Constructing Action Graphs for Material Synthesis Procedures

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6.864 Final Project

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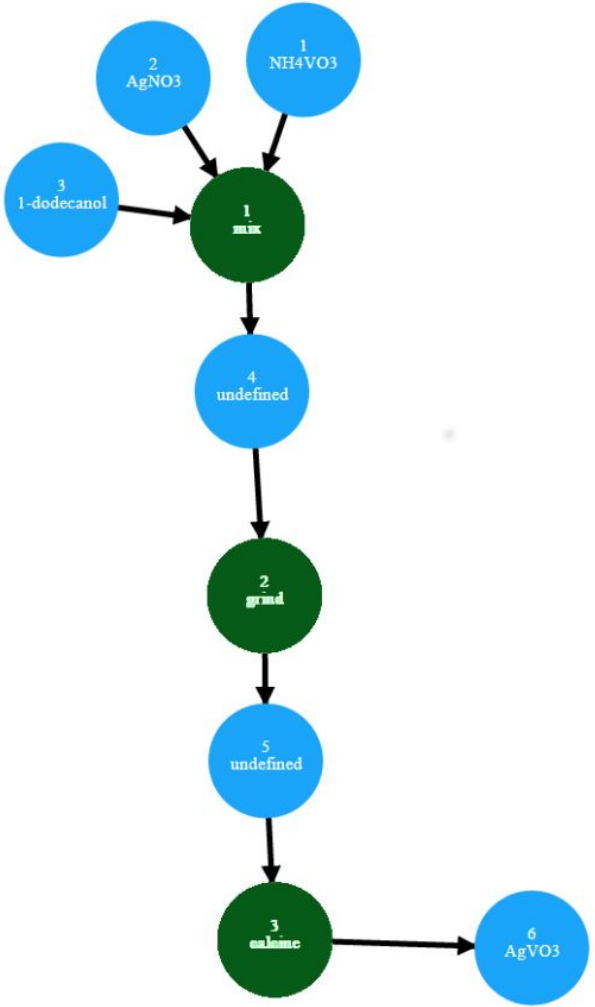
Action Graphs

Summarize the raw procedure:

Ammonium metavanadate (NH4VO3 , 99%), silver nitrate (AgNO3 , 99%), and 1-dodecanol (99%) used in the experimental work were of analytical grade, supplied by SigmaeAldrich and used as received.

*The typical synthesis procedure is as follow: ammonium metavanadate (0.1 mmol), silver nitrate (0.1 mmol) and 1.0 mL of 1-dodecanol were **mixed**, **ground** for 1 h in a mortar and then **calcined** at 450 # C for 5 h in a muffle furnace.*

The resulting AgVO3 nanoparticles were collected and subjected to further analysis.



Subproblems

1. Main action detection
    a. Extraneous description removal
2. Input and output extraction
3. Sequencing of actions

Dataset: 23 synthesis procedures with annotated graphs

- Average number of sentences = 8
- Average number of verbs per procedure = **25**
- Average number of gold verbs in annotated graphs = **6**
- Average number of true nouns in annotated graphs = **205**
- Average number of ‘undefined’ in annotated graphs = **52**

I. Main Action Detection // Extraneous Removal

*Example: The solution was **dried** at 120 C for 6 hours and then **pressed** into ceramic body at 70 MPa.*

Baseline model based on heuristic rules:

- Verb, POS of has to be a past participle (VBN)
- Extract several VBNs based on conjunctions

Supervised models with MaxEnt

- Feature templates: verb indices, POS tags, dependency arc labels

I. Results

With 10-fold cross validation

	Precision	Recall	F1 Score
Baseline #1) PCFG parse with rules	0.378	0.649	0.478
Baseline #2) Dependency parse: root word	0.371	0.287	0.324
Baseline #3) All verbs	0.201	0.874	0.327
MaxEnt Model	**0.793**	**0.874**	**0.831**

I. Difficulties in Action Detection

Example 1:

