A graph-convolutional NN model for the prediction of chemical reactivity

Egor Gladin

MIPT

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Plan

Статья

Connor W. Coley, Wengong Jin, Luke Rogers, Timothy F. Jamison, Tommi S. Jaakkola, William H. Green, Regina Barzilay, Klavs F. Jensen

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Постановка задачи

Задача

Предсказать продукты реакции по веществам и растворам, участвующим в реакции

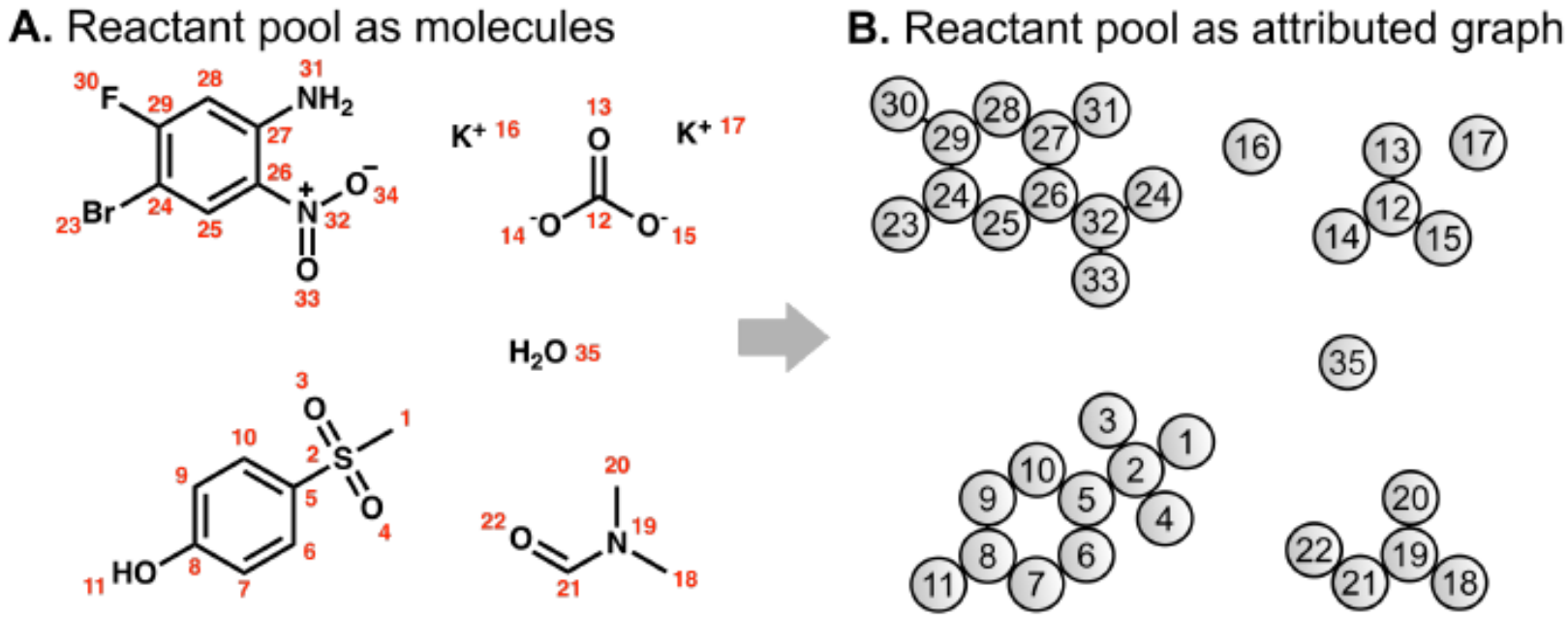


Схема подхода

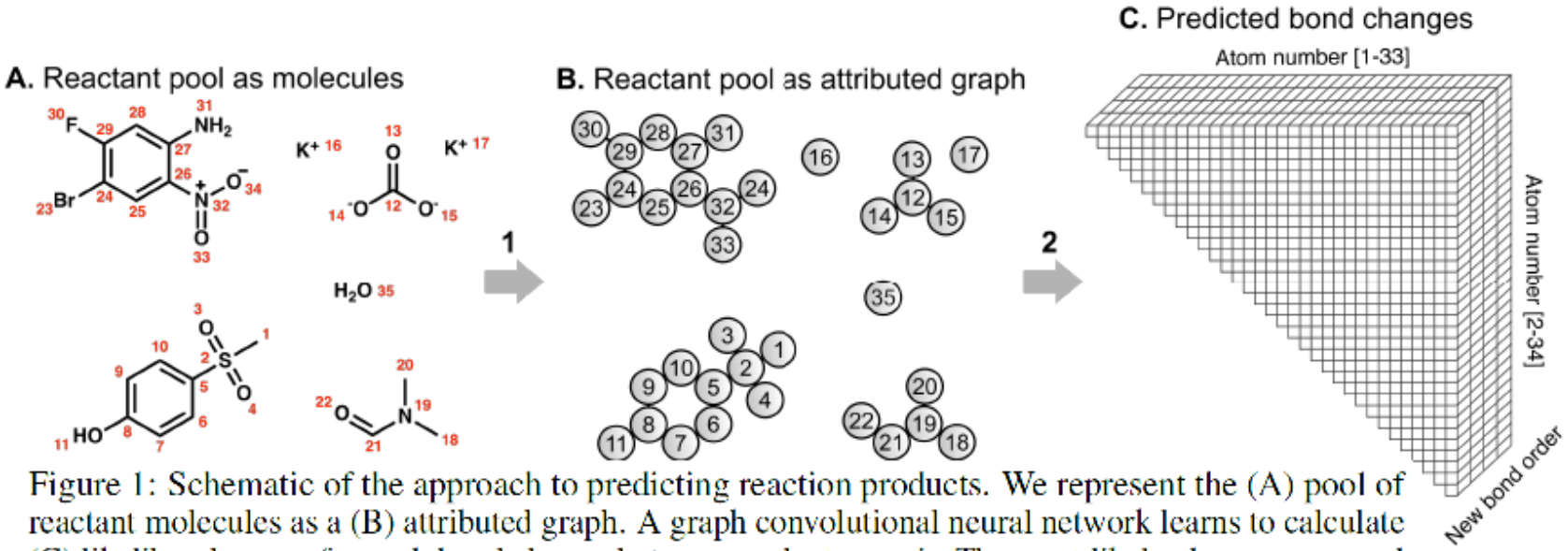
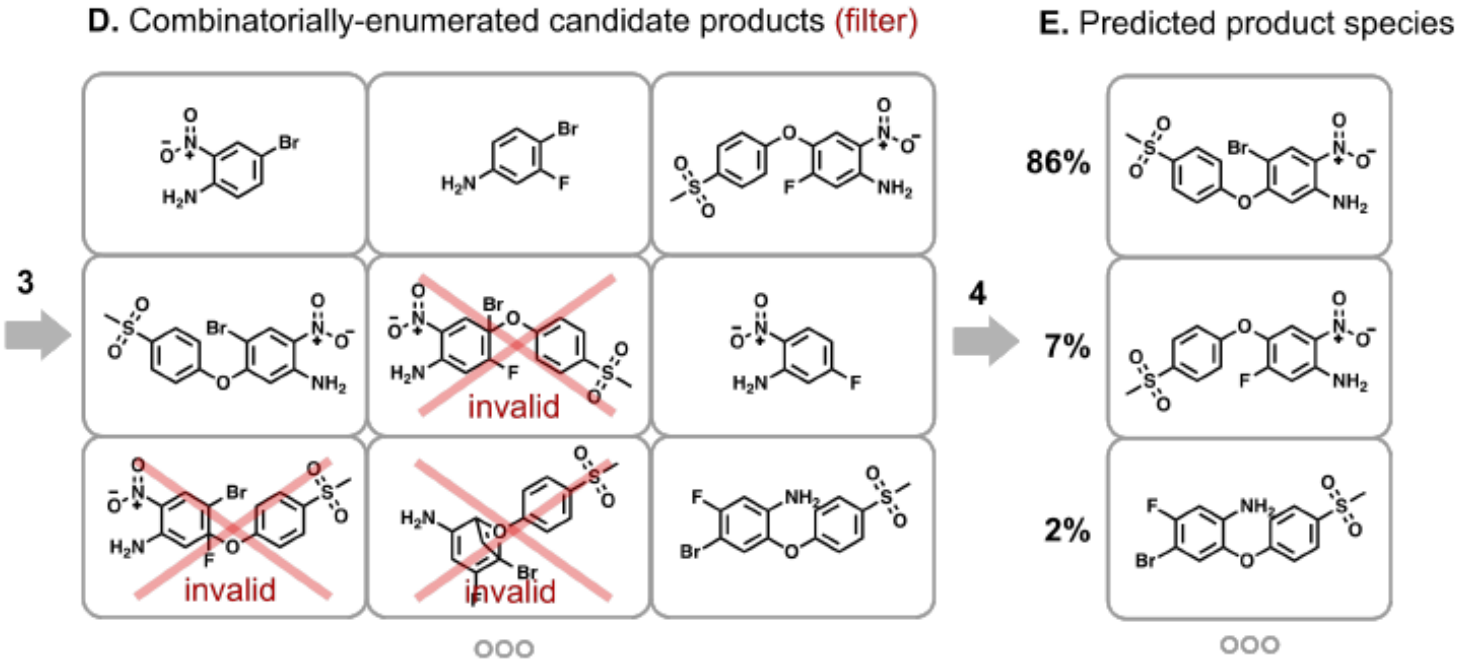


