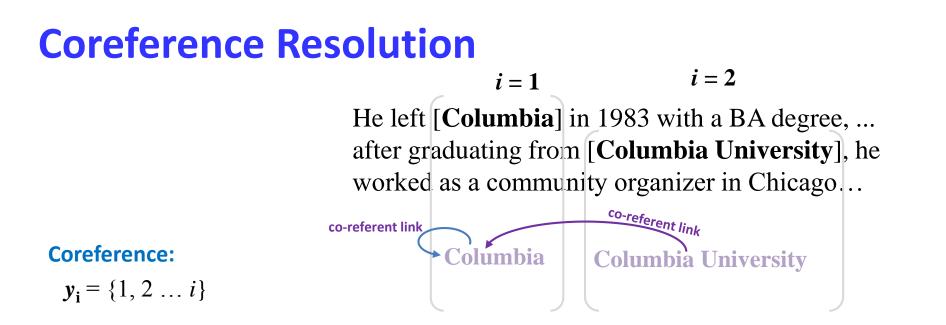
He left [**Columbia**] in 1983 with a BA degree, ... after graduating from [**Columbia University**], he worked as a community organizer in Chicago...

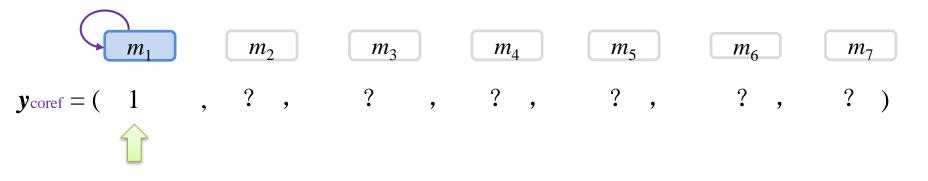
Coreference Resolution

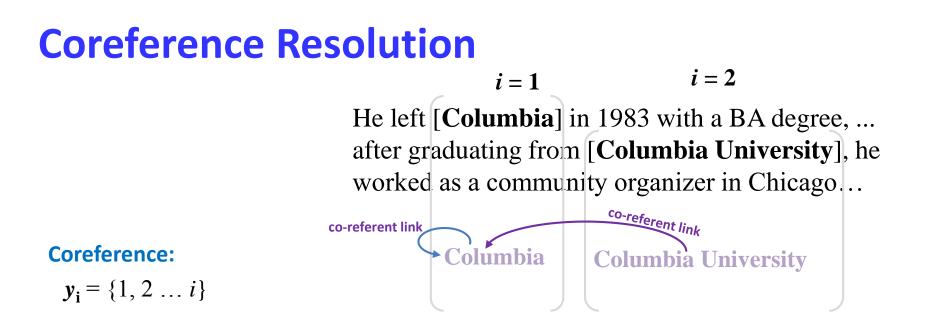


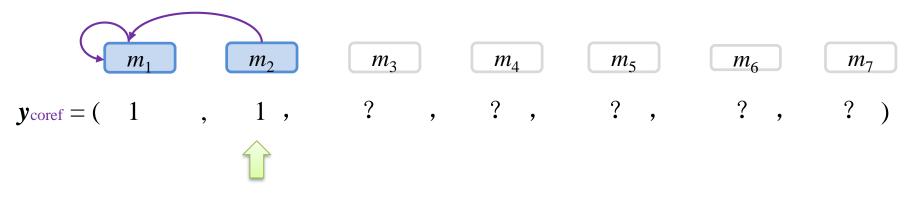


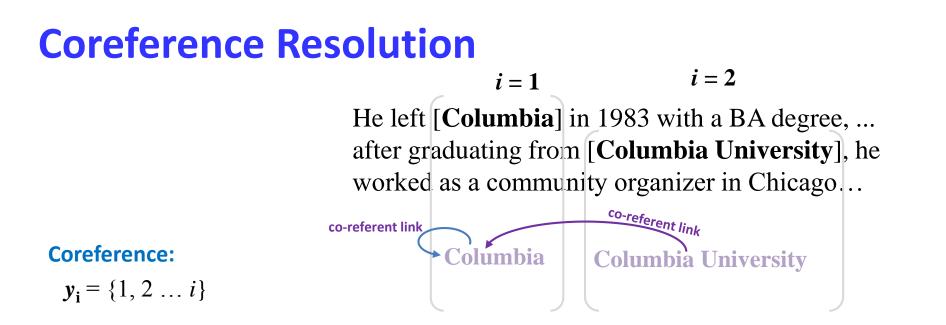


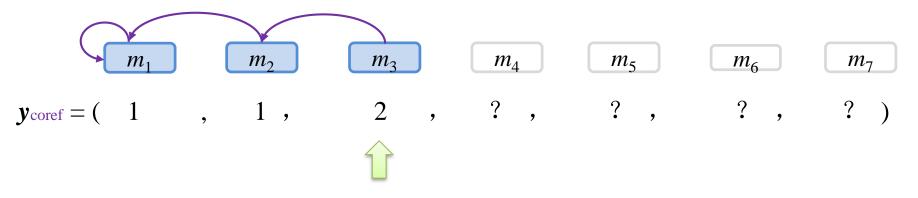


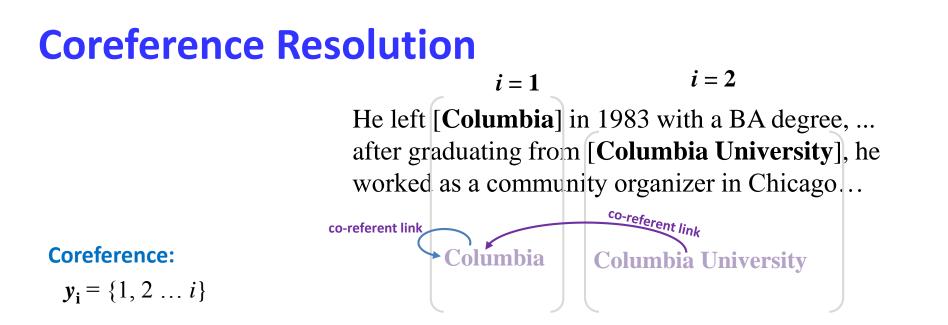


