HyperSearch: Prediction of New Hyperedges through Unconstrained yet Efficient Search - Supplementary Document

APPENDIX

A. *Details on ILP Formulation for the Scoring Function (Supplementing Sect. V-B)*

To compute the score for a candidate hyperedge e', we formulate the problem as an Integer Linear Programming (ILP) problem, inspired by proportional fault-tolerant frequent itemset mining [1], [2].

Let $E = \{e_1, e_2, \ldots, e_{|E|}\}$ be the set of observed hyperedges, and $e' = \{v_1, v_2, \ldots, v_{|e'|}\}$ be a candidate hyperedge. We define a binary decision variable $x_j \in \{0, 1\}$ for each $e_j \in E$, indicating whether e_j is included in the subset $\widetilde{E}$.

Let $A \in \{0, 1\}^{|e'| \times |E|}$ be a binary matrix such that $A_{i,j} = 1$ if node $v_i \notin e_j$, and 0 otherwise. We then define the following constraints:

- **Node relaxation constraint:** Each node $v_i \in e'$ can be missing from at most an ϵ_v proportion of selected hyperedges:

$$\sum_{j=1}^{|E|} A_{i,j} \cdot x_j \leq \epsilon_v \cdot \sum_{j=1}^{|E|} x_j \quad \forall i \in [m] \tag{1}$$

- **Hyperedge relaxation constraint:** Each selected hyperedge may miss at most an ϵ_e fraction of the nodes in e':

$$\sum_{i=1}^{|e'|} A_{i,j} \leq \epsilon_e \cdot |e'| \quad \forall j \text{ such that } x_j = 1 \tag{2}$$

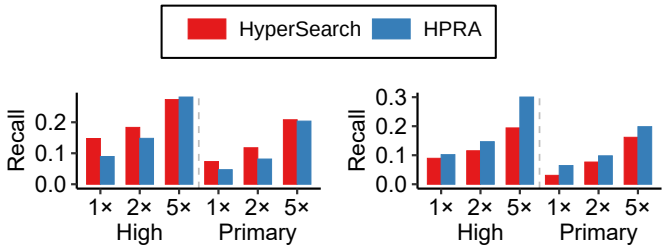
- **Total relaxation constraint:** The total number of node-hyperedge mismatches must be within the allowed global relaxation:

$$\sum_{i=1}^{|e'|} \sum_{j=1}^{|E|} A_{i,j} \cdot x_j \leq \epsilon_t \cdot |e'| \cdot \sum_{j=1}^{|E|} x_j \tag{3}$$

The objective is to maximize the number of selected hyperedges:

$$\max \sum_{j=1}^{|E|} x_j \tag{4}$$

Solving this ILP yields the largest subset $\widetilde{E}$ of observed hyperedges that satisfies the node-, hyperedge-, and total-level relaxation constraints with respect to the candidate e'. We implement this ILP formulation using the SCIP solver provided through Google OR-Tools.



(a) All Candidates (b) Size-3 Candidates

Fig. 1. (a) The superiority of HyperSearch in predictive accuracy diminishes as the number of predicted hyperedges increases. (b) HyperSearch is outperformed by HPRA on size-3 hyperedges, likely due to the lack of promising candidates based on our scoring function. This highlights a limitation of HyperSearch in identifying *structurally novel* hyperedges composed of node combinations absent in observed hyperedges.

B. *Additional Details on Dataset Preprocessing (Supplementing Sect. VI-A)*

The Cora, High, Primary, Ubuntu, and Math datasets contain only hyperedges of size up to 5. For the other five datasets, we retained only hyperedges with sizes up to 10 (before splitting them into E_1 and E_2) for computational efficiency. This preprocessing step was applied to all methods.

Moreover, we identified hyperedge sizes i where the proportion of hyperedges was below 1% and removed them. As shown in Table I, after such preprocessing, in each dataset, at least 90% of the original hyperedges remained.

C. *Hyperparameter Search Spaces for HNN Models (Supplementing Sect. VI-A)*

Table II summarizes the hyperparameter search spaces used for the HNN models employed in our experiments. The hyperparameters are selected based on the original settings proposed in their respective papers and further optimized based on validation performance. Common hyperparameters (e.g., epochs, hidden dimensions, optimizer, learning rate, batch size) are consistently aligned across methods, while method-specific parameters are indicated separately.