*The precursor powders of LiFePO4 were **prepared** by chemical co-precipitation method using stoichiometric LiH2PO4 (Alfa, 97%), FeSO47H2O (Alfa, 99%) and LiOHH2O (Alfa, 98%) as starting materials.*

- Extracted: prepare
- Annotated: **mix**

Example 2:

*To obtain LiFePO4/C composites, the precursor powders were well **mixed** with glucose and **treated** at 975 K and 1025 K at Ar-4%H2 atmosphere.*

- Extracted: mix → treat
- Annotated: mix → **heat**

II. Inputs and Output Extraction

Two Kinds of Relationship:

1. Argument → Action (e.g. powders → **grind**)
2. Action → Product (e.g. **calcine** → powders)

Supervised Binary MaxEnt Classification
For any given pair in corpus, classify whether it belongs to Argument-Action, Verb-Action, or neither

Key Challenge: Identifying implicit argument/products ('undefined')

Features for pair of words:
POS tags, is_named_entity, dependency parse tree structures, sentence index offset

II. Results

(Baseline Heuristic: Pair all verbs and nouns)

For **Argument-Action**:

	Precision	Recall	F1 Score
Baseline: Heuristic	0.014	0.7395	0.028
MaxEnt Model	**0.89**	**0.92**	**0.90**

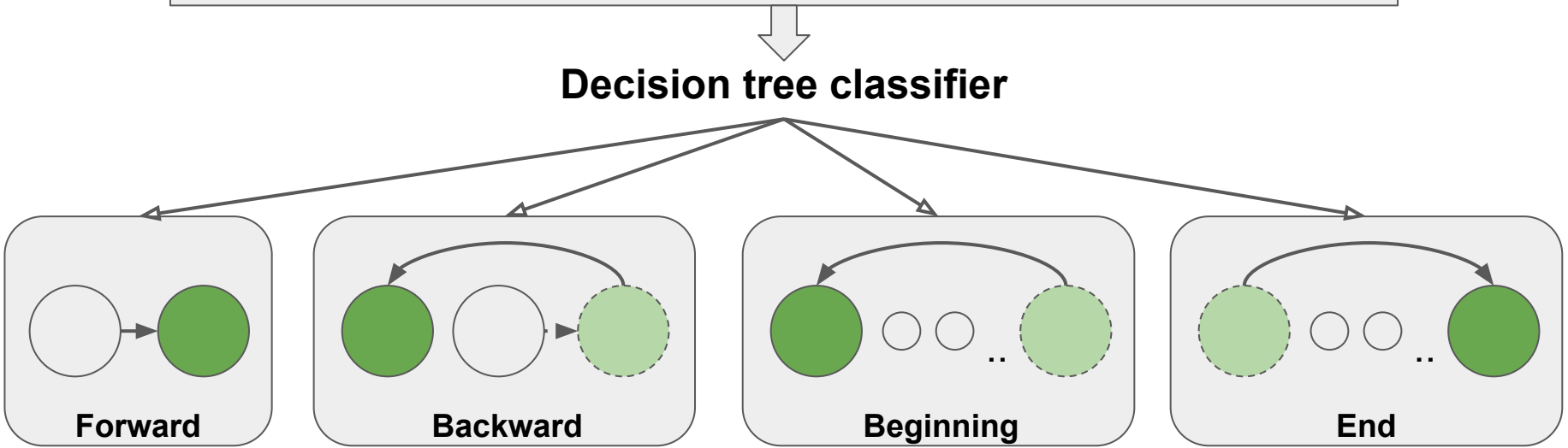
For **Action-Product**:

	Precision	Recall	F1 Score
Baseline: Heuristic	0.008	0.28	0.016
MaxEnt Model	**0.91**	**0.82**	**0.87**

III. Sequence Ordering

Classify prepositions, adverbs, and subordinating conjunctions to **partial moves**:

