

Automatically Extracting Action Graphs From Materials Science Synthesis Procedures

Sheshera Mysore

Edward Kim

Emma Strubell

Ao Liu

Haw-Shiuan Chang

Srikrishna Kompella

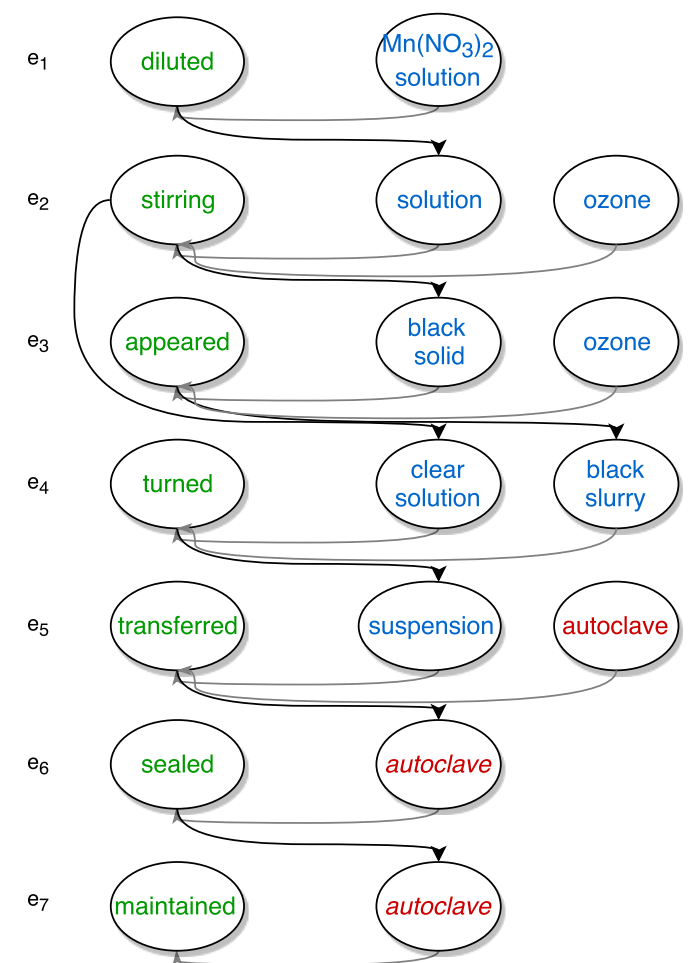
Kevin Huang

Andrew McCallum

Elsa Olivetti

Typical synthesis procedure text

In a typical procedure for the synthesis of β -MnO₂ nanowires, 2.5 mL of 50 wt.% Mn(NO₃)₂ solution was diluted to 25.0 mL, and ozone was fed into the bottom of the solution for 30 min under vigorous stirring. With the indraught of ozone, black solid appeared gradually and the clear solution turned into black slurry finally. Then the suspension was transferred into an autoclave of 48.0 mL, sealed and maintained at 200 °C for 8 h. After this, the autoclave was cooled to room temperature naturally. The resulting solid products were washed with water, and dried at 120 °C for 8 h.



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- Want to accelerate materials science via large-scale analysis, prediction of inorganic synthesis routes

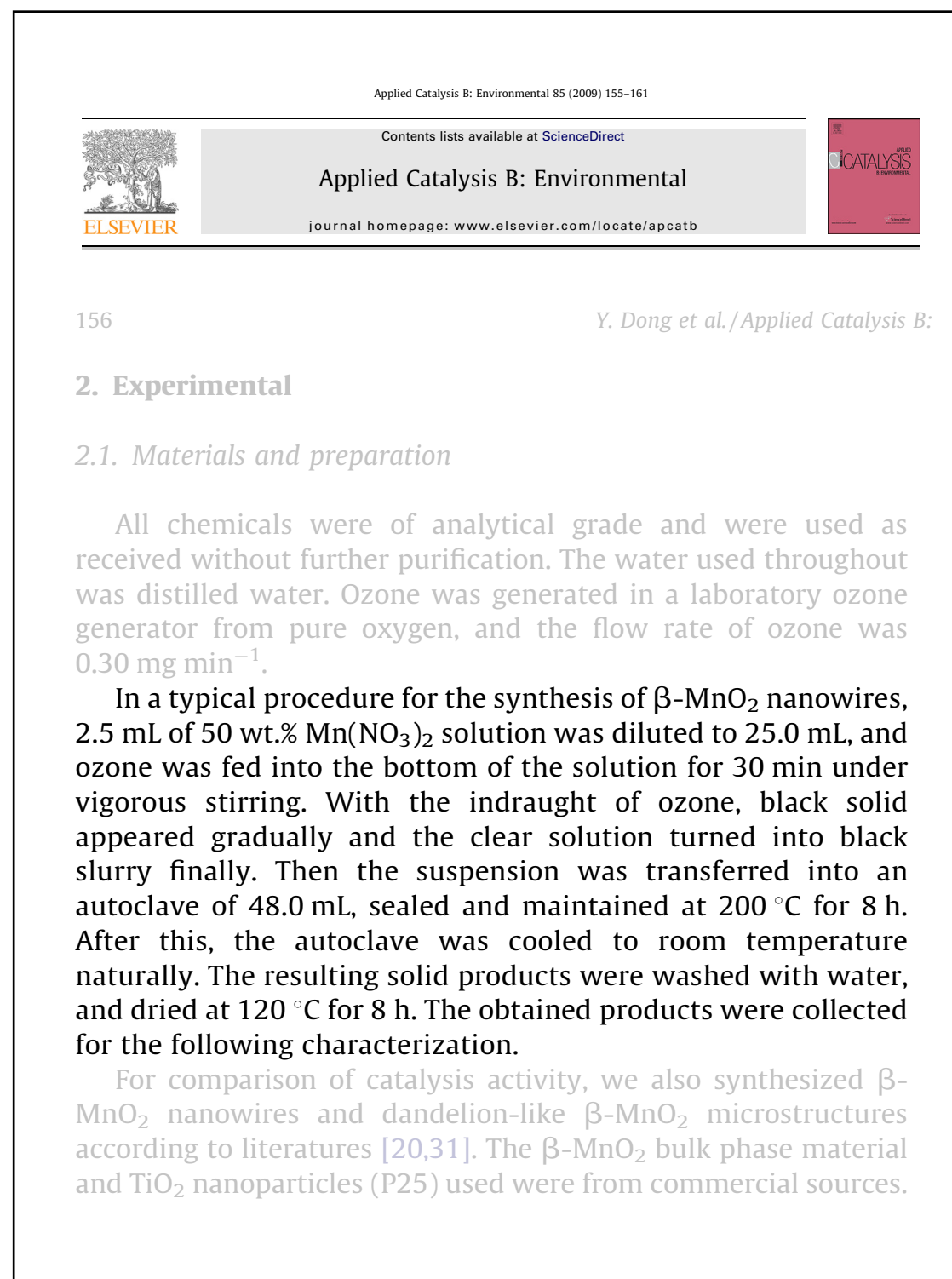
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- Want to accelerate materials science via large-scale analysis, prediction of inorganic synthesis routes
- Unlike organic synthesis, no tabulation of synthesis routes — have to read papers!