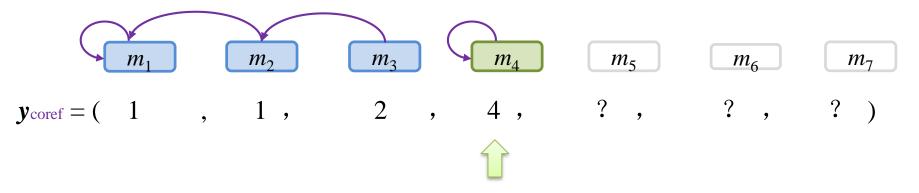


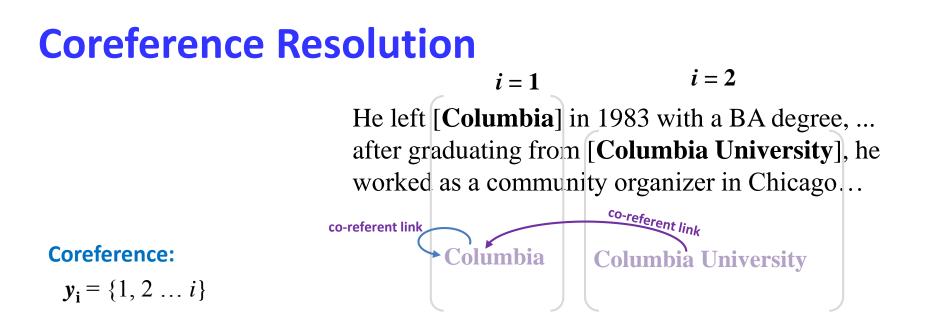


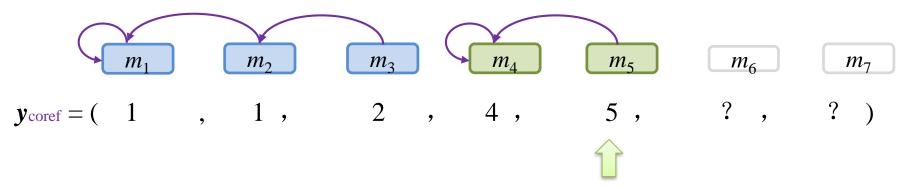


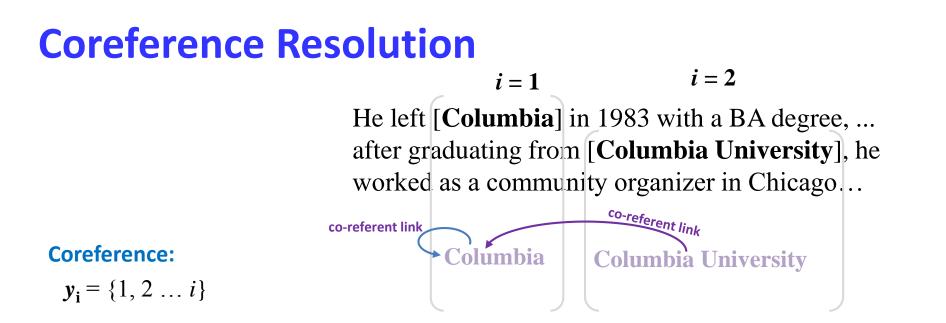


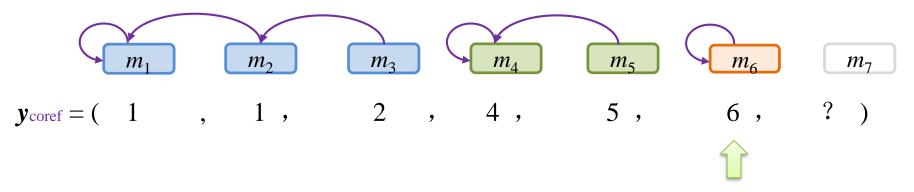


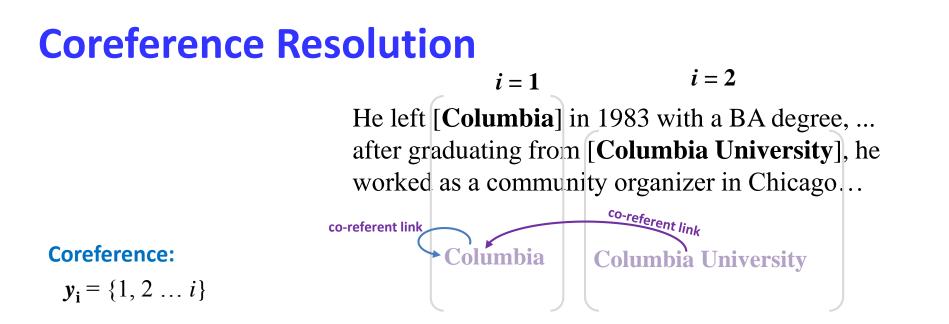


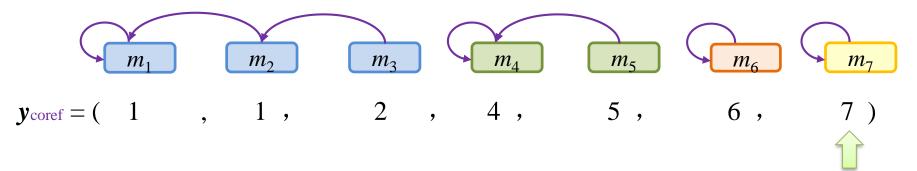


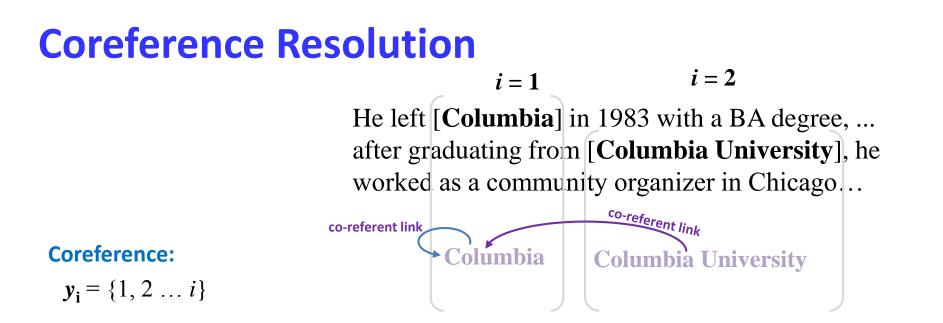


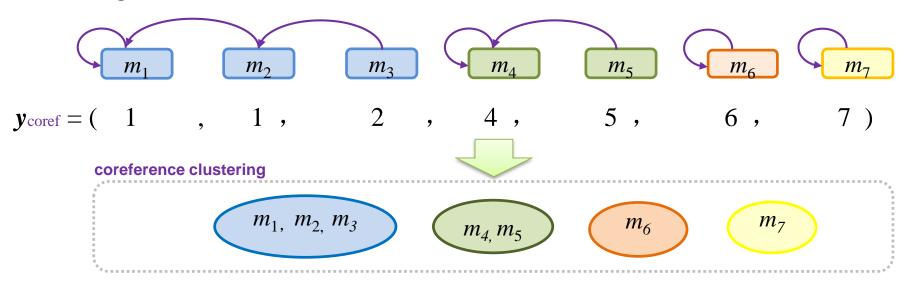




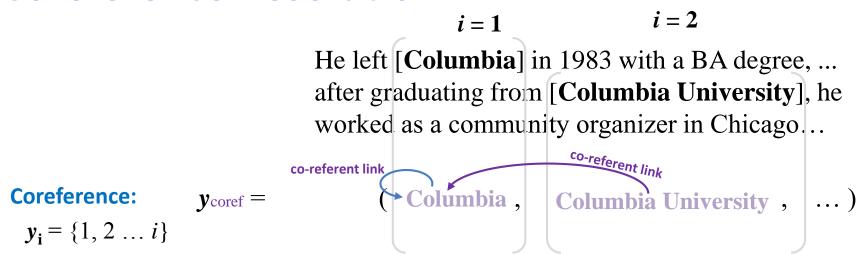