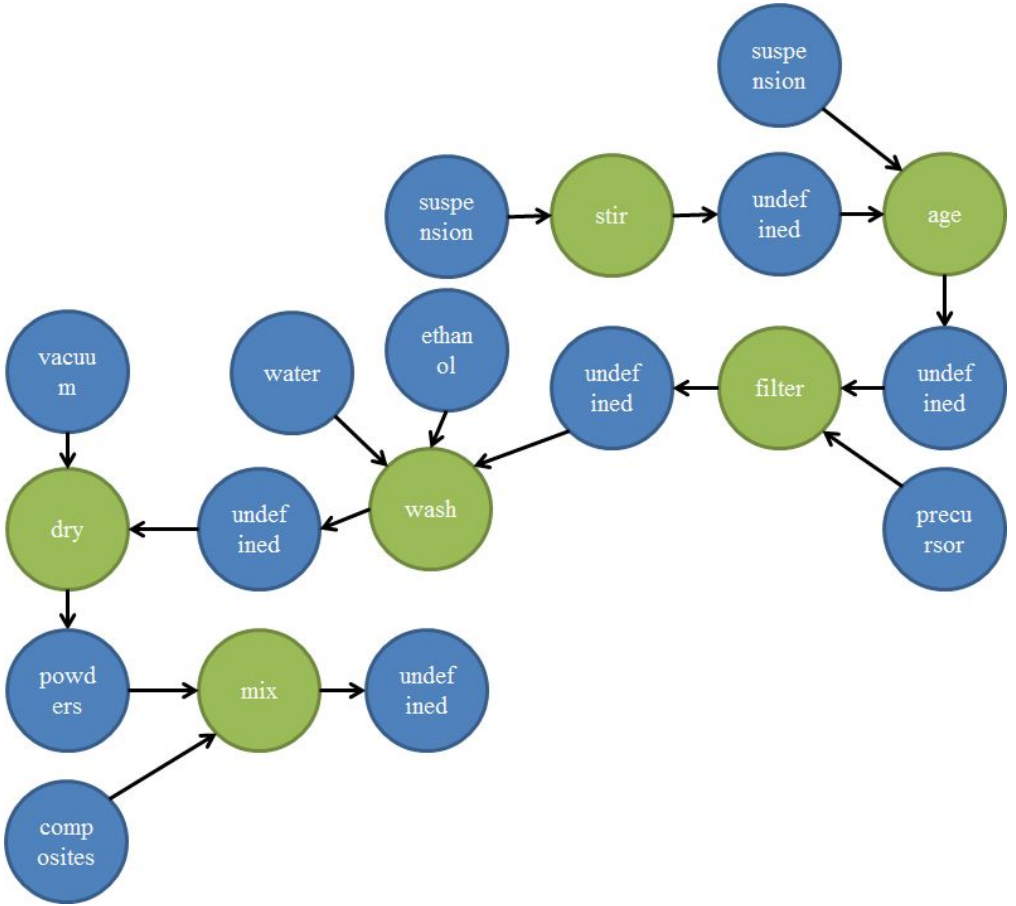
"followed by", "subsequently", "finally", "once after", "meanwhile", "before", "after", "which was previously", "when _____", "then", ...