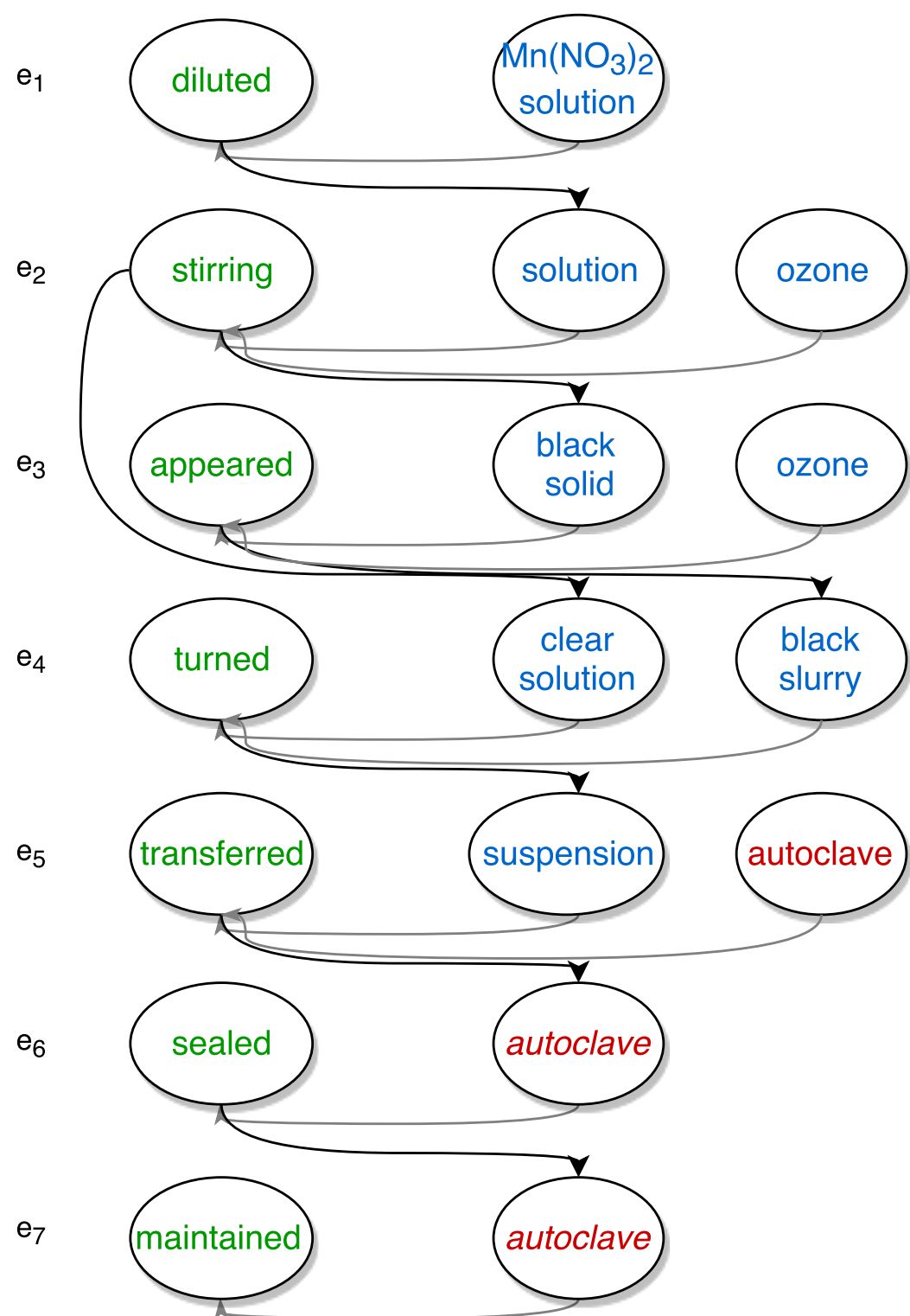


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Goal: automatically extract materials synthesis procedures from text.



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2. Experimental

2.1. Materials and preparation

All chemicals were of analytical grade and were used as received without further purification. The water used throughout was distilled water. Ozone was generated in a laboratory ozone generator from pure oxygen, and the flow rate of ozone was 0.30 mg min⁻¹.

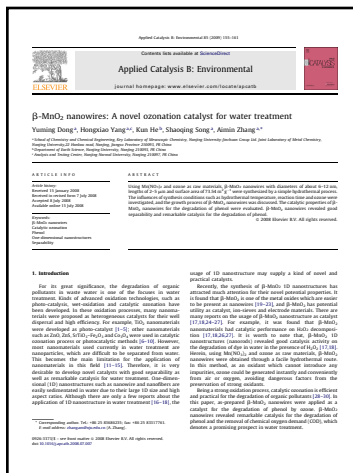
In a typical procedure for the synthesis of β-MnO₂ nanowires, 2.5 mL of 50 wt.% Mn(NO₃)₂ solution was diluted to 25.0 mL, and ozone was fed into the bottom of the solution for 30 min under vigorous stirring. With the indraught of ozone, black solid appeared gradually and the clear solution turned into black slurry finally. Then the suspension was transferred into an autoclave of 48.0 mL, sealed and maintained at 200 °C for 8 h. After this, the autoclave was cooled to room temperature naturally. The resulting solid products were washed with water, and dried at 120 °C for 8 h. The obtained products were collected for the following characterization.

For comparison of catalysis activity, we also synthesized β-MnO₂ nanowires and dandelion-like β-MnO₂ microstructures according to literatures [20,31]. The β-MnO₂ bulk phase material and TiO₂ nanoparticles (P25) used were from commercial sources.

Overall pipeline architecture



Overall pipeline architecture



PDF to text



... the suspension was transferred to an autoclave and sealed...

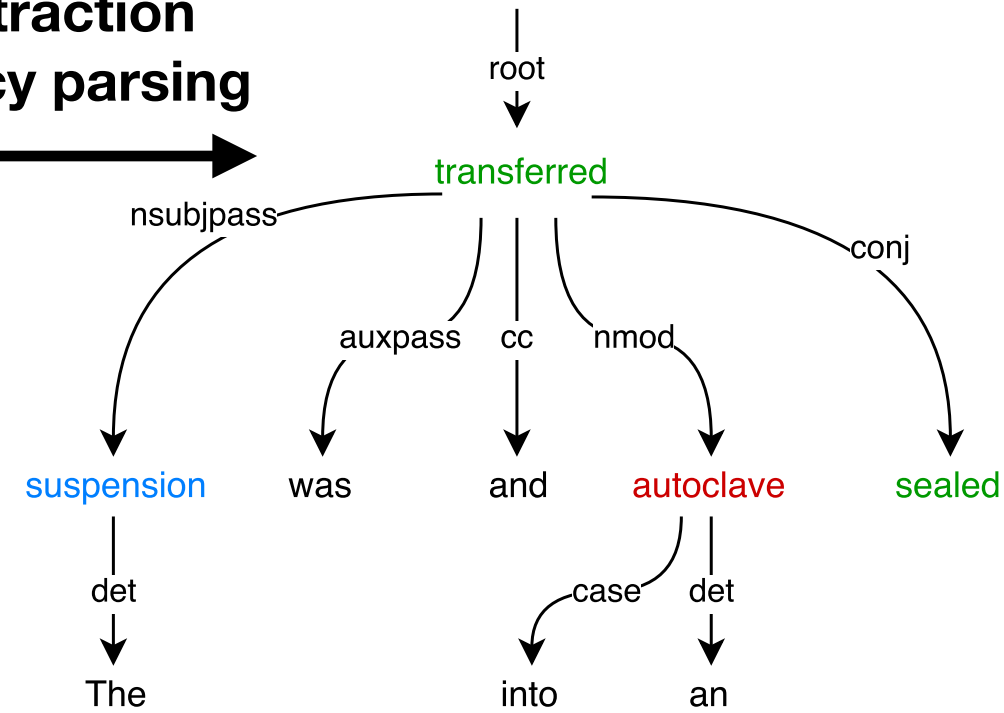
Overall pipeline architecture



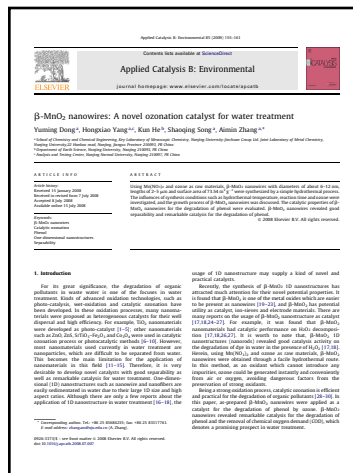
PDF to text

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Entity extraction
Dependency parsing



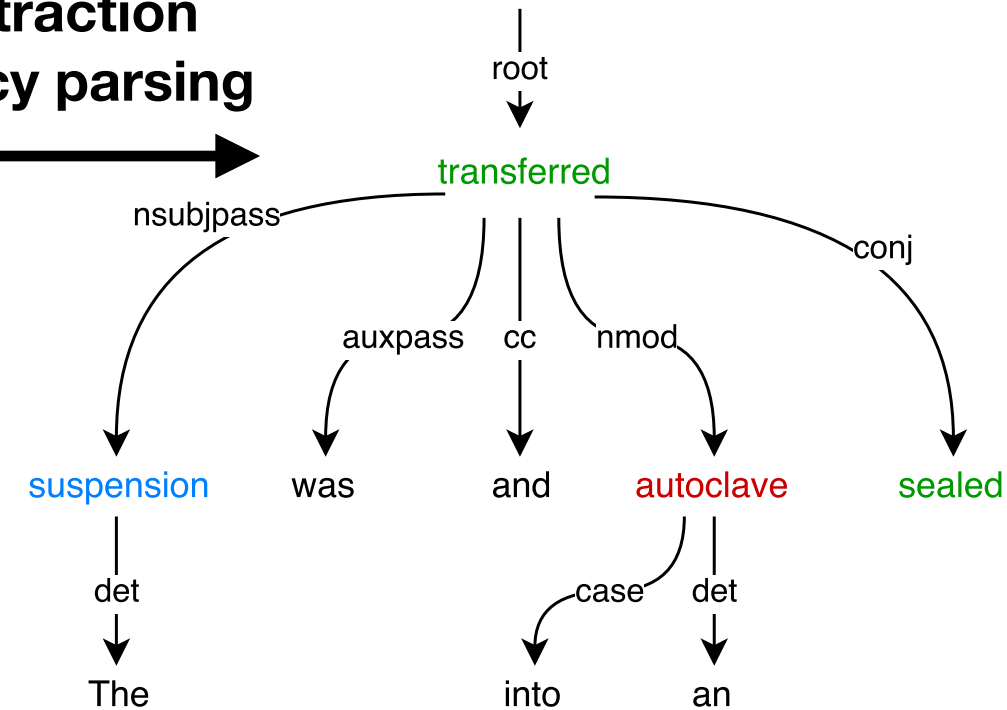
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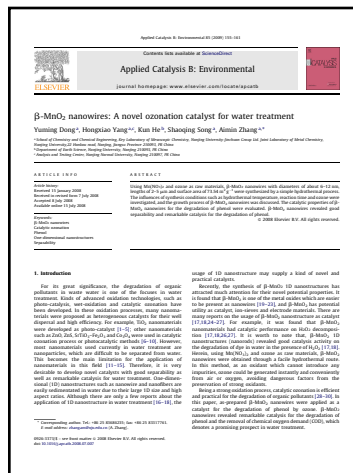
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(suspension, transferred, autoclave)
(suspension, sealed, autoclave)
(suspension, maintained, autoclave)

