# Integrating Learning and Search for Structured Prediction

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### **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

sky	sky	sky	sky	sky	sky	sky	sky	sky	sky
sky	sky	sky	sky	sky	sky	sky	sky	sky	sky
sky	sky	sky	sky	sky	sky	sky	sky	sky	sky
sky	sky	sky	sky	sky	sky	s ky	sky	sky	sky
sky	sky	rocks	rocks	rocks	sky	ks	sky	sky	sky
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
sand	sand	sand	water	water	water	water	water	water	water

# **Biological Image Analysis**



Nematocyst Image



#### Body parts of the nematocyst

# **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**



## **Automated Planning**

# Planning

A planning problem gives:

- an initial state
- > a goal condition
- > a list of actions and their semantics (e.g. STRIPS)



**Objective:** find action sequence from initial state to goal

## **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

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

γ



**Training Data**  $\{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$ Х Learning ? Algorithm

Example problem:

X - image of a face

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



Example problem:

X - image of a face

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

# Learning for <u>Simple</u> Outputs



# Learning for <u>Simple</u> Outputs





Y = set of all possible POS tag sequences

#### **Exponential !!**



### **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."



Y = set of all possible letter sequences

#### **Exponential !!**



### **Image Labeling**



sky	sky	sky	sky	sky	sky	sky	sky	sky	sky
sky	sky	sky	sky	sky	sky	sky	sky	sky	sky
sky	sky	sky	sky	sky	sky	sky	sky	sky	sky
sky	sky	sky	sky rocks	sky recks	sky	s ky rocks	sky	sky	sky
sky	sky rocks	rocks	rocks	rocks	sky	Ks	sky	sky	sky
rocks	rocks	rocks	rocks	rocks	rocl	o ćks	sky	sky	sky
rocks	rocks	rocks	rocks	rocks	rocks	rocks	rocks water	water	water
sand	sand	sand water	sand water	water	water	water	water	water	water
sand	sand	water	water	water	water	water	water	water	water
sand	sand	sand	water	water	water	water	water	water	water

# 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**

- Most algorithms learn parameters of linear models
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$$F(\mathbf{x}) = \arg\min_{y \in Y} w \cdot \phi(x, y)$$

#### **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



# 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  $\phi(x, y)$ 

# 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 inference algorithms exist only for simple features

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

## **Focus of Tutorial**

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

#### • Key Idea:

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

### Part 3: A Brief Overview of Search Concepts

### **Combinatorial Search: Key Concepts**

#### Search Space

- Where to start the search?
- How to navigate the space?

### Search Procedure / Strategy

How to conduct search?

#### Search Control Knowledge

How to guide the search? (Intelligence)

## **Search Space Definition**

#### Initial State Function: I

Where to start the search?

#### Successor State Function: S

- What are the successor (next) states for a given state?
- Generally, specified as a set of actions that modify the given state to compute the successor states

#### Terminal State Function: T

When to stop the search?

## (Ordered) Search Space: Example



## **Search Procedure**

- Search Tree (or Graph): Instantiation of the search space. How to navigate?
- Uninformed (Blind) Search Procedure
  - Breadth-First Search (BFS)
  - Depth-First Search (DFS)
- Informed (Intelligent) Search Procedure
  - Greedy Search
  - Beam Search
  - Best-First Search

## **Informed Search Procedures**

- Maintain an internal memory of a set of open nodes (M)
- Intelligent search guided by the control knowledge
- Algorithmic Framework for Best-First Search style search strategies:
  - Selection: score each open node in the memory M and select a subset of node(s) to expand
  - Expansion: expand each selected state using the successor function to generate the candidate set
  - Pruning: Retains a subset of all open nodes (update M) and prune away all the remaining nodes

### **Best-First Search Style Algorithms**

- Best-first Search  $(M = \infty)$ 
  - selects the best open node
  - no pruning

- Greedy Search (M = 1)
  - selection is trivial
  - prunes everything except for the best open node in the candidate set

### **Best-First Search Style Algorithms**

- Best-first Beam Search (M = B)
  - selects the best open node
  - prunes everything except for the best *B* open nodes in the candidate set

- Breadth-First Beam Search (M = B)
  - selection is trivial all B nodes
  - prunes everything except for the best *B* open nodes in the candidate set

## **Search Control Knowledge**

#### Greedy Policies

Classifier that selects the best action at each state

#### Heuristic Functions

- computes the score for each search node
- heuristic scores are used to perform selection and pruning