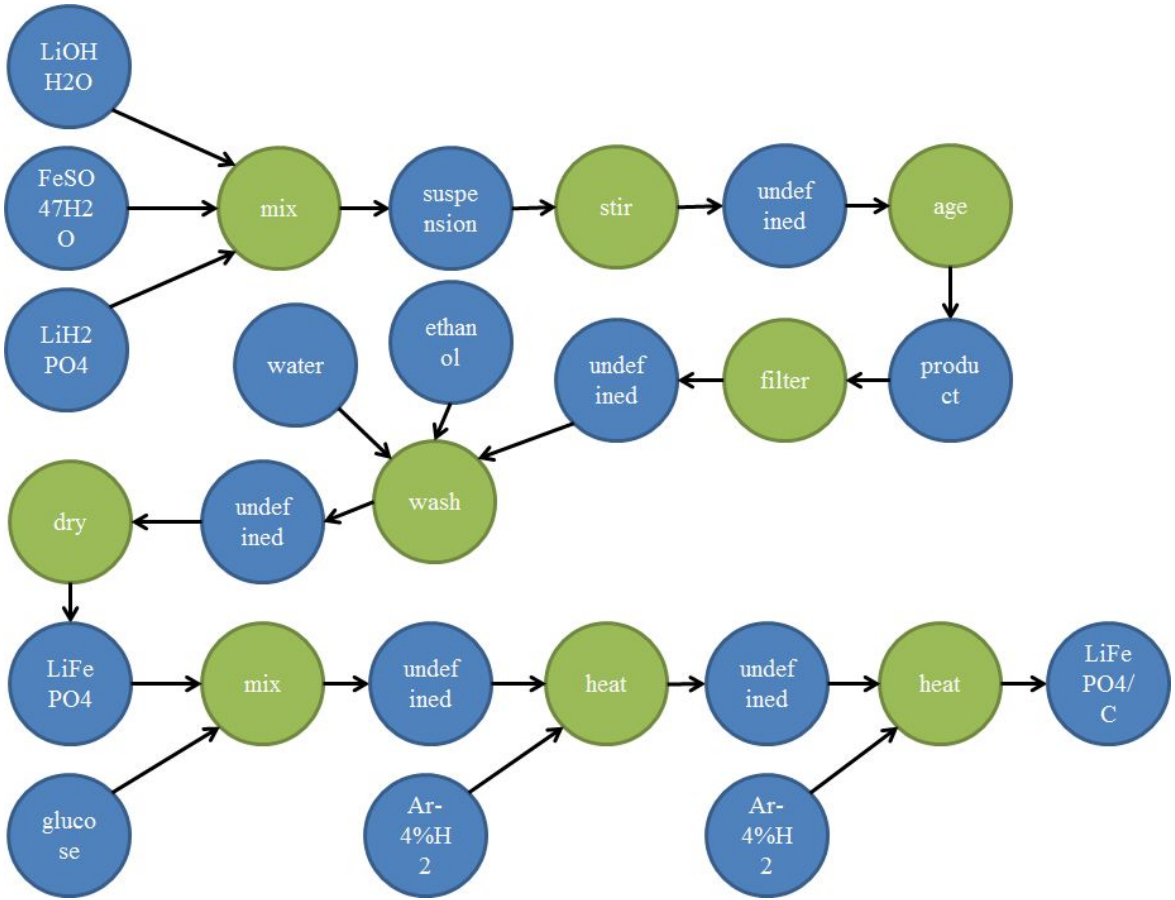
III. Results: Sequence Ordering

With MaxEnt Action Detect			
	Precision	Recall	F1 Score
Chronological Baseline	0.607	0.688	0.645
Partial Ordering Model	0.589	0.667	0.625
Assuming Perfect Action Detection			
	Precision	Recall	F1 Score
Chronological Baseline	0.951	0.951	0.951
Partial Ordering Model	0.923	0.943	0.933

Example Predicted Graph



Ground Truth



Text

The precursor powders of LiFePO4 were prepared by chemical co-precipitation method using stoichiometric LiH2PO4 (Alfa, 97%), FeSO47H2O (Alfa, 99%) and LiOHH2O (Alfa, 98%) as starting materials.

The suspension was stirred at 0-4 #C for about 30 min and aged for about 2 h.

The final precursor powder product was then filtered, washed with deionized water and ethanol, and dried at 100 #C in a vacuum oven for 2 h.

To obtain LiFePO4/C composites, the precursor powders were well mixed with glucose and treated at 975 K and 1025 K at Ar-4%H2 atmosphere.

Conclusion

- Even with much noisier data compared to cooking recipes, action detector and input/output detector performed reasonably well
  - Strong predictive signal with supervised learning
- Similar to cooking recipes, once extraneous descriptors are pruned out, actions are generally written in chronological order
- Visualizing action graphs for c

Future Work

- Semi-supervised, unsupervised approach by leveraging large database of scholarly articles
- Joint generative model across all variables of ***a*** = *(c,I,o)*
- Clustering phrases and labeling them to replicate annotators' summarization behavior