Event extraction

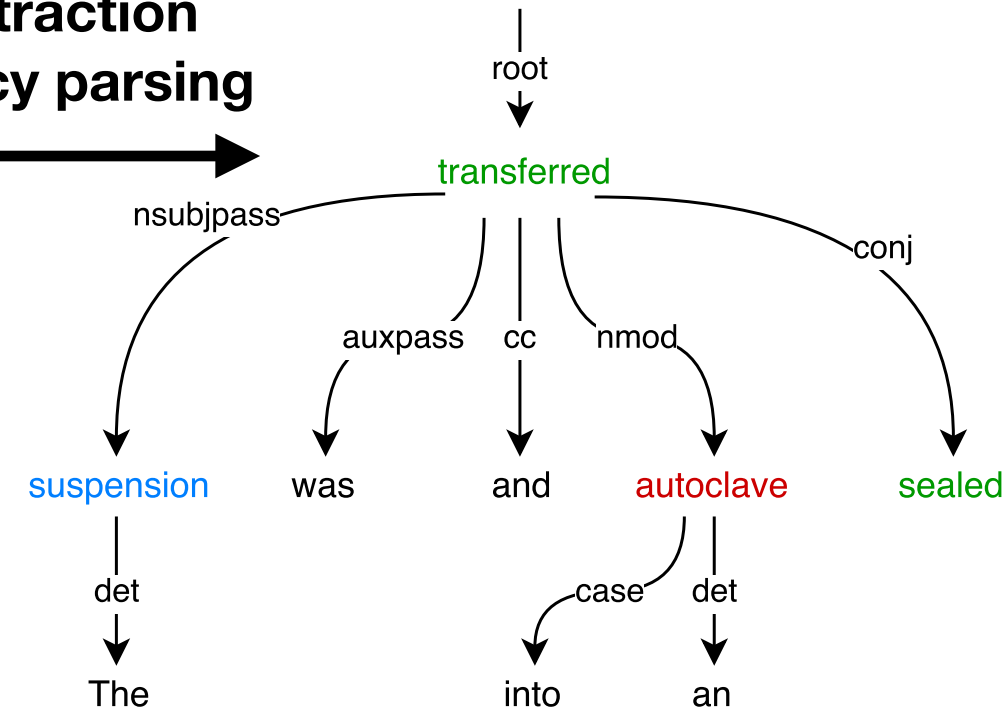
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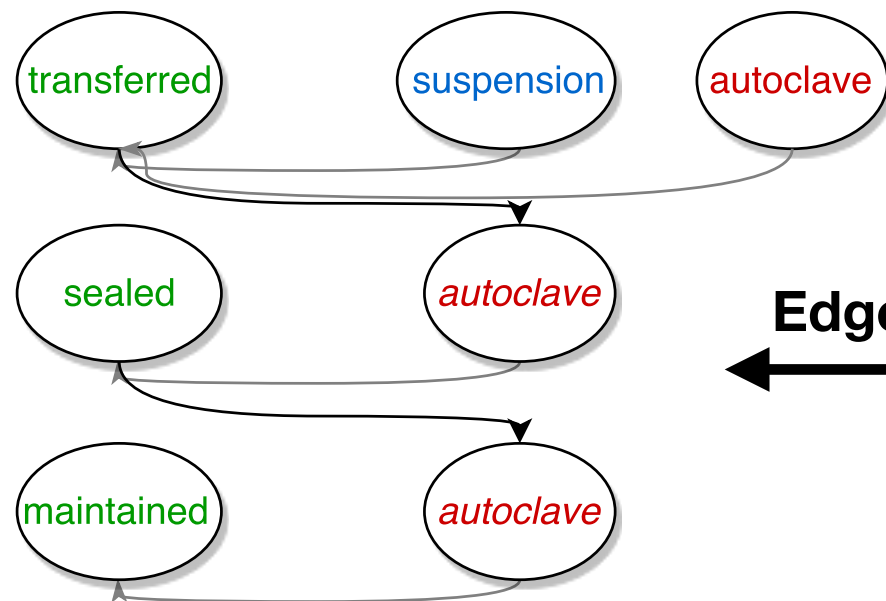
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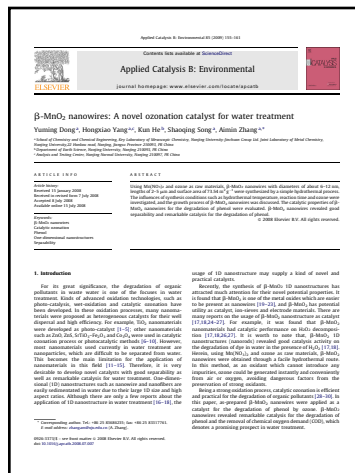
Edge induction



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Event extraction

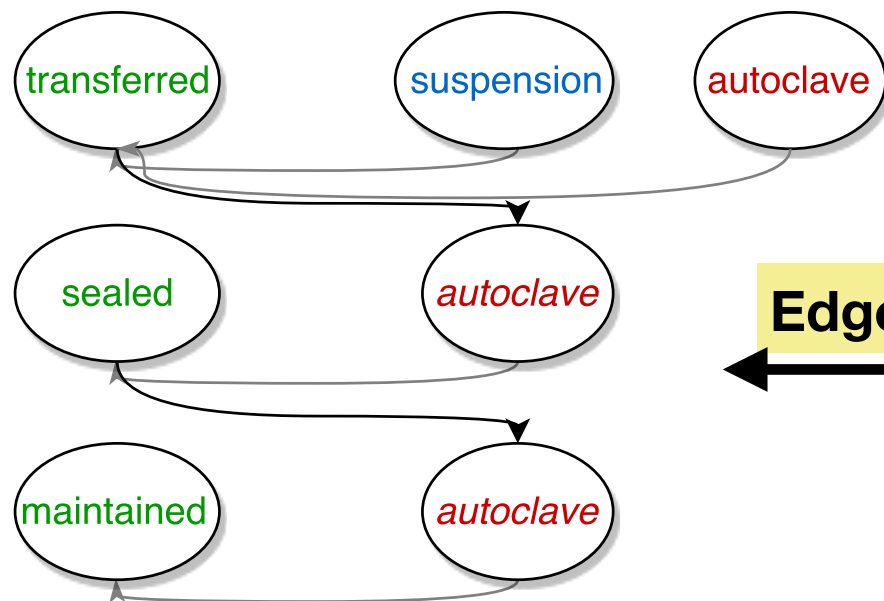
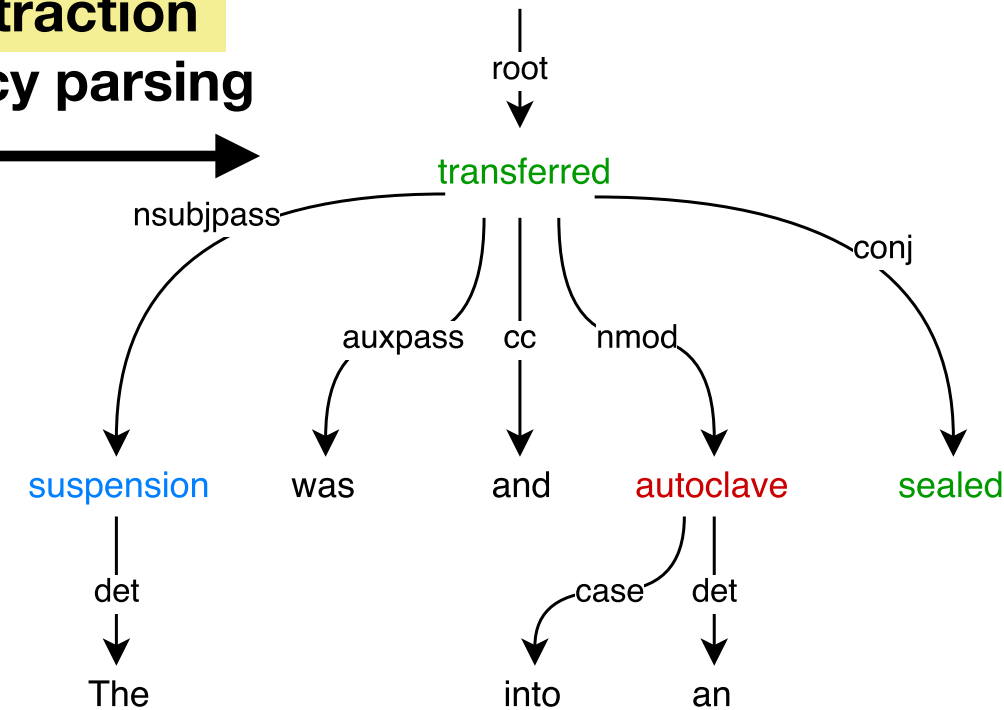
Overall pipeline architecture