Figure 1: Schematic of the approach to predicting reaction products. We represent the (A) pool of reactant molecules as a (B) attributed graph. A graph convolutional neural network learns to calculate (C) likelihood scores for each bond change between each atom pair. The most likely changes are used to perform a focused, ranked enumeration of (D) candidate products, which are filtered by chemical valence rules. These candidates are then rescored by another graph convolutional network to yield (E) a probability distribution over predicted product species.

Схема подхода



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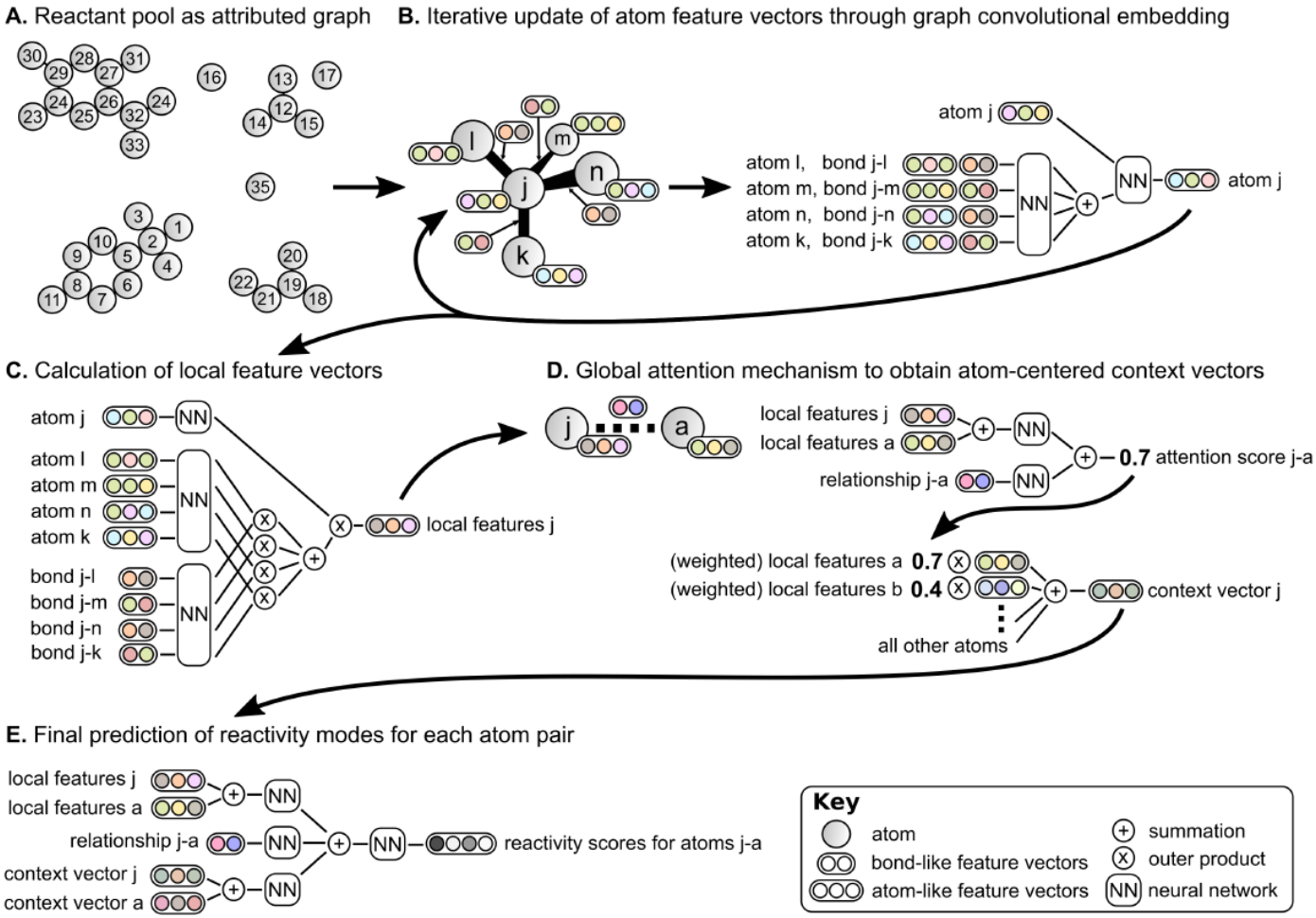
WLN for predicting likely changes in bond order