D. *Additional Evaluation Metric: Average F1 Score (Supplementing Sect. VI-A and Sect.VI-B)*

To supplement the Recall@$\mathcal{K}$ evaluation in the main article, we also report the results using the *Average F1 Score*, which quantifies the closeness between predicted and ground-truth hyperedges. Specifically, for each predicted hyperedge, we compute the F1 score against its best-matching ground-truth hyperedge, and vice versa, then average the two values across

TABLE I
PROPORTION OF HYPEREDGES BASED ON THEIR SIZE (≤ 10).

Size (Unit: %)	Citeseer	Cora	Cora-A	DBLP-A	Enron	Eu	High	Primary	Ubuntu	Math
Total (≤ 10)	**98.61**	**100.00**	**92.16**	**92.51**	**98.56**	**96.68**	**100.00**	**100.00**	**100.00**	**100.00**
2	48.61	37.90	41.65	41.86	55.53	52.21	70.32	60.99	19.41	14.92
3	24.10	29.80	19.69	19.88	21.76	20.29	26.75	36.21	36.05	37.75
4	11.35	20.30	10.52	10.90	9.47	9.35	2.84	2.73	27.01	30.12
5	6.37	12.00	7.84	6.71	4.32	5.57	0.09	0.07	17.53	17.21
6	3.59	-	4.64	4.33	2.95	3.63	-	-	-	-
7	2.19	-	2.89	3.15	1.85	2.29	-	-	-	-
8	1.00	-	2.16	2.41	1.51	1.44	-	-	-	-
9	0.60	-	1.13	1.73	0.41	1.12	-	-	-	-
10	0.80	-	1.65	1.55	0.75	0.78	-	-	-	-

TABLE II
HYPERPARAMETER SEARCH SPACES FOR HNN MODELS.

Hyperparameter	MHP	AHP	Hyper-SAGNN	NHP
Epochs	500	500	500	500
Hidden Dimension	{64, 128}	400	64	{64, 128, 256}
Optimizer	Adam	Adam	Adam	Adam
Learning Rate	{1e-3, 5e-4, 1e-4}	Generator & Discriminator: {1e-3, 1e-4, 1e-5, 1e-6}	{1e-2, 1e-3, 1e-4}	{1e-2, 1e-3}
Batch Size	{128, 256, 512}	128	128	{32, 64, 128}
Number of Samples	{2, 5, 8, 10, 12, 15}	-	-	-
Normalization Factor (α, β)	-	{(0,0), (1,1)}	-	-
Dropout	-	{0, 0.5}	-	-
node2vec (p,q)	-	-	{(1,1), (50,0.5), (50,1), (100,0.5)}	-

the dataset. This provides a complementary perspective that captures partial correctness, especially in cases where predicted and true hyperedges have significant but not complete overlap.

Formally, the Average F1 Score is defined as:

$$\text{Average F1 Score} := \frac{1}{2}\left(\begin{array}{l}\dfrac{1}{|E_2|}\displaystyle\sum_{e_i\in E_2} F1(e_i, e'_{g(i)}) \\ +\dfrac{1}{|E'|}\displaystyle\sum_{e'_i\in E'} F1(e_{g'(i)}, e'_i)\end{array}\right) \quad (5)$$

where:

- E_2 is the set of missing hyperedges (test set),
- E' is the set of predicted hyperedges,
- $g(i)$ returns the index of the best-matching predicted hyperedge e'_j for each e_i, i.e., $g(i) = \arg\max_j \text{F1}(e_i, e'_j)$,
- $g'(i)$ returns the index of the best-matching ground-truth hyperedge e_j for each e'_i, i.e., $g'(i) = \arg\max_j \text{F1}(e_j, e'_i)$.

Tables III and IV summarize the results. Compared to Recall@$\mathcal{K}$, which focuses on exact matching, Average F1 Score highlights subtler differences in hyperedge structure and matching behavior.

E. Additional Results On "Q1. Accuracy" (Supplementing Sect.VI-B)

As shown in Fig.1(a), the superiority of HyperSearch in predictive accuracy diminishes as the number of predicted hyperedges increases. As depicted in Fig.1(b), HyperSearch is outperformed by HPRA w.r.t. the performance on size-3 hyperedges, this is likely because there are not many size-3 promising candidates based on our scoring function, which reveals a potential limitation of HyperSearch in identifying "structurally novel" hyperedges consisting of node combinations that do not exist in observed hyperedges.