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MATERIAL

OPERATION

APPARATUS

OPERATION

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Entity extraction

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PRP

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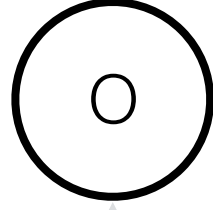
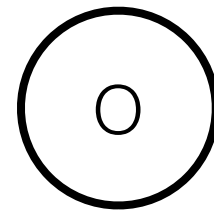
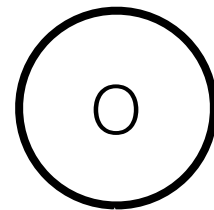
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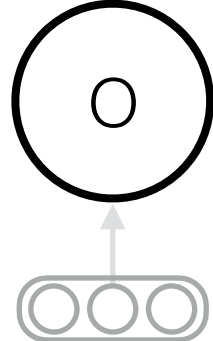
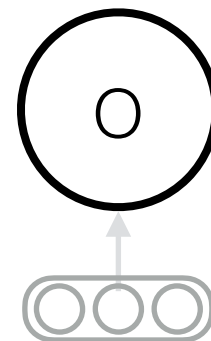
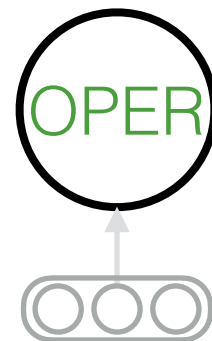
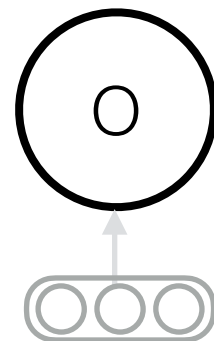
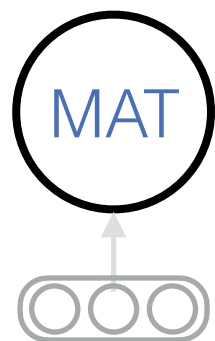
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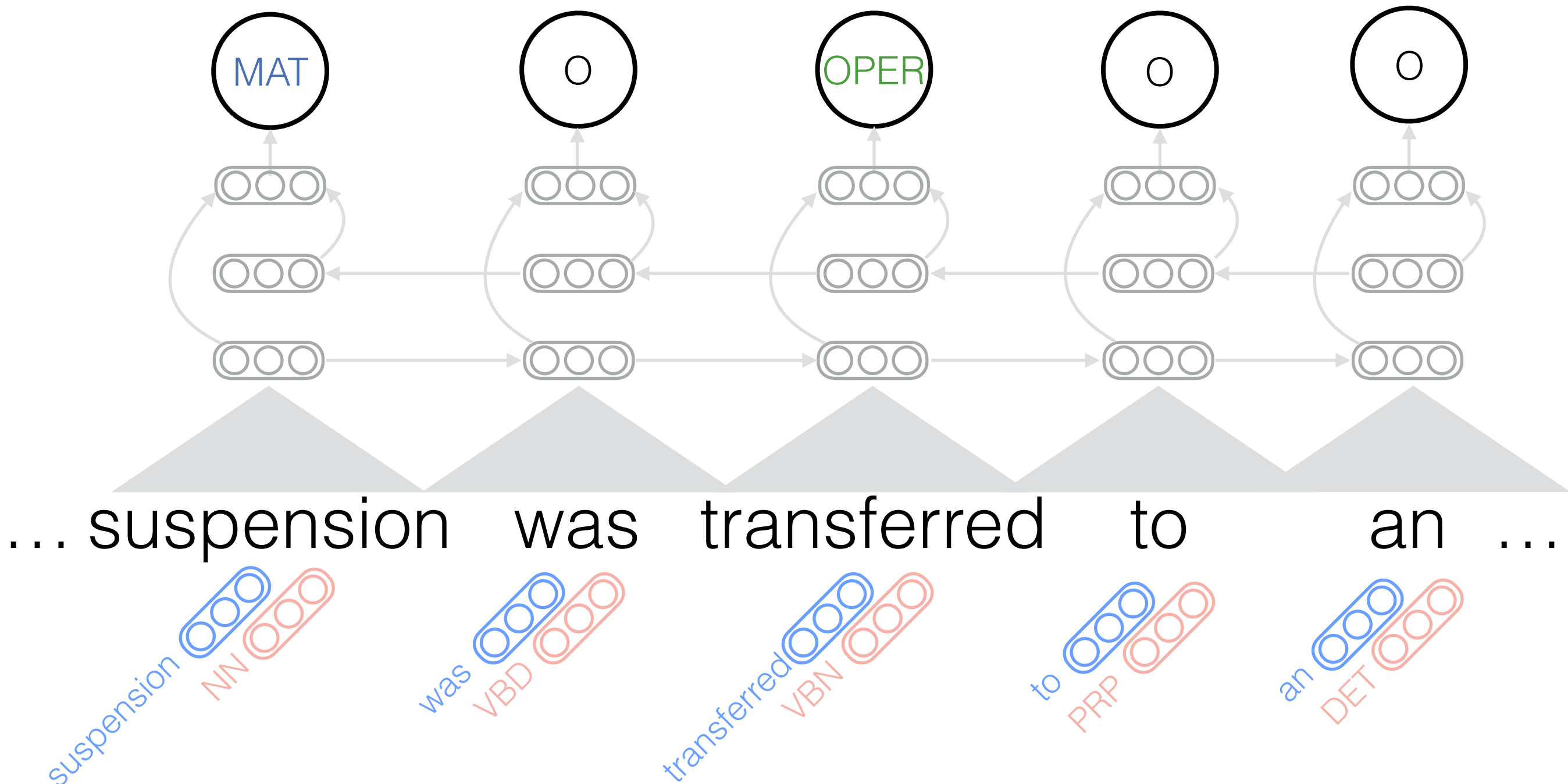
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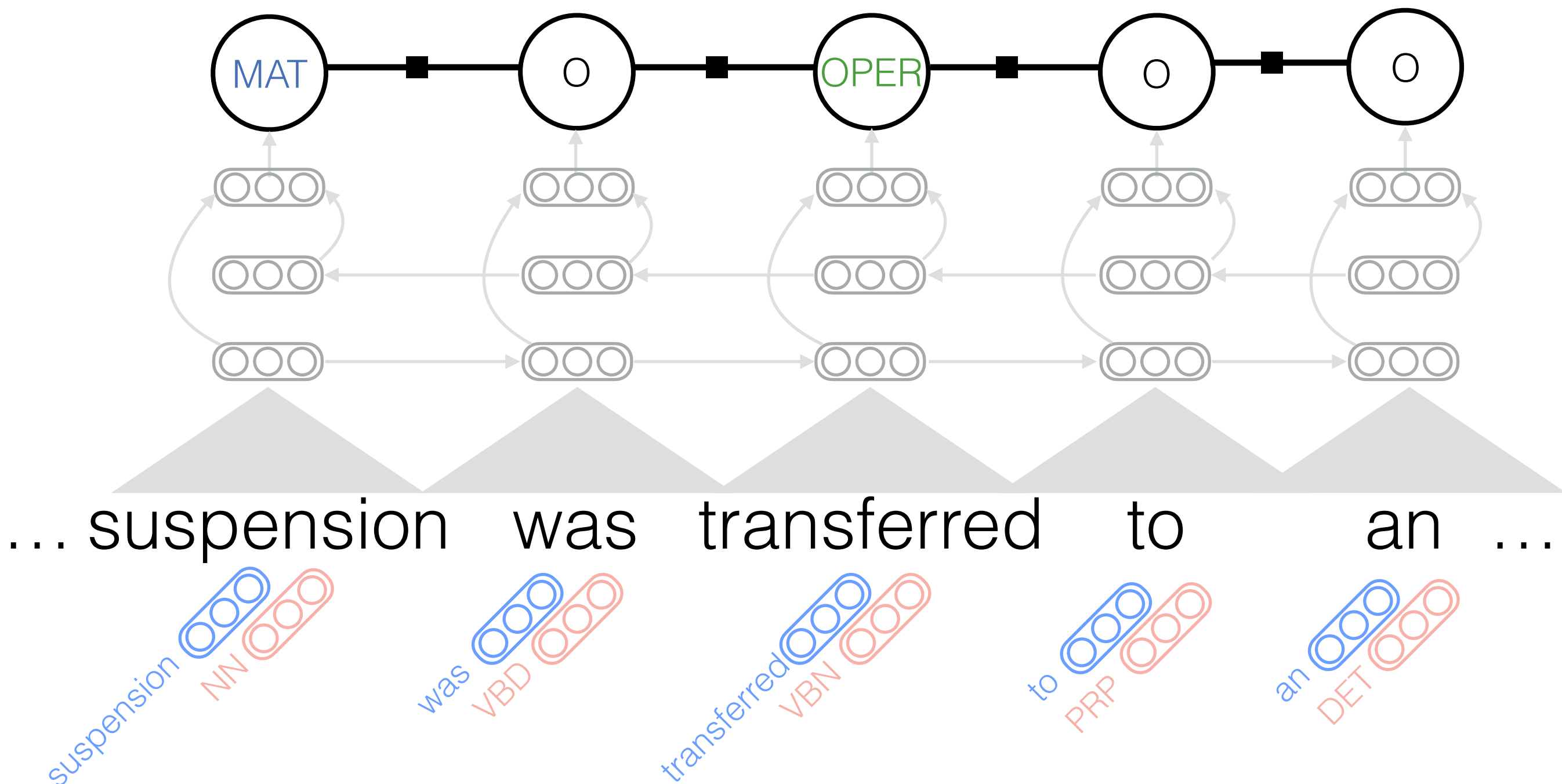
MATERIAL