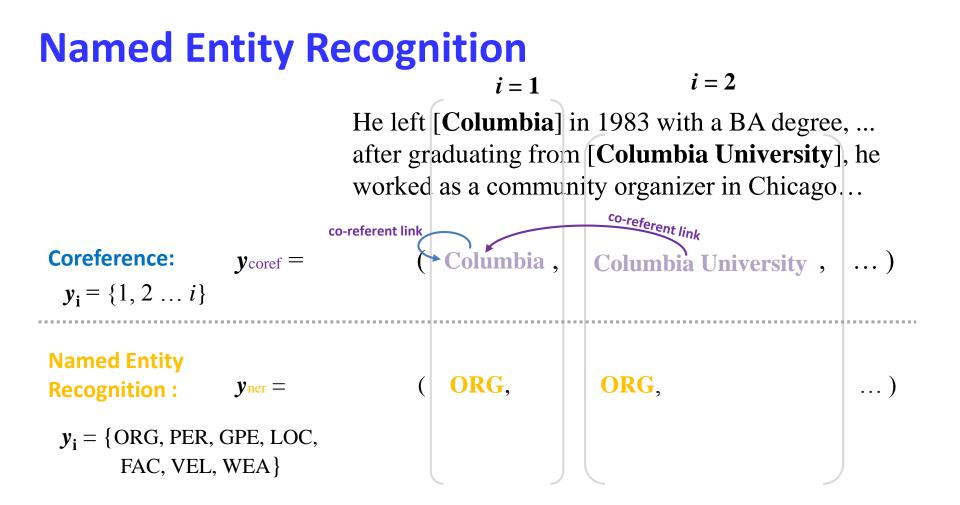




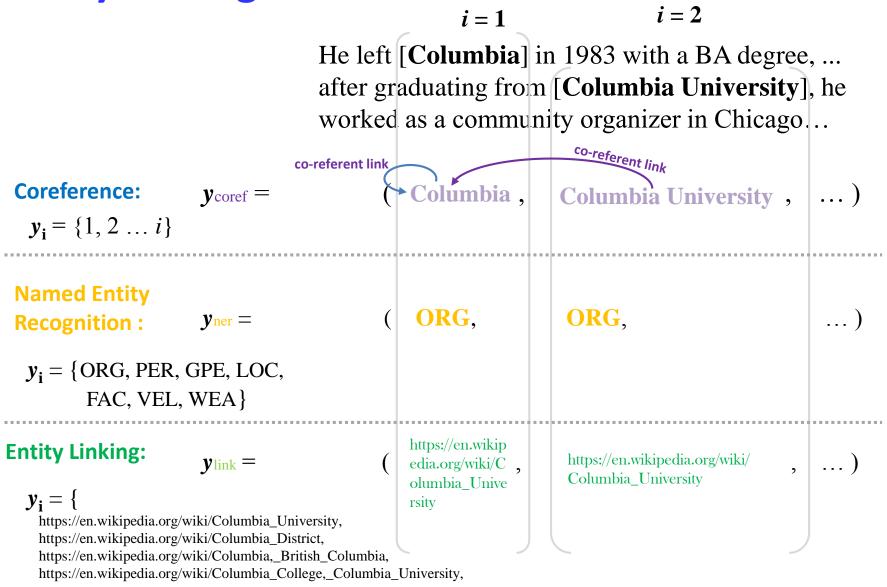


Coreference Resolution



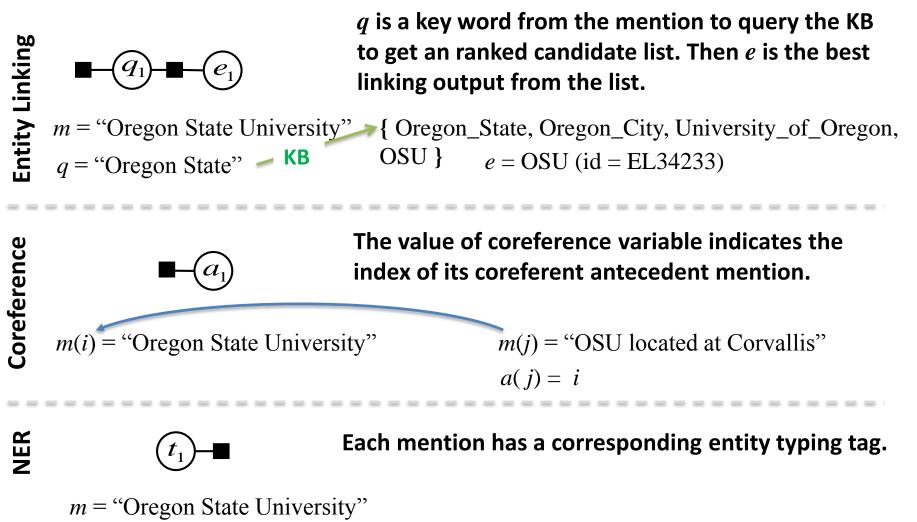


Entity Linking



Graphic Model: Joint Entity Linking, Typing, and Coreference Task [Greg Durrett and Dan Klein. TACL 2014]

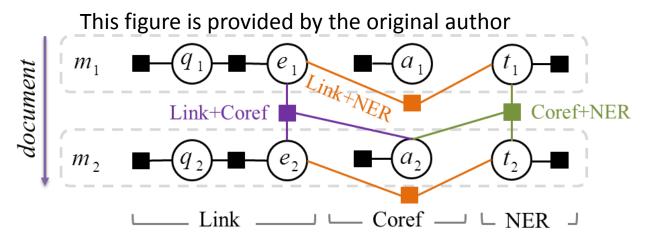
Insolate models



t = ORG

Graphic Model: Joint Entity Linking, Typing, and Coreference Task [Greg Durrett and Dan Klein. TACL 2014]