Local atom representation

Обозначения

- f_v^l - feature vector атома v на итерации l
- f_{uv} - стартовый feature vector связи (u, v)
- U_i, V_i, W_i - матрицы WLN (обучаемые веса)
- c_v - конечное локальное представление атома v

$$f_v^l = \tau\left(U_1 f_v^{l-1} + U_2 \sum_{u \in N(v)} \tau(V_1 f_u^{l-1} + V_2 f_{uv})\right) \quad (1 \le l \le L)$$

$$c_v = \sum_{u \in N(v)} W_1 f_u^L \odot W_2 f_{uv} \odot W_3 f_v^L$$

Global atom representation

Обозначения

- α_{vz} - attention score of atom v upon atom z
- b_{uv} - feature vector, отвечающий за отношение (u, v)
- P_a, P_b, u - обучаемые веса модели

$$\alpha_{vz} = \sigma(u^T \tau(P_a c_v + P_a c_z + P_b b_{vz}))$$

$$\tilde{c}_v = \sum_v \alpha_{vz} c_z$$

Reaction center

Центр реакции

(u, v, b) находится в центре реакции $\iff$ тип связи между атомами u и v сменился на b

Обозначения

- $s_{u,v,b}$ - вероятность того, что (u, v, b) в центре реакции
- M_a, M_b, P_a, u_b - обучаемые веса модели
- $y_{u,v,b} = 1 \iff (u, v, b)$ в центре реакции

$$s_{u,v,b} = \sigma\left(u_b^T \tau(M_a \tilde{c}_u + M_a \tilde{c}_v + P_a c_u + P_a c_v + M_b f_{uv})\right)$$

$$- \sum_{u,v,b;u \neq v} y_{u,v,b} \log s_{u,v,b} + (1 - y_{u,v,b}) \log(1 - s_{u,v,b})$$

Reaction center prediction

Обозначения

- r - реагенты
- p_i - i-й потенциальный продукт реакции
- $c_v^{(p_i)}$ - feature vector атома v в продукте p_i
- $d_v^{(p_i)} \triangleq c_v^{(p_i)} - c_v^{(r)}$, $h_v^{(p_i,0)} = d_v^{(p_i)}$
- $RC(p_i)$ - множество связей, изменившихся в p_i

$$h_v^{(p_i,l)} = \tau\left(U_1 h_v^{(p_i,l-1)} + U_2 \sum_{u \in N(v)} \tau\left(V_1 h_u^{(p_i,l-1)} + V_2 f_{uv}\right)\right) \qquad (1 \le l \le L)$$

$$g_v^{(p_i)} = \sum_{u \in N(v)} W_1 h_u^{(p_i,L)} \odot W_2 f_{uv} \odot W_3 h_v^{(p_i,L)}$$

$$s(p_i) = u^T \tau\left(M \sum_{v \in p_i} g_v^{(p_i)}\right) + \sum_{(u,v,b) \in RC(p_i)} s_{u,v,b}$$

Results

Точность на уровне экспертов
Скорость: 100 ms per example on a single consumer GPU

Method	$\|\theta\|$	Top-1 [%]	Top-2 [%]	Top-3 [%]	Top-5 [%]
WLN/WLDN [16]	3.2 M	79.6	-	87.7	89.2
Sequence-to-sequence [31]	30 M*	80.3	84.7	86.2	87.5
This work	2.6 M	**85.6**	**90.5**	**92.8**	**93.4**