OPERATION

APPARATUS

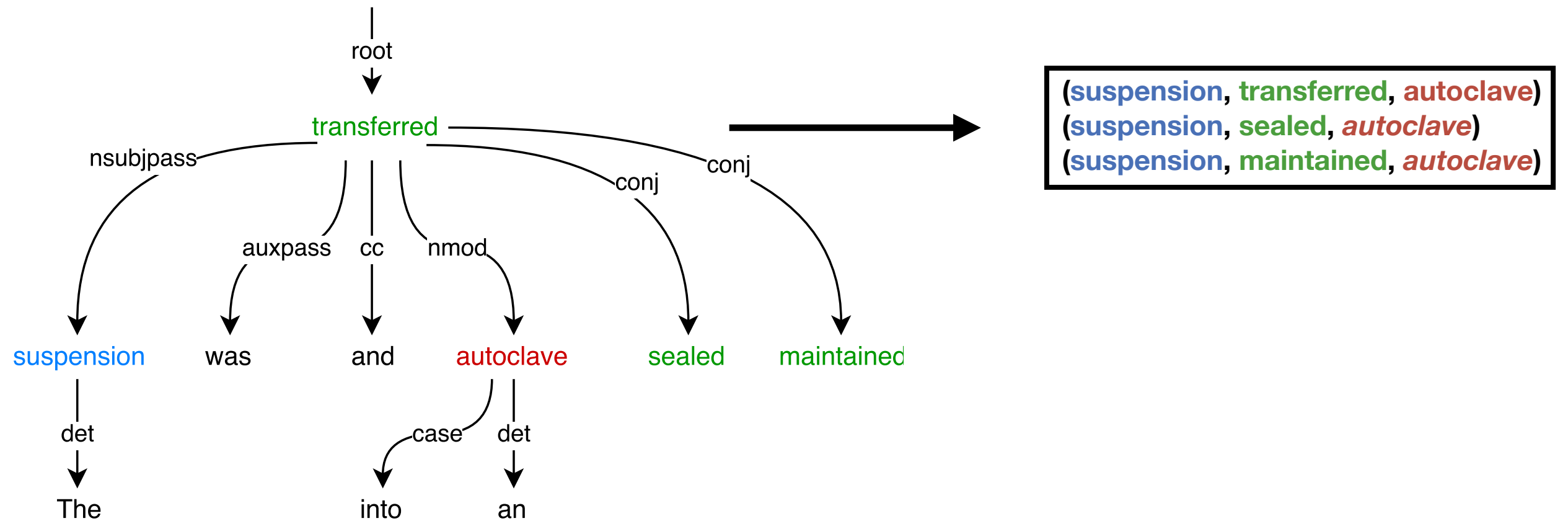
OPERATION

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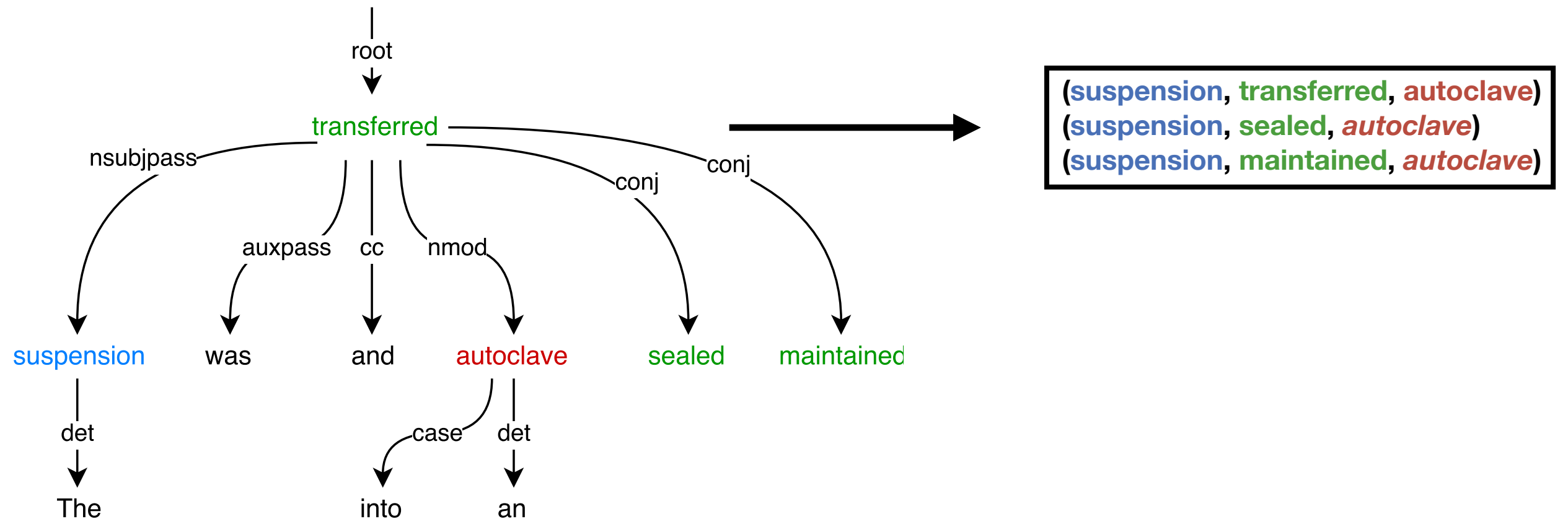
Event extraction

Event extraction



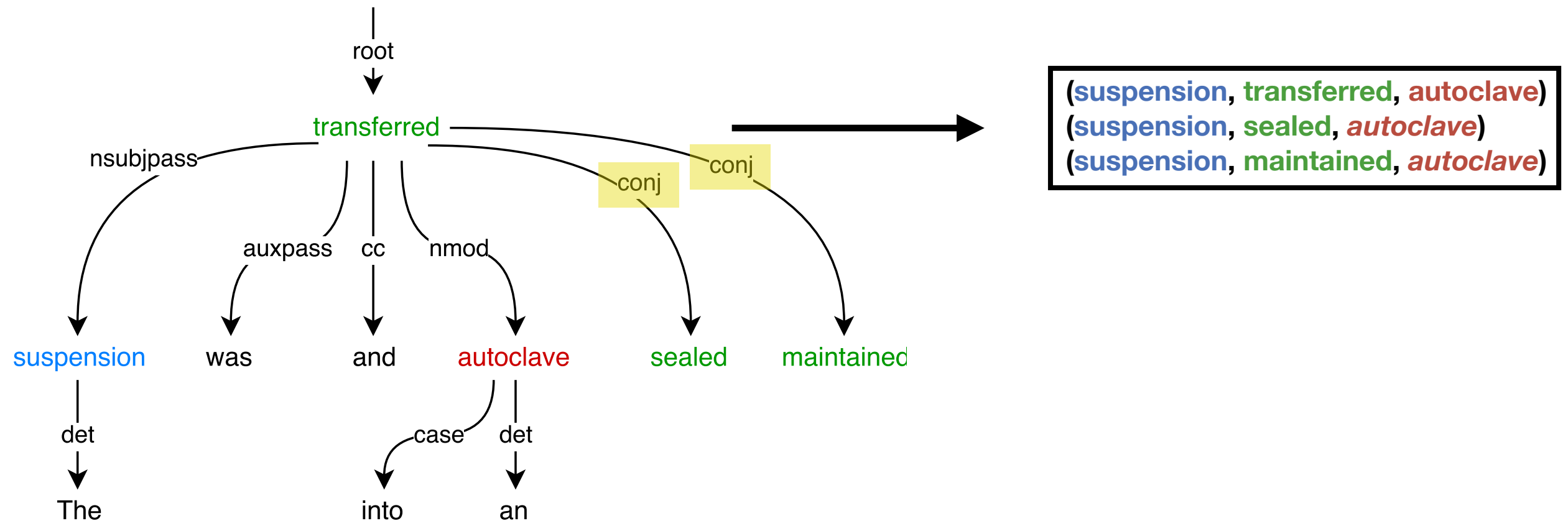
Event extraction

- Rules over dependency parse tree + entities



Event extraction

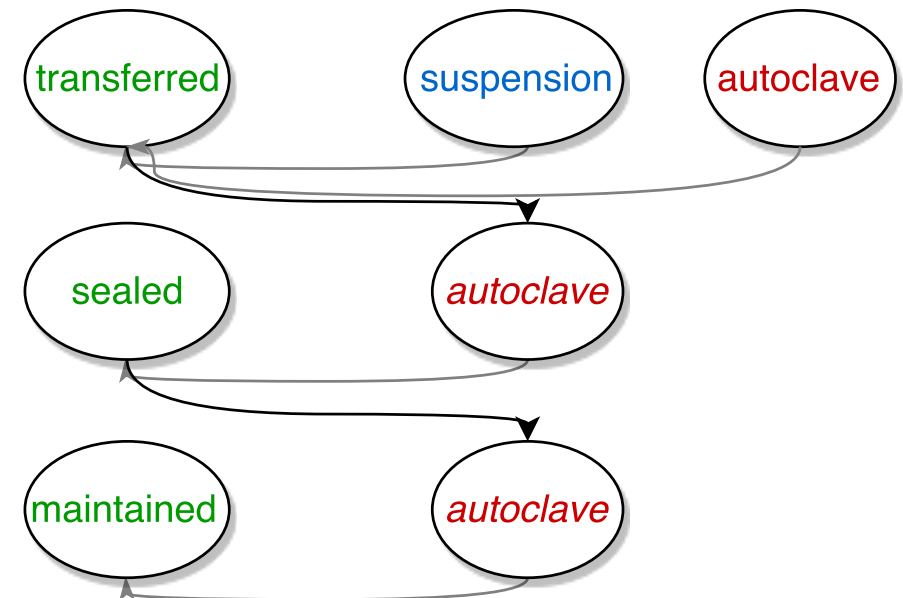
- Rules over dependency parse tree + entities