F. Refinement with HNNs (Supplementing Sects. VI-A & VI-B)

To further refine and enhance the quality of the predicted hyperedges, we incorporate a filtering step using Hypergraph Neural Networks (HNNs). This step applies an HNN model to the hyperedge candidates generated in the earlier stages, leveraging learned representations to improve prediction performance. Specifically, it involves the following steps:

1) **Training**: The existing HNN method is trained for the hyperedge prediction task, on the same dataset split used in the earlier stages.
2) **Scoring**: The trained HNN is applied to the hyperedge candidates generated in the first step to estimate their likelihood of being ground-truth hyperedges.
3) **Filtering**: The top-ranked candidates, based on the HNN scoring function, are retained for the final prediction.

For instance, if the target number of hyperedge candidates is $\mathcal{K}$, we first predict $2\mathcal{K}$ candidates in the first step of the algorithm. These candidates are then refined using the trained HNN, with the final output consisting of the most promising $\mathcal{K}$ hyperedge candidates. This two-step approach ensures that the initial candidate generation process remains efficient while leveraging the expressive power of HNNs for more accurate predictions.

TABLE III

AVERAGE F1 SCORE. HYPERSEARCH ACHIEVES STRONG PERFORMANCE UNDER AVERAGE F1 SCORE ACROSS MOST SETTINGS. WE REPORT THE AVERAGE VALUES AND STANDARD DEVIATIONS OVER THE FIVE RANDOM SPLITS OF AVERAGE F1 SCORE, EVALUATED ON THE FOUR DATASETS WITHOUT EDGE TIMESTAMPS. FOR EACH SETTING, THE BEST AND SECOND-BEST METHODS ARE HIGHLIGHTED IN GREEN AND YELLOW, RESPECTIVELY.

Dataset	**Citeseer**			**Cora**			**Cora-A**			**DBLP-A**		
Method (↓) / $\mathcal{K}$ (→)	1×	2×	5×	1×	2×	5×	1×	2×	5×	1×	2×	5×
HyperSearch (Proposed)	40.0 (3.6)	43.8 (2.8)	49.5 (2.0)	48.7 (1.6)	51.3 (1.3)	54.2 (0.8)	18.8 (3.5)	23.6 (1.8)	29.7 (1.3)	17.7 (0.8)	20.5 (0.7)	27.0 (0.5)
CNS	37.5 (1.2)	41.9 (0.7)	48.1 (0.5)	45.3 (1.8)	49.0 (1.0)	53.5 (1.1)	17.1 (1.0)	21.0 (0.7)	26.9 (1.1)	16.7 (0.2)	20.7 (0.2)	26.7 (0.2)
HPRA	25.9 (1.2)	31.4 (2.1)	36.6 (0.8)	33.2 (1.3)	37.1 (0.8)	42.8 (0.9)	12.8 (1.7)	18.1 (1.2)	26.5 (0.8)	12.2 (0.2)	17.5 (0.2)	28.5 (0.1)
MHP	33.9 (1.9)	39.1 (2.0)	44.5 (1.3)	39.9 (0.5)	42.8 (0.4)	46.8 (0.8)	19.3 (2.2)	24.2 (1.9)	31.2 (1.7)	-	-	-
MHP-C	31.7 (2.2)	37.0 (1.9)	-	46.2 (1.1)	48.2 (0.9)	-	19.4 (1.9)	21.2 (1.5)	26.0 (1.3)	-	-	-
AHP-C	34.8 (3.0)	39.1 (2.8)	-	41.8 (1.7)	44.7 (1.4)	-	16.3 (2.0)	19.7 (2.2)	24.0 (2.2)	-	-	-
SAGNN-C	30.2 (1.3)	34.4 (2.0)	-	42.0 (1.9)	44.9 (1.7)	-	15.0 (1.5)	17.7 (1.3)	20.7 (1.4)	13.8 (0.3)	16.6 (0.3)	20.1 (0.4)
NHP-C	36.9 (1.3)	42.2 (1.2)	-	51.8 (0.7)	55.4 (0.2)	-	19.6 (1.7)	23.7 (1.2)	28.9 (2.0)	16.0 (0.4)	20.1 (0.4)	25.8 (0.2)
MHP-H	31.6 (2.2)	36.9 (2.0)	-	46.2 (1.1)	48.3 (0.9)	53.0 (0.6)	19.2 (1.8)	21.1 (1.5)	26.0 (1.2)	-	-	-
AHP-H	24.5 (6.7)	27.6 (7.0)	-	31.4 (3.5)	35.4 (3.4)	40.8 (2.7)	12.4 (3.0)	15.8 (3.6)	22.2 (4.6)	-	-	-
SAGNN-H	17.6 (2.2)	20.1 (1.4)	-	28.4 (1.5)	32.2 (1.2)	36.0 (1.4)	10.0 (1.5)	13.4 (1.3)	19.5 (1.4)	11.3 (0.3)	15.5 (0.3)	-
NHP-H	21.9 (2.2)	24.9 (1.3)	-	35.8 (1.6)	39.1 (1.2)	43.1 (0.9)	7.8 (1.0)	10.2 (1.1)	14.7 (0.9)	12.7 (0.3)	17.5 (0.3)	-

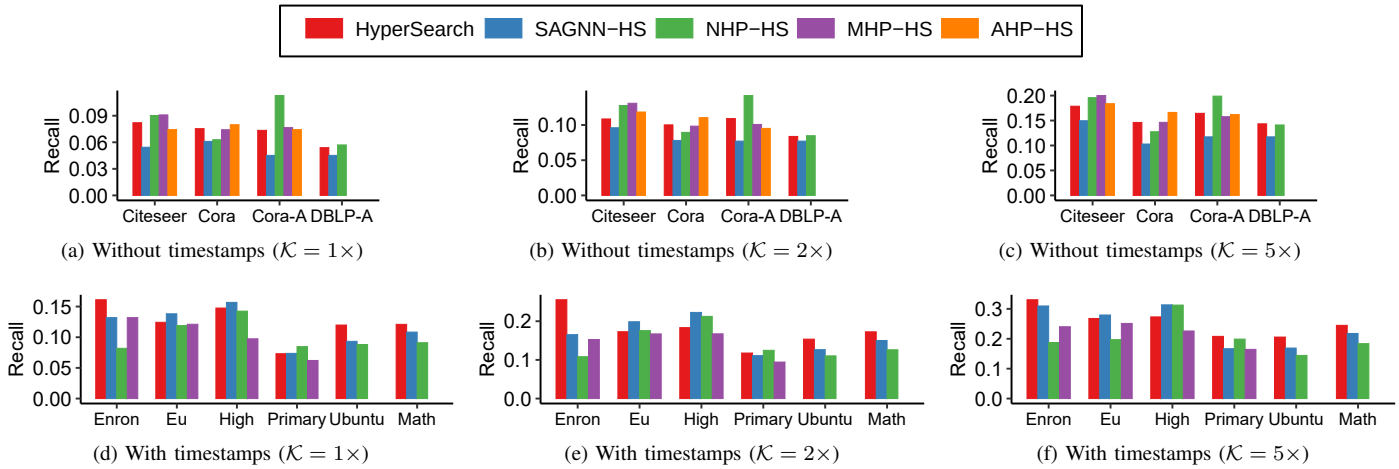
-: out-of-time (> 2 days).

TABLE IV

AVERAGE F1 SCORE. HYPERSEARCH ACHIEVES STRONG PERFORMANCE UNDER AVERAGE F1 SCORE IN MOST SETTINGS. WE REPORT THE AVERAGE F1 SCORE ON THE SIX DATASETS WITH EDGE TIMESTAMPS (NO STANDARD DEVIATION SINCE THERE IS ONLY ONE CHRONOLOGICAL SPLIT). FOR EACH SETTING, THE BEST AND SECOND-BEST METHODS ARE HIGHLIGHTED IN GREEN AND YELLOW, RESPECTIVELY.

Dataset	**Enron**			**Eu**			**High**			**Primary**			**Ubuntu**			**Math-sx**		
Method (↓) / $\mathcal{K}$ (→)	1×	2×	5×	1×	2×	5×	1×	2×	5×	1×	2×	5×	1×	2×	5×	1×	2×	5×
HyperSearch (Proposed)	60.6	62.1	63.4	58.5	59.9	62.4	58.8	61.9	64.4	57.8	60.8	63.2	73.3	73.7	74.2	74.6	75.5	76.4
CNS	54.6	57.9	63.0	56.0	59.0	63.3	58.5	59.1	59.6	57.7	58.5	59.5	62.4	64.1	66.7	66.5	68.7	71.7
HPRA	51.7	53.9	55.7	57.5	59.0	61.7	60.2	62.6	65.6	58.3	59.8	64.1	61.7	63.2	65.1	68.4	69.8	71.8
MHP	45.5	47.8	51.2	46.7	47.7	49.6	49.6	50.2	53.0	53.2	56.5	62.0	-	-	-	-	-	-
MHP-C	55.6	56.2	61.1	58.5	59.2	62.5	57.4	59.5	60.5	57.0	58.6	61.1	-	-	-	-	-	-
SAGNN-C	45.6	48.5	51.3	59.5	62.5	66.3	52.3	54.3	54.7	57.2	57.9	59.0	64.3	66.2	68.7	69.5	71.7	74.5
NHP-C	52.9	55.9	59.7	54.9	57.7	61.9	56.2	56.4	56.7	55.9	56.6	57.2	61.1	62.9	65.1	-	-	-
MHP-H	57.7	58.2	62.1	56.5	57.5	61.5	58.3	60.0	61.2	57.2	58.9	60.9	-	-	-	-	-	-
SAGNN-H	49.4	51.5	53.5	59.7	61.6	64.6	60.8	62.3	66.5	56.6	58.8	61.8	64.5	66.0	-	70.6	72.1	-
NHP-H	51.7	53.2	55.4	56.5	58.3	60.8	59.6	61.1	64.6	57.7	59.6	62.4	60.2	61.5	-	67.3	68.7	-

-: out-of-time (> 2 days).



(a) Without timestamps ($\mathcal{K} = 1\times$) (b) Without timestamps ($\mathcal{K} = 2\times$) (c) Without timestamps ($\mathcal{K} = 5\times$)

(d) With timestamps ($\mathcal{K} = 1\times$) (e) With timestamps ($\mathcal{K} = 2\times$) (f) With timestamps ($\mathcal{K} = 5\times$)

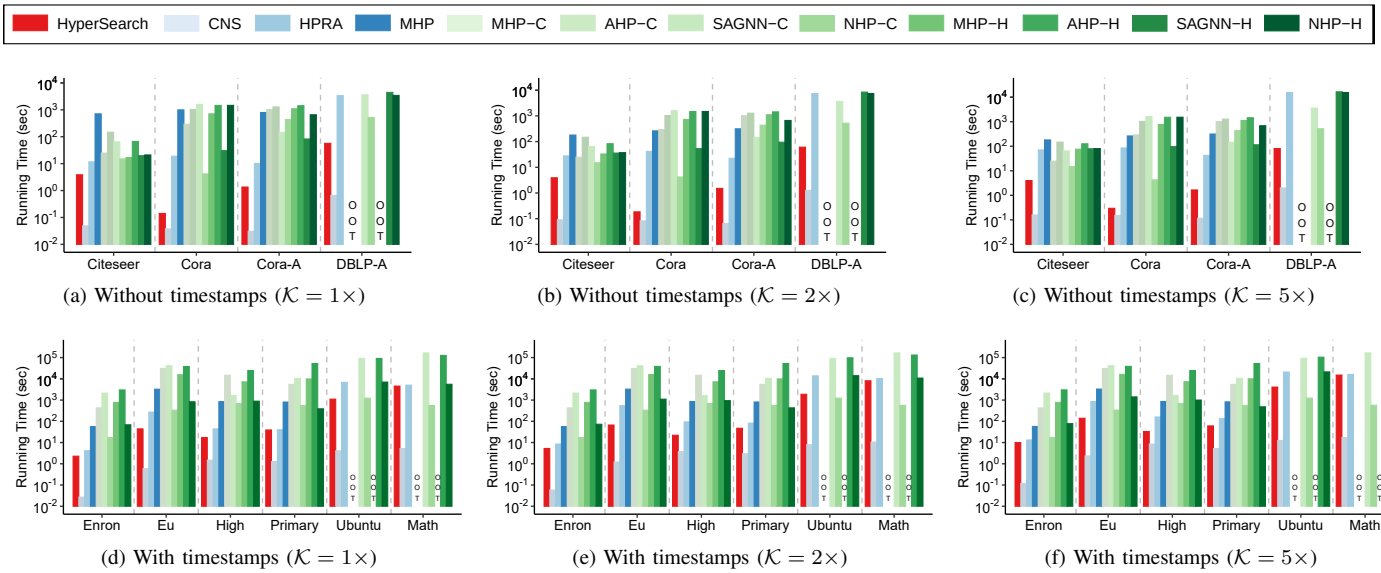
Fig. 2. Refinement with HNNs does not consistently enhance the prediction accuracy of HyperSearch.

Results. We assessed the impact of incorporating refinement with Hypergraph Neural Networks (HNNs). Specifically, we compared the performance of HyperSearch with variants that applied two HNN models, MHP and AHP. As shown in Fig