#### Pruning Rules

additional control knowledge to prune bad actions / states

#### Cost Function

Scoring function to evaluate the terminal states

## Part 4: Control Knowledge Learning Framework: Greedy Methods

# **Greedy Control Knowledge Learning**

### • Given

- Search space definition (ordered or unordered)
- Training examples (input-output pairs)

### Learning Goal

Learn a policy or classifier to make good predictions

#### • Key Idea:

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

### **Ordered vs. Unordered Search Space**

#### Ordered Search Space

- Fixed ordering of decisions (e.g., left-to-right in sequences)
- Classifier based structured prediction

- Unordered Search Space
  - Learner dynamically orders the decisions
  - Easy-First approach

### **Classifier-based Structured Prediction**

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

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

## **DAgger for Handwriting Recognition**



### **Ordered vs. Unordered Search Space**

#### Ordered Search Space

- Fixed ordering of decisions (e.g., left-to-right in sequences)
- Classifier based structured prediction

- Unordered Search Space
  - Learner dynamically orders the decisions
  - Easy-First approach

### Easy-First Approach for Structured Prediction

## **Easy-First Approach: Motivation**

#### 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

## **Example: Cross-Document Coreference**

**One of the key suspected mafia bosses** arrested yesterday **had hanged** himself.

Doc 1

Doc 2

Police said Lo Presti has hanged himself.

One of the key suspected mafia bosses had hanged Lo Presti has hanged

Hard Easy

## **Example: Cross-Document Coreference**





- Once we decide that the two verbs are coreferent, the two noun mentions serve the same semantic role to the verb cluster
- Strong evidence for coreference

## **Easy-First Approach: Overview**

Consider a set of inter-dependent decisions in a sequential manner

• At each step, make the easiest decision first

 This allows us to accumulate more information to help resolve more challenging decisions later

## **Applications of Easy-First**

- Cross-document joint entity and event coreference
  - ▲ Lee et. al. EMNLP-CoNLL '12

Within-document co-reference Resolution
Stoyanov and Eisner, COLING'12

- Dependency parsing
  - Goldberg and Elhadad, HLT-NAACL' 10

### • Search space

A state corresponds to a partial solution



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- A state corresponds to a partial solution
- In each state, we consider a set of fixed possible actions



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- A state corresponds to a partial solution
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- Each action is described by a feature vector  $x \in \mathbb{R}^d$



### • Search space

- A state corresponds to a partial solution
- In each state, we consider a set of fixed possible actions
- Each action is described by a feature vector  $x \in \mathbb{R}^d$
- An action is defined to be *good* if it leads to an improved state


#### **Easy-First Approach: Key Elements**

- Search space
- Scoring function  $f: \mathbb{R}^d \to \mathbb{R}$ - e.g.,  $f(x) = w \cdot x$

- In each state, evaluate all possible actions



#### **Easy-First Approach: Key Elements**

- Search space
- Scoring function  $f: \mathbb{R}^d \to \mathbb{R}$ - e.g.,  $f(x) = w \cdot x$ 
  - In each state, evaluate all possible actions
  - Take the highest scoring action (easiest)



## **Scoring Function Learning**

**Possible goal:** learn a scoring function such that: in every state all good actions are ranked higher than all bad actions

A better goal: learn a scoring function such that in every state *a good action* is ranked higher than all bad actions

## **Alternate Methods**

 In a training step, if the highest scoring action is bad, perform weight update

- Different update approaches
  - Best (highest scoring) good vs. best (highest scoring) bad
  - Average good vs. average bad

Issue: they do not directly optimize toward our goal!

# **Optimization Objective for Update**

- **Goal:** find a linear function such that it ranks one good action higher than all bad actions
  - This can be achieved by a set of constraints

 $\max_{g \in G} w \cdot x_g > w \cdot x_b + 1$ <br/>for all  $b \in B$ 

- Optimization Objective:
  - Use hinge loss to capture the constraints
  - Regularization to avoid overly aggressive update

$$\underset{w}{\operatorname{argmin}} \frac{1}{|B|} \sum_{b \in B} (1 - \max_{g \in G} w \cdot x_g + w \cdot x_b)_+ + \lambda \|w - w_c\|^2$$

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# **Optimization: Majorization-Minimization**

[Xie et al., 2015]

$$\underset{w}{\operatorname{argmin}} \frac{1}{|B|} \sum_{b \in B} (1 - \max_{g \in G} w \cdot x_g + w \cdot x_b)_+ + \lambda \|w - w_c\|^2$$