Edge induction

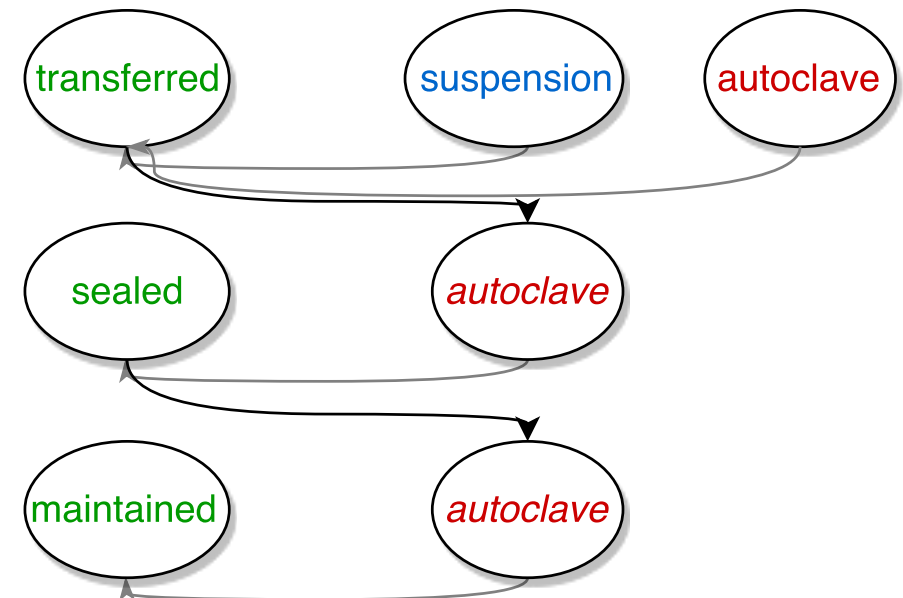
Edge induction

(suspension, transferred, autoclave)
(suspension, sealed, autoclave)
(suspension, maintained, autoclave)



Edge induction

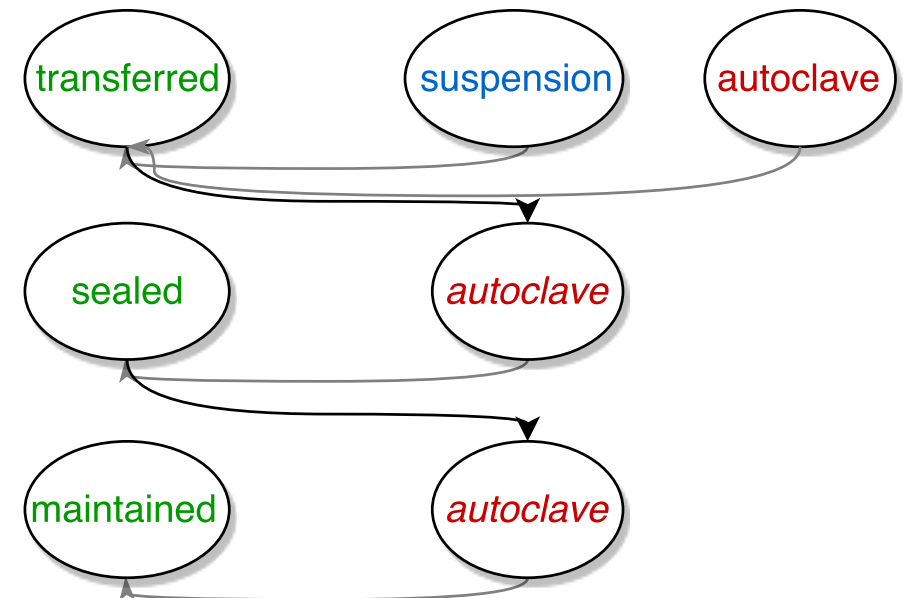
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(suspension, maintained, autoclave)



Baseline sequential model:

Edge induction

(suspension, transferred, autoclave)
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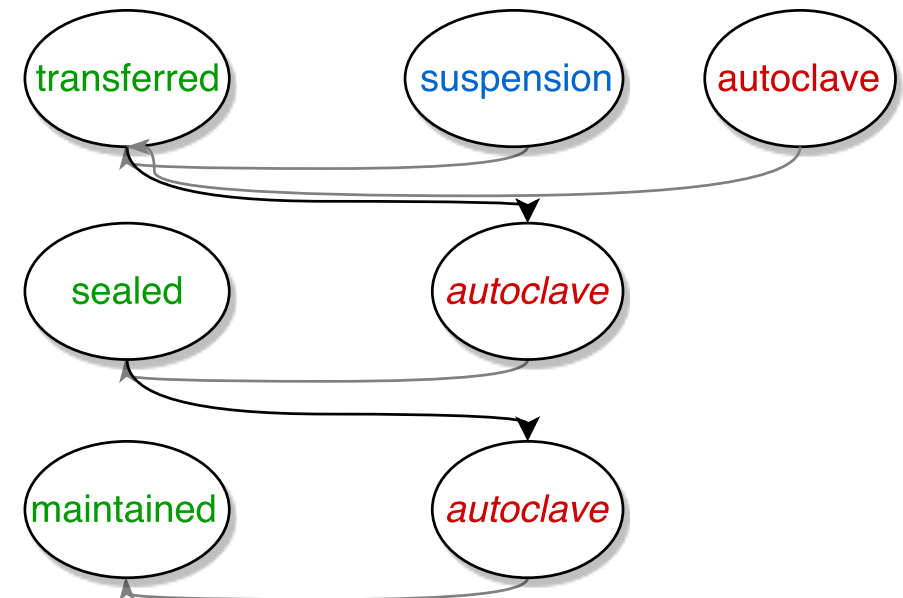


Baseline sequential model:

- Attach each event to the previous event in text.

Edge induction

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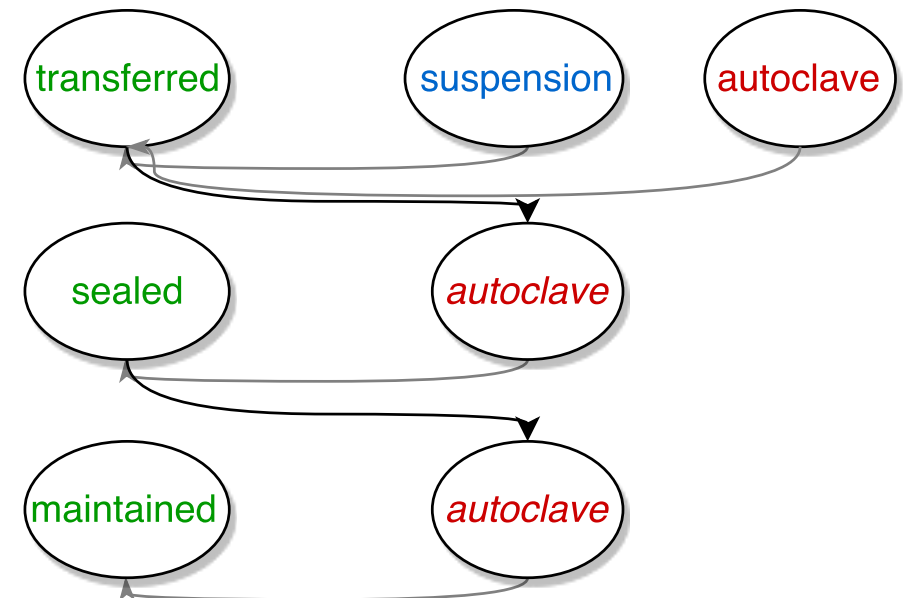
Baseline sequential model:

- Attach each event to the previous event in text.