Learning

• The objective can be optimized using AdaGrad algorithm.

Inference

- **Belief propagation** is still the best choice, but not efficient enough.
 - **Solution**: use a threshold to prune away most of bad links in for coreference variables, but keep only *k* remaining.

Summary of Graphic Model Approaches

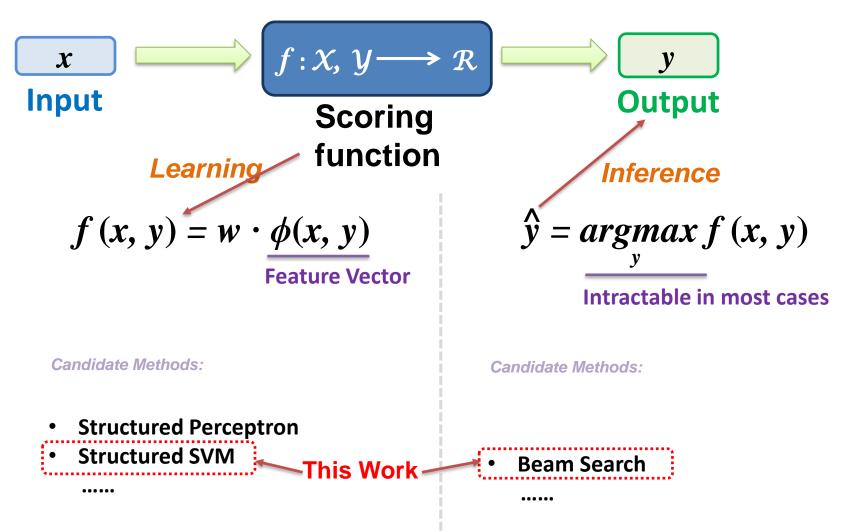
Advantages

- The powerful capability of representation.
- Easy to deal with missing labels.