Can be solved using a Majorization-Minimization (MM) algorithm to get local optima solution

#### • In each MM iteration:

- Let  $x_q^*$  be the current highest scoring good action
- Solve following convex objective (via subgradient descent):

$$\underset{w}{\operatorname{argmin}} \frac{1}{|B|} \sum_{b \in B} (1 - \max_{g \in G} w \cdot x_g + w \cdot x_b)_+ + \lambda \|w - w_c\|^2$$

$$\frac{w \cdot x_g^*}{w \cdot x_g^*}$$

## **Contrast with Alternate Methods**



## Experiment I: Cross-document entity and event Coreference

Results on EECB corpus (Lee et al., 2012)

■ BGBB ■ R-BGBB ■ BGVB ■ R-BGVB ■ Lee et al.



[Xie et al., 2015]

### Experiment I: Within document Coreference



■ BGBB ■ R-BGBB ■ BGVB ■ R-BGVB



[Xie et al., 2015]

# **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
  - "scheduled sampling"
    - Samy Bengio, Oriol Vinyals, Navdeep Jaitly, Noam Shazeer: Scheduled Sampling for Sequence Prediction with Recurrent Neural Networks. NIPS 2015

## Part 5: 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: Learning Instantiations

Early update

Max-violation update

Learning as Search Optimization (LaSO)

## **Beam Search Framework: Early Update**

- Search error: NO target node in the beam
  - We cannot reach the goal node (correct structured output)

- Weight update: standard structured perceptron
  - Score of correct output > score of bad output

Beam update: reset beam with initial state OR discontinue search

## **Beam Search Framework: Early Update**

### repeat

- For every training example (x, y)
  - Perform search with current heuristic (weights)

If search error, update weights

Reset beam with initial state

(Dis)continue search

• until convergence or max. iterations

Beam Search Framework: Learning Instantiations

Early update

Max-violation update

Learning as Search Optimization (LaSO)

## Beam Search Framework: Max-Violation Update

- Improves on the drawback of Early update
  - Slow learning: learns from only earliest mistake

#### Max-Violation fix

- Consider worst-mistake (maximum violation) instead of earliest-mistake for the weight update
- More useful training data
- Converges faster than early update

# POS Tagging: Max-violation vs. Early vs. Standard

#### Early and Max-violation >> Standard at small beams

- Advantage shrinks as beam size increases
- Max-violation converges faster than Early (and slightly better)

**Source:** Huang et al., 2012



## **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
  - $\bullet w_{new} = w_{old} + \alpha \cdot (\psi_{avg}(target) \psi_{avg}(non target))$
  - $\psi_{avg}(target)$  = 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

## LaSO: Example Planning Results

#### Blocksworld

30 testing problems

Source: Xu et al., 2009

- Trained with beam width 10
- Features: RPL heuristic and features induced in prior work



Part 6: 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
- Experiments and Results
- Engineering Methodology for applying HC-Search
- Relation to Alternate Methods

# **Outline of HC-Search Framework**

#### Introduction

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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**



























![](_page_126_Figure_1.jpeg)

![](_page_127_Figure_1.jpeg)

![](_page_128_Figure_1.jpeg)

## **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**

#### Introduction

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- Engineering Methodology for applying HC-Search
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![](_page_132_Figure_1.jpeg)

![](_page_133_Figure_1.jpeg)

![](_page_134_Figure_1.jpeg)

![](_page_135_Figure_1.jpeg)

![](_page_135_Figure_2.jpeg)

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

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

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

![](_page_137_Figure_0.jpeg)

 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.

![](_page_138_Figure_0.jpeg)

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

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

![](_page_139_Figure_0.jpeg)

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- 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)

# **Outline of HC-Search Framework**

#### Introduction

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

# **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**

![](_page_143_Figure_1.jpeg)

![](_page_143_Picture_2.jpeg)
# **Greedy Search: Imitation with true loss**



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

# **Greedy Search: Ranking examples**





. . .