Unsupervised probabilistic model:

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(suspension, transferred, autoclave)
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Baseline sequential model:

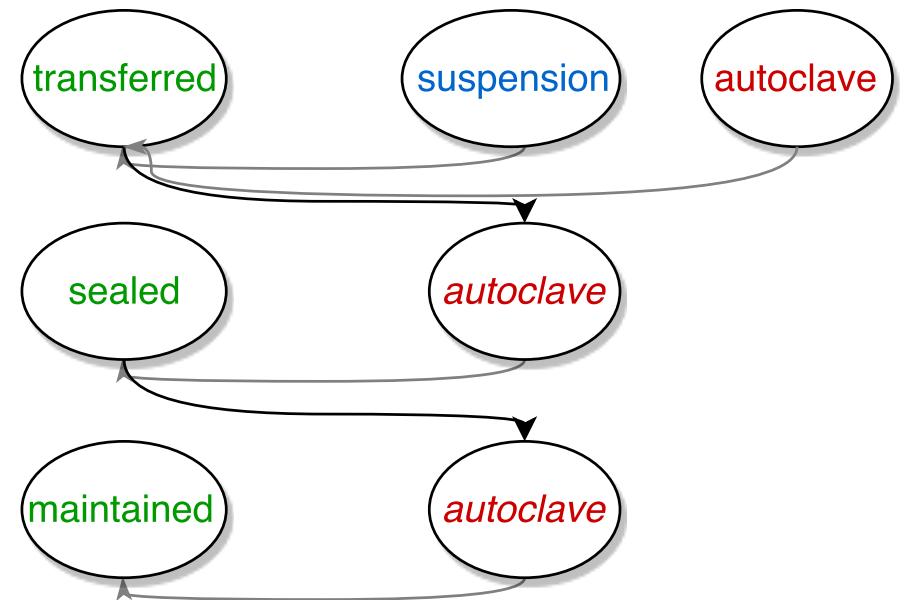
- Attach each event to the previous event in text.

Unsupervised probabilistic model:

- Define prior over connections: $P(C)$

Edge induction

(suspension, transferred, autoclave)
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Baseline sequential model:

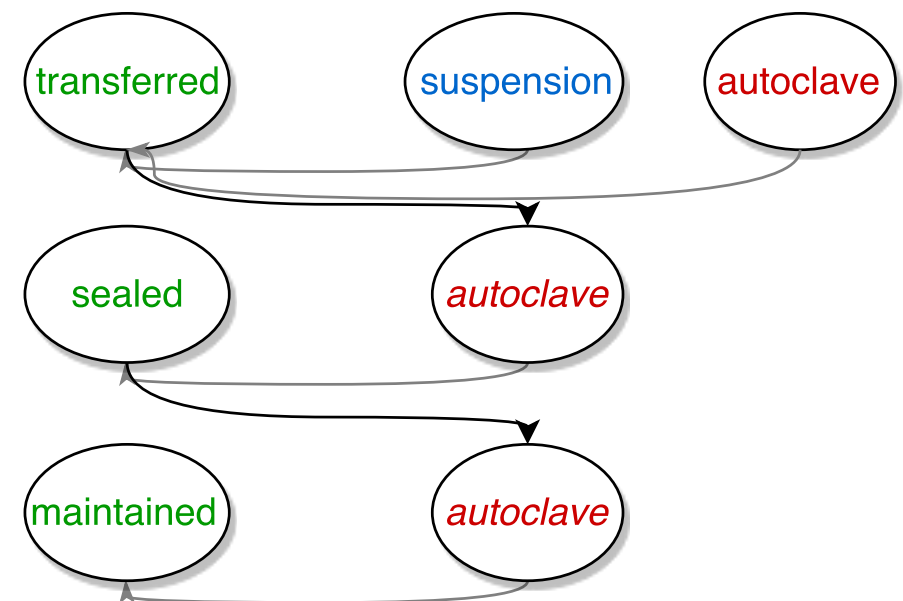
- Attach each event to the previous event in text.

Unsupervised probabilistic model:

- Define prior over connections: $P(C)$
 - Example: given dependency label, probability of incoming connections?

Edge induction

(suspension, transferred, autoclave)
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Baseline sequential model:

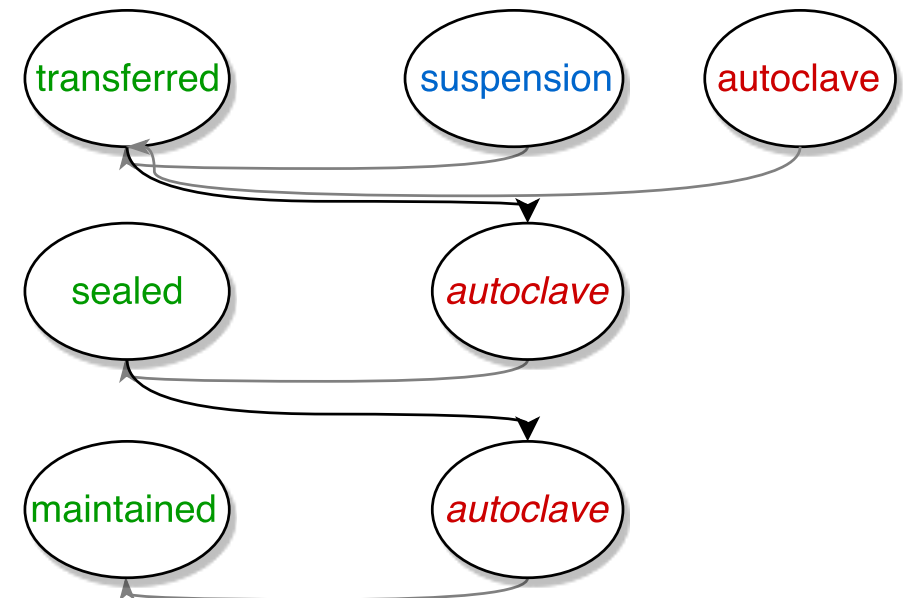
- Attach each event to the previous event in text.

Unsupervised probabilistic model:

- Define prior over connections: $P(C)$
 - Example: given dependency label, probability of incoming connections?
- Model probability of entities, text given connections: $P(S|C)$

Edge induction

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(suspension, sealed, autoclave)
(suspension, maintained, autoclave)



Baseline sequential model:

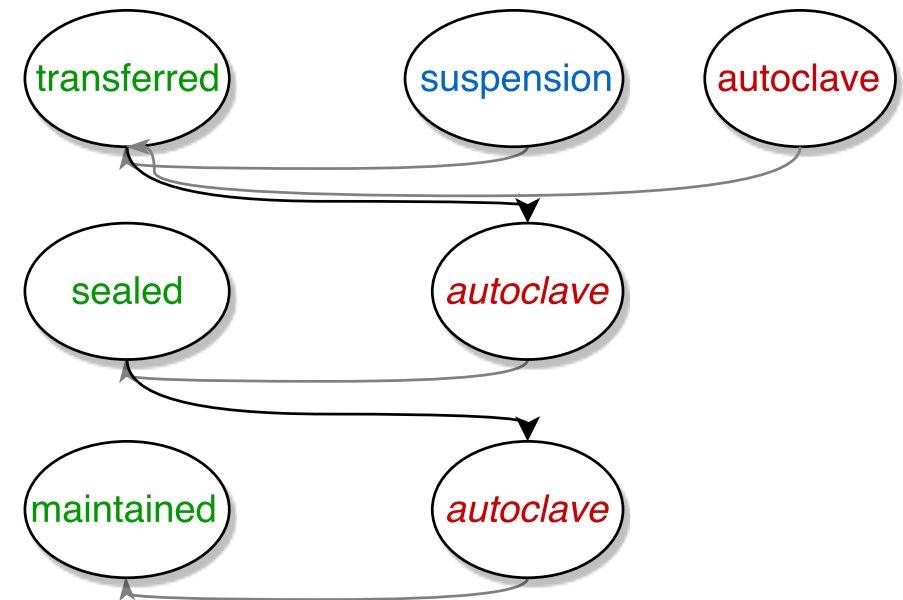
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Unsupervised probabilistic model:

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 - Example: given dependency label, probability of incoming connections?
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 - Example: *ozone* more likely to be added while *stirring* than while *heating*

Edge induction

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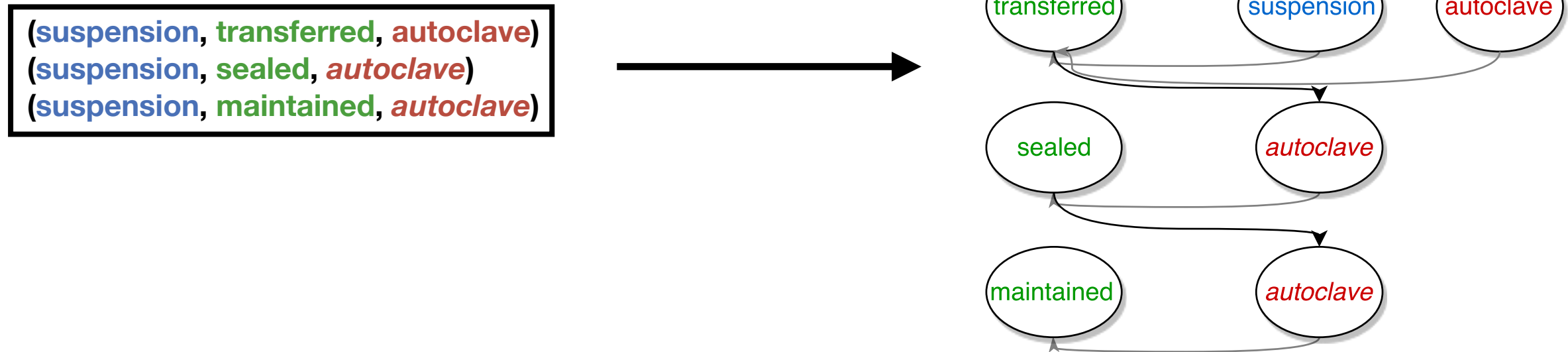
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 - Example: *suspension* more likely an intermediate than a raw ingredient