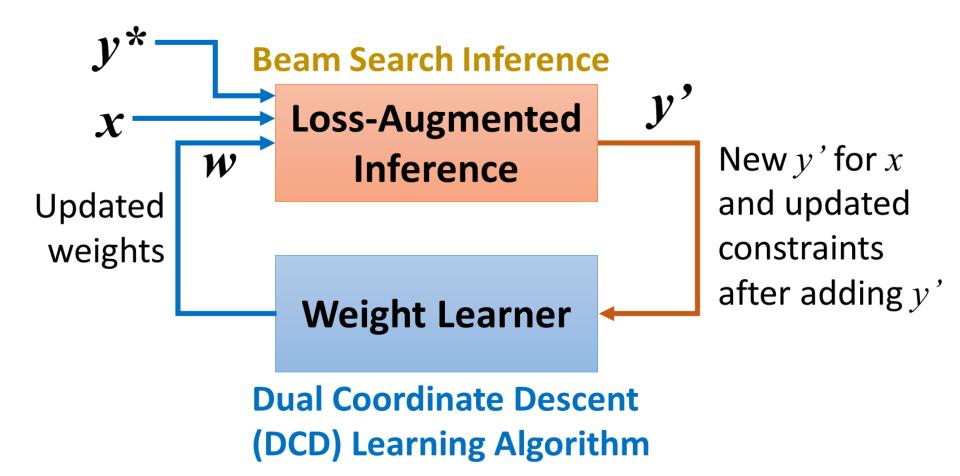
Challenges

- The main learning difficulty in these graphic models is its complicate structure
 - Graph decomposition during learning and inference by ignoring some other parts of the graph.
- Huge number of (hidden) variables and parameters.
 - Pruning candidate values;
 - Fixing some of variable values at early stages

Search-based inference for Structured Prediction

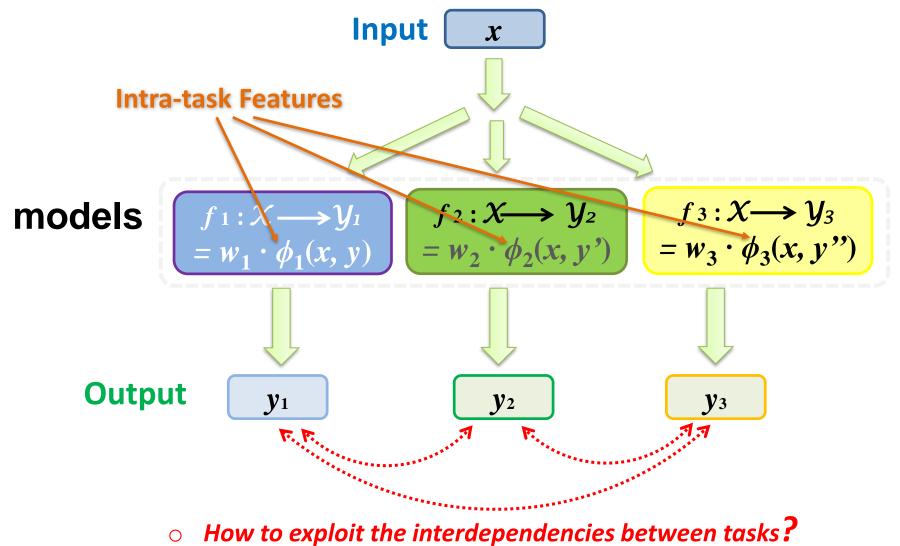


Structured SVM Learning with Search-based Inference



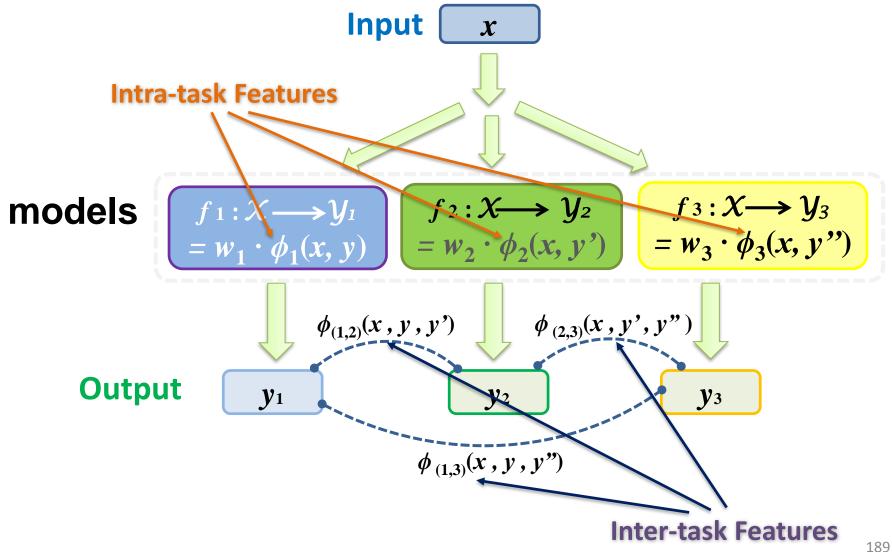
Multi-Task Structured Prediction

Multi-Task Structured Prediction (MTSP):

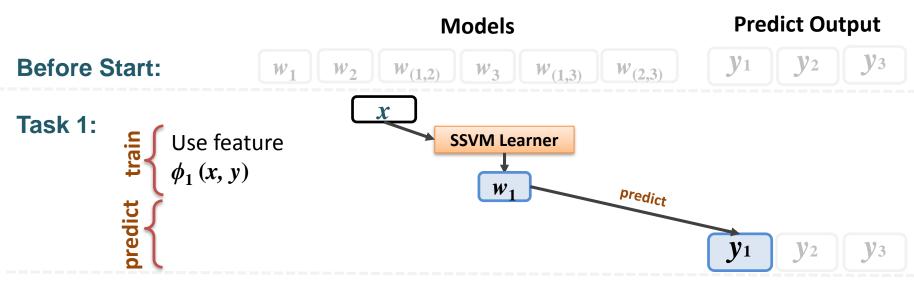


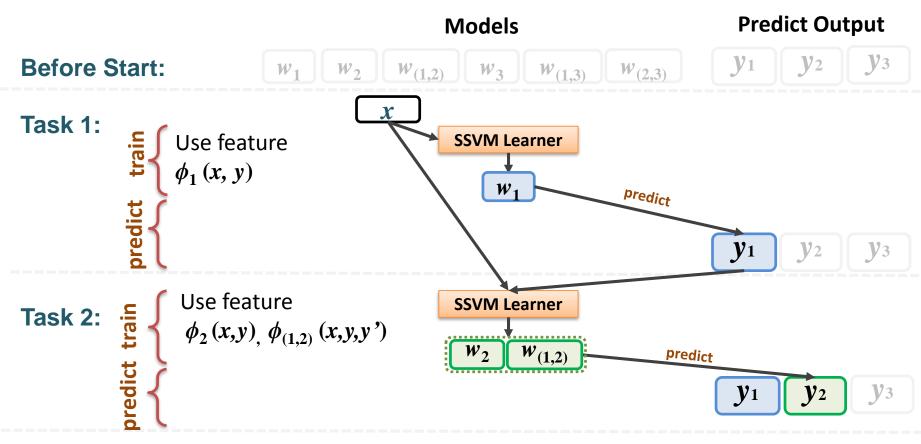
Multi-Task Structured Prediction

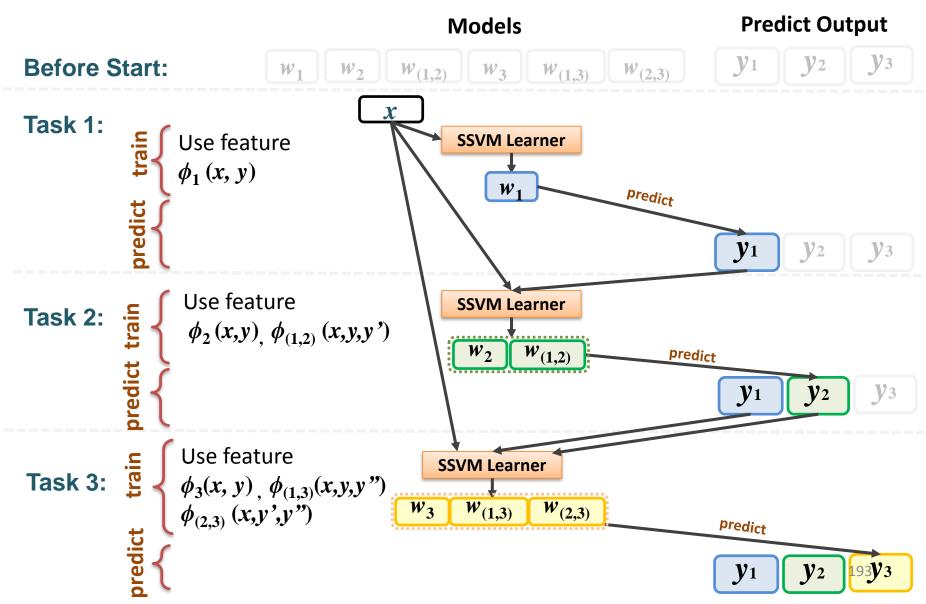
Introduce Inter-task Features:



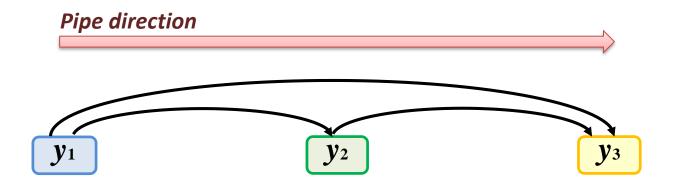








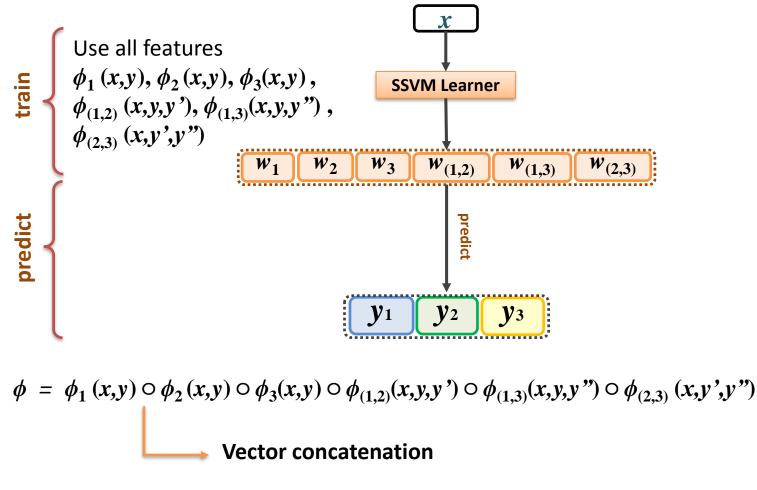
Pipeline Performance Depends on Task Order



The task performs better when it is placed last in order.
 There is **no** ordering that allows the pipeline to reach peak performance on all the three tasks.

Joint Architecture

Task 1 & 2 & 3:



Big Problem: Huge branching factor for search

Pruning

A pruner is a classifier to prune the domain of each variable using state features.

Score-agnostic Pruning



- Can accelerate the training time;
- May or may not improve the testing accuracy;

Score-sensitive Pruning



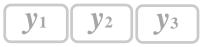
- Can improve the testing accuracy;
- No training speedup, but evaluation does speed up.

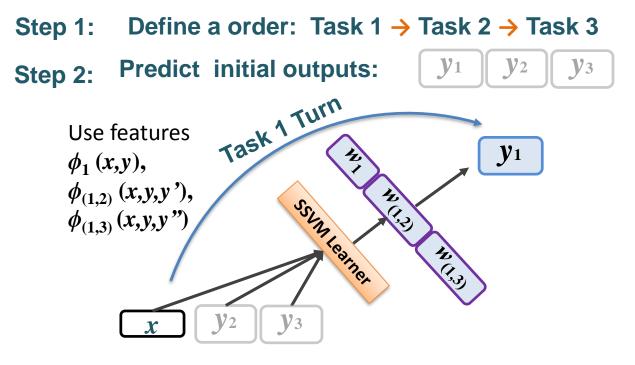
Pipeline architecture



Connect the tail of pipeline to the head?

- Step 1: Define a order: Task 1 → Task 2 → Task 3
- Step 2: Predict initial outputs:



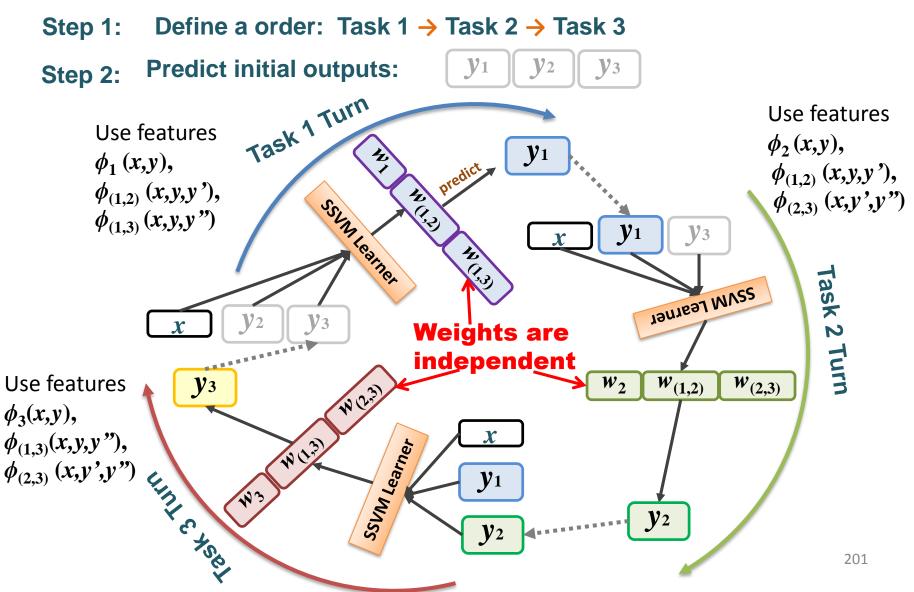


Unshared-Weight-Cyclic Training



Predict initial outputs: **y**₁ **V**2 **V**3 Step 2: Task 1 Turn Use features Use features **y**₁ $\phi_2(x,y),$ $\phi_1(x,y),$ predict $\phi_{(1,2)}(x,y,y'),$ $\phi_{(1,2)}(x,y,y'),$ 12 (1.2) SSUMLearner $\phi_{(2,3)}(x,y',y'')$ $\phi_{(1,3)}(x,y,y'')$ **y**3 **y**1 x 40 (1.3) Task 2 Turn Jaujeat WV22 v_2 **V**3 x **w**_(1,2) **W**_(2,3) W_2

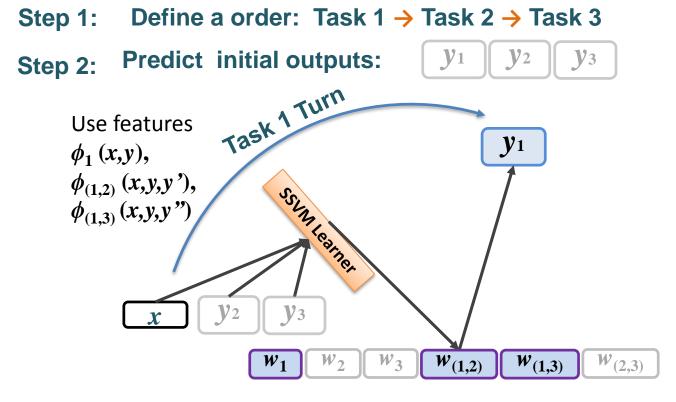
y₂

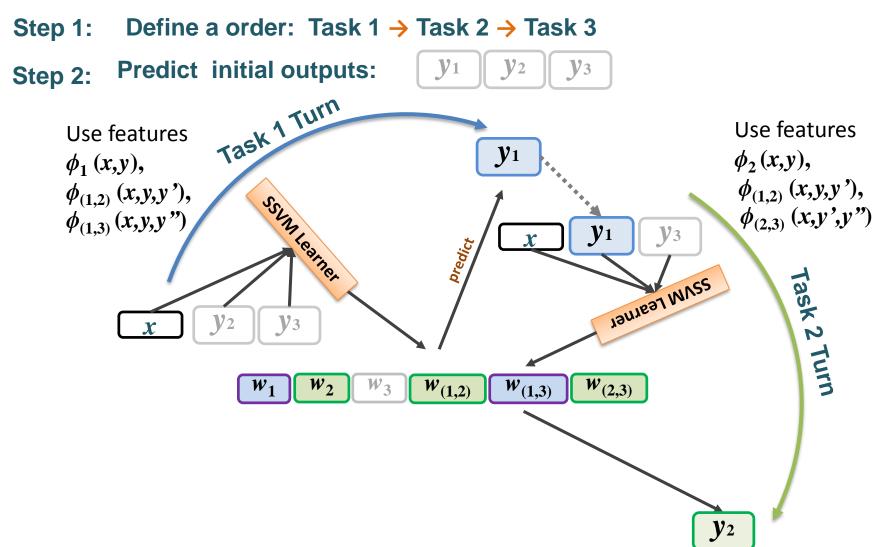


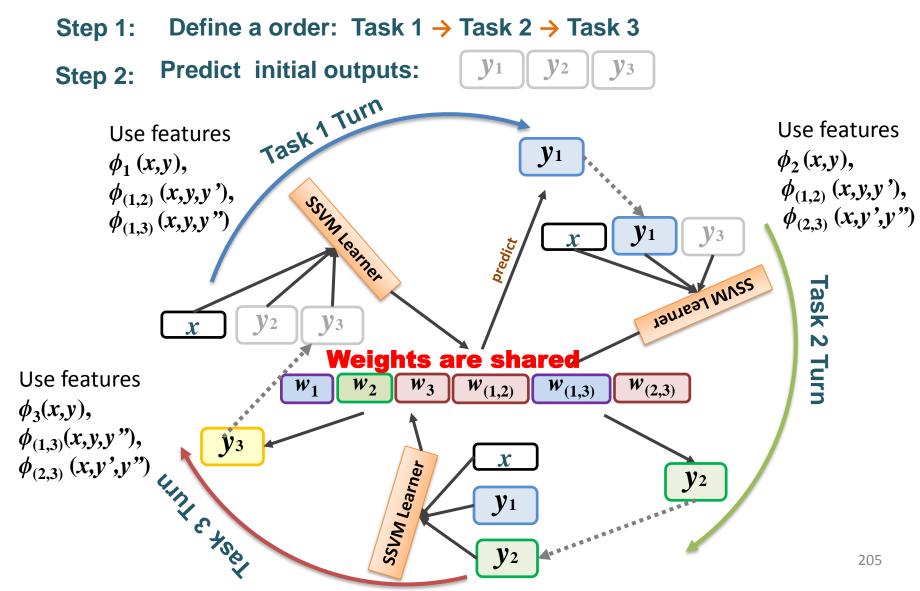
- Step 1: Define a order: Task $1 \rightarrow$ Task $2 \rightarrow$ Task 3
- Step 2: Predict initial outputs:











Summary of Search-based Approaches

- MTSP outperform the STSP by exploiting interdependency, which is captured by inter-task features.
- 2. Search-based inference for large structured prediction problems suffers from local optima and is mitigated by a good initialization.
- 3. Pipeline architecture is the fastest on both training and testing, but low accuracy; Joint architecture is good on accuracy, but slow speed; Cyclic is a trade-off between these two.
- 4. Score-sensitive pruning of joint MTSP performs the best and takes most time.
- 5. Unshared weights usually performs better than shared weights.

Summary

Different frameworks for structured prediction [Jana]

- Cost function learning framework and recent advances
- Control knowledge learning framework (greedy and beam search)
- HC-Search: A Unifying framework

Integrating deep learning and structured prediction [Liping]

- Deep learning ∩ cost function learning
- ▲ Deep learning ∩ control knowledge learning

Multi-task structured prediction [ChaoMa]

- Graphical models approach
- Search based learning and inference architectures

Future Directions

- Design and optimization of search spaces for complex structured prediction problems
 - very under-studied problem
- Leveraging deep learning advances to improve the performance of structured prediction approaches
 - Loose vs. tight integration
- Learning to trade-off speed and accuracy of structured prediction
 - Active research topic, but relatively less work
- What architectures are more suitable for "Anytime" predictions? How to learn for anytime prediction?

Future Directions

- Theoretical analysis: sample complexity and generalization bounds
 - Lot of room for this line of work in the context of "learning" + "search" approaches
- Understanding and analyzing structured predictors in the context of integrated applications
 - Pipelines in NLP and Vision among others
- Amortized inference or speedup learning for other inference formulations
- (Multi-task) structured prediction with weak supervision
 - Dan Roth: Incidental Supervision: Moving beyond Supervised Learning. AAAI 2017