# **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)
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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]

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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**



# **Limited Discrepancy Search: Idea**

- Limited Discrepancy Search [Harvey and Ginsberg, 1995]
  - Key idea: correct the response of recurrent classifier at a small no. of critical errors to produce high-quality outputs



 See IJCAI'16 paper on LDS for AND/OR search w/ applications to optimization tasks in graphical modelS

# **Limited Discrepancy Search: Illustration**

- Limited Discrepancy Search [Harvey and Ginsberg, 1995]
  - Key idea: correct the response of recurrent classifier at a small no. of critical errors to produce high-quality outputs



# **Limited Discrepancy Search: Illustration**

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  - Key idea: correct the response of recurrent classifier at a small no. of critical errors to produce high-quality outputs



# **LDS Space: Illustration**



# **Quality of LDS Space**

Expected target depth



# **Quality of LDS Space**

Expected target depth



 $\circ~$  We can learn a classifier to optimize the I.I.D error  $\epsilon$ 

Doppa, J.R., Fern, A., Tadepalli, P. Structured Prediction via Output Space Search. *Journal of Machine Learning Research (JMLR), vol 15,* 2014.

# **Quality of LDS Space**

Expected target depth



- $\circ~$  We can learn a classifier to optimize the I.I.D error  $\epsilon$
- Important contribution that helped HC-Search achieve state-of-the-art results

# **Quality of Search Space: LDS vs. Flip-bit**

Expected target depth of a search space



# **Sparse LDS Space (k)**

### Complete LDS space is expensive

- each successor state generation requires running greedy policy with the given discrepancy set
- # successors = L.T, where T is the size of the structured output and L is the number of labels

### Sparse Search Space: Key Idea

- Sort discrepancies using recurrent classifier scores and pick top-k choices
- # successors = k.T
- Parameter k = # discrepancies for each variable controls the trade-off between speed and accuracy
- In practice, very small k suffice
- How can we deal with dependence on T?

# **Aside: Very simple HC-Search Instantiation**

### Heuristic function

Greedy recurrent classifier (or policy)

### • Search procedure

 Depth-first or Breadth-first Limited Discrepancy Search w/ bounded depth

### Cost function

Score the outputs generated by search procedure

# Computer Vision Tasks: Randomized Segmentation Space [Lam et al., 2015]

 Key Idea: probabilistically sample likely object configurations in the image from a hierarchical segmentation tree





Candidate generation

# **Pre-requisite: Hierarchical Segmentation Tree**

### Berkeley segmentation tree

- Regions are very robust
- Regions are closed
- UCM level 0 corresponds to all super-pixels



# Randomized Segmentation Space: Segmentation Selection



# Randomized Segmentation Space: Candidate Generation



For each segment, give it a label (based on segment's current labels and neighboring segment labels) and add it to the candidate set

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# **Benchmark Domains**

### • Handwriting recognition [Taskar et al., 2003]

HW-Small and HW-Large

- NET-Talk [Sejnowski and Rosenberg, 1987]
  - Stress and Phoneme prediction
    - x = "photograph" y = /f-Ot@graf-/
- Scene labeling [Vogel et al., 2007]





# **Experimental Setup**

- Search space: LDS space
- Search procedure: Greedy search
- Time bound: 15 steps for sequences and 150 for scene labeling
- Loss function: Hamming loss
- Baselines
  - Recurrent
  - CRFs
  - SVM-Struct
  - SEARN
  - CASCADES
  - C-Search

# **Results: comparison to state-of-the-art**

#### **Error-rates of different structured prediction algorithms**

	HW-Small	HW-Large	Phoneme	Scene labeling
HC-Search	12.81	03.23	16.05	19.71
C-Search	17.41	07.41	20.91	27.05
CRF	19.97	13.11	21.09	-
SVM-Struct	19.64	12.49	21.70	-
Recurrent	34.33	25.13	26.42	43.36
SEARN	17.88	09.42	22.74	37.69
CASCADES	13.02	03.22	17.41	-
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CASCADES	13.02	03.22	17.41	-

 HC-Search outperforms all the other algorithms including C-Search (our prior approach that uses a single function C to serve the dual roles of heuristic and cost function)



	Phoneme			Scene labeling		
Error	e	$\epsilon_{H}$	$\epsilon_H \epsilon_{C H}$		$\epsilon_{H}$	$\epsilon_{C H}$
HC-Search	16.05	03.98	12.07	19.71	5.82	13.89

	Phoneme			Scene labeling		
Error	E	$\epsilon_H \epsilon_{C H}$		e	$\epsilon_{H}$	$\epsilon_{C H}$
HC-Search	16.05	03.98	12.07	19.71	5.82	13.89

• Selection loss  $\epsilon_{C|H}$  contributes more to the overall loss

	Phoneme			Scene labeling		
Error	Е	$\epsilon_{H}$	$\epsilon_{C H}$	E	$\epsilon_{H}$	$\epsilon_{C H}$
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 Improvement of HC-Search over C-Search is due to the improvement in the selection loss

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- Improvement of HC-Search over C-Search is due to the improvement in the selection loss
- Clearly shows the advantage of separating the roles of heuristic and cost function

#### **Multi-Label Prediction: Problem**

Input



Output

#### **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: Challenges**



- o Joint prediction of labels to exploit the relationships between labels
- Automatically optimize the evaluation measure of the real-world task

## **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

Dataset	Domain	#TR	#TS	#F	#L	<b>E</b> [ <b>d</b> ]
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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)



#### **Multi-Label Prediction: Results**

#### • F1 Accuracy Results

Algorithm	Scene	Emotions	Medical	Genbase	Yeast	Enron	LLog	Slashdot
BR	52.60	60.20	63.90	98.70	63.20	53.90	36.00	46.20
CC	59.10	57.50	64.00	99.40	63.20	53.30	26.50	44.90
ECC	68.00	62.60	65.30	99.40	64.60	59.10	32.20	50.20
M2CC	68.20	63.20	65.40	99.40	64.90	59.10	32.30	50.30
CLR	62.20	66.30	66.20	70.70	63.80	56.50	22.70	46.60
CDN	63.20	61.40	68.90	97.80	64.00	58.50	36.60	53.10
CCA	66.43	63.27	49.60	98.60	61.64	53.83	25.80	48.00
PIR	74.45	60.92	80.17	99.41	65.47	61.14	38.95	57.55
SML	68.50	64.32	68.34	99.62	64.32	57.46	34.95	55.73
RML	74.17	64.83	80.73	98.80	63.18	57.79	35.97	51.30
DecL	73.76	65.29	78.02	97.89	63.46	61.19	37.52	54.67
HC-Search	75.89	66.17	78.19	98.12	63.78	62.34	39.76	57.98

Doppa, J.R., Yu, J., Ma C., Fern, A., Tadepalli, P. HC-Search for Multi-Label Prediction: An Empirical Study. *American Association of Artificial Intelligence (AAAI) Conference* 2014.

### **Detecting Basal Tubules of Nematocysts**



#### Challenges:

- Imaged against significant background clutter (unavoidable)
- Biological objects have highly-deformable parts

## **Detecting Basal Tubules of Nematocysts**

#### Experimental Setup

#### 80 images (training); 20 images (validation); 30 images (testing)

1024



197

## **Detecting Basal Tubules of Nematocysts**

#### Baselines

- IID Classifier
- Pairwise CRFs (w/ ICM, LBP, Graph-cuts)

#### • HC-Search

- Flipbit space (IID classifier + flip patch labels)
- Randomized Segmentation space

Algorithm	Precision	Recall	F1
SVM	0.675	0.147	0.241
Logistic Regression	0.605	0.129	0.213

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Pairwise CRF (w/ ICM)	0.432	0.360	0.393
Pairwise CRF (w/ LBP)	0.545	0.091	0.156
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Pairwise CRF (w/ GC)	0.537	0.070	0.124
HC-Search (w/ Flipbit)	0.472	0.545	0.506

Lam, M., Doppa, J.R., Xu, S.H., Todorovic, S., Dietterich, T.G., Reft, A., Daly, M. Learning to Detect Basal Tubules of Nematocysts in SEM Images. *IEEE Workshop on Computer Vision for Accelerated Biosciences (CVAB)* 2013.

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HC-Search (w/ Randomized)	0.831	0.651	0.729

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• **HC-Search** significantly outperforms all the other algorithms

• Performance critically depends on the **quality of the search space** 

#### • Visual results:



Ground-truth output



CRF w/ Graph cuts



**HC-Search** 



CRF w/ LBP

## **Results: Stanford Background Dataset**

Benchmark for scene labeling in vision community

Method	Accuracy (%)
Region Energy	76.4
SHL	76.9
RNN	78.1
ConvNet	78.8
ConvNet + NN	80.4
ConvNet + CRF	81.4
Pylon (No Bnd)	81.3
Pylon	81.9
HC-Search (w/ Randomized)	81.4

HC-Search without using features from deep learning

# **Outline of HC-Search Framework**

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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*

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

# **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

#### **Part 7: Future Directions**

# **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

# **Important References**

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#### Recurrent classifier:

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## **Important References**

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