Edge induction



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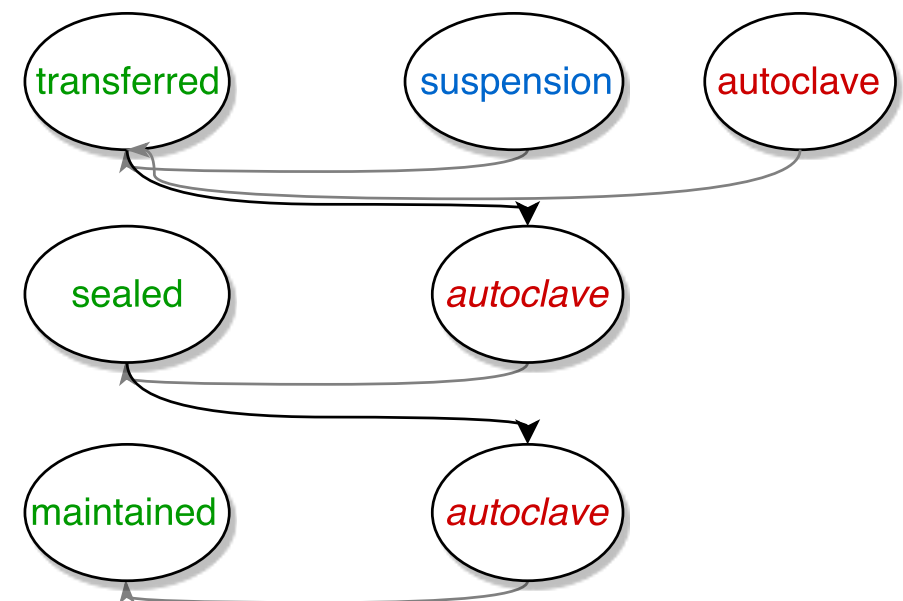
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 - Example: *ozone* more likely to be added while *stirring* than while *heating*
 - Example: *suspension* more likely an intermediate than a raw ingredient
- Maximize $P(S, C) = P(S|C)P(C)$ w/ hard EM

Edge induction

(suspension, transferred, autoclave)
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(suspension, maintained, autoclave)



Baseline sequential model:


- Attach each event to the previous event in text.

Unsupervised probabilistic model: [Kiddon et al. 2015, food recipes]


- Define prior over connections: $P(C)$
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 - Example: *ozone* more likely to be added while *stirring* than while *heating*
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β -MnO₂ nanowires: A novel ozonation catalyst for water treatment

Yuming Dong^a, Hongxiao Yang^{a,c}, Kun He^b, Shaoqing Song^a, Aimin Zhang^{a,*}

^aSchool of Chemistry and Chemical Engineering, Key Laboratory of Mesoscopic Chemistry, Nanjing University-Jinchuan Group Ltd. Joint Laboratory of Metal Chemistry, Nanjing University, 22 Hankou road, Nanjing, Jiangsu Province 210093, PR China
^bDepartment of Earth Science, Nanjing University, Nanjing 210093, PR China
^cAnalysis and Testing Center, Nanjing Normal University, Nanjing 210097, PR China

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ABSTRACT

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Keywords:
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Phenol
One-dimensional nanostructures
Separability

1. Introduction

For its great significance, the degradation of organic pollutants in waste water is one of the focuses in water treatment. Kinds of advanced oxidation technologies, such as photo-catalysis, wet-oxidation and catalytic ozonation have been developed. In these oxidation processes, many nanomaterials were proposed as heterogeneous catalysts for their well dispersal and high efficiency. For example, TiO₂ nanomaterials were developed as photo-catalyst [1–5]; other nanomaterials such as ZnO, ZnS, SrTiO₃–Fe₂O₃ and Co₃O₄ were used in catalytic ozonation process or photocatalytic methods [6–10]. However, most nanomaterials used currently in water treatment are nanoparticles, which are difficult to be separated from water. This becomes the main limitation for the application of nanomaterials in this field [11–15]. Therefore, it is very desirable to develop novel catalysts with good separability as well as remarkable catalysis for water treatment. One-dimensional (1D) nanostructures such as nanowire and nanofibers are easily sedimentated in water due to their large 1D size and high aspect ratios. Although there are only a few reports about the application of 1D nanostructure in water treatment [16–18], the

usage of 1D nanostructure may supply a kind of novel and practical catalysts.

Recently, the synthesis of β -MnO₂ 1D nanostructures has attracted much attention for their novel potential properties. It is found that β -MnO₂ is one of the metal oxides which are easier to be present as nanowires [19–23], and β -MnO₂ has potential utility as catalyst, ion-sieves and electrode materials. There are many reports on the usage of β -MnO₂ nanostructure as catalyst [17,18,24–27]. For example, it was found that β -MnO₂ nanomaterials had catalytic performance on H₂O₂ decomposition [17,18,26,27]. It is worth to note that, β -MnO₂ 1D nanostructures (nanorods) revealed good catalysis activity on the degradation of dye in water in the presence of H₂O₂ [17,18]. Herein, using Mn(NO₃)₂ and ozone as raw materials, β -MnO₂ nanowires were obtained through a facile hydrothermal route. In this method, as an oxidant which cannot introduce any impurities, ozone could be generated instantly and conveniently from air or oxygen, avoiding dangerous factors from the preservation of strong oxidants.

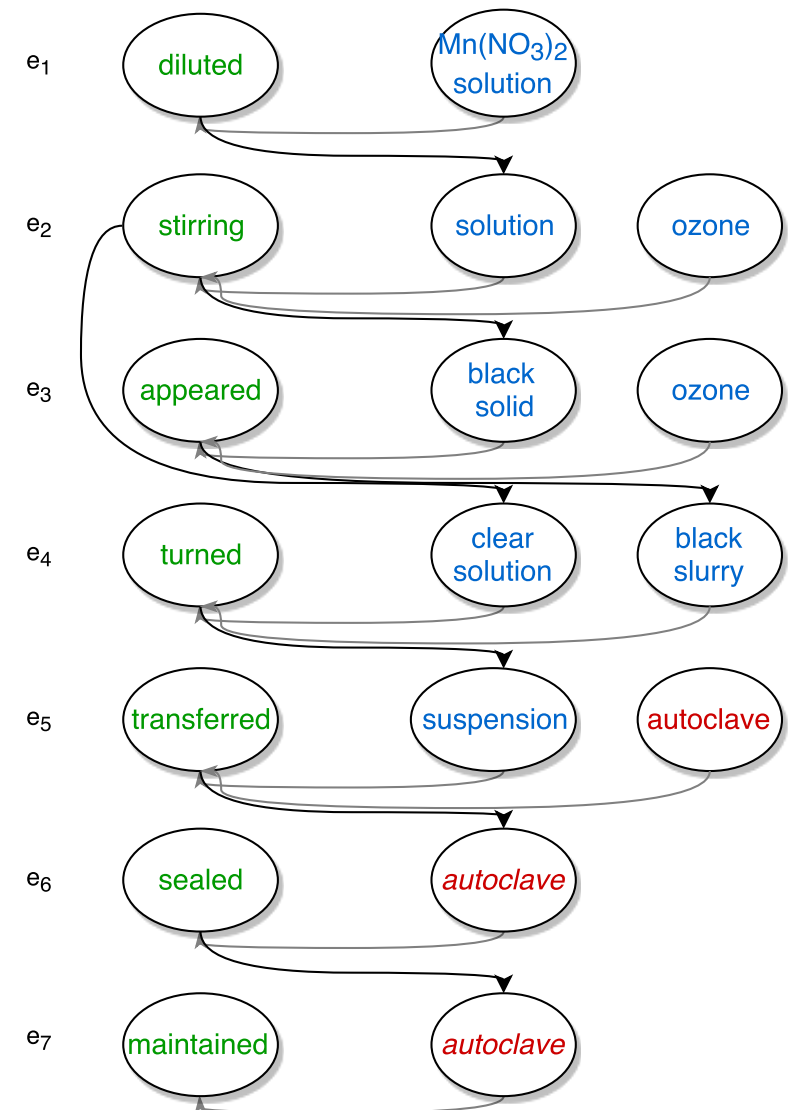
Being a strong oxidation process, catalytic ozonation is efficient and practical for the degradation of organic pollutants [28–30]. In this paper, as-prepared β -MnO₂ nanowires were applied as a catalyst for the degradation of phenol by ozone. β -MnO₂ nanowires revealed remarkable catalysis for the degradation of phenol and the removal of chemical oxygen demand (COD), which denotes a promising prospect in water treatment.

* Corresponding author. Tel.: +86 25 83686235; fax: +86 25 83317761.
E-mail address: zhangam@nju.edu.cn (A. Zhang).

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Typical synthesis procedure text

In a typical procedure for the synthesis of β -MnO₂ nanowires, 2.5 mL of 50 wt.% Mn(NO₃)₂ solution was diluted to 25.0 mL, and ozone was fed into the bottom of the solution for 30 min under vigorous stirring. With the indraught of ozone, black solid appeared gradually and the clear solution turned into black slurry finally. Then the suspension was transferred into an autoclave of 48.0 mL, sealed and maintained at 200 °C for 8 h. After this, the autoclave was cooled to room temperature naturally. The resulting solid products were washed with water, and dried at 120 °C for 8 h.



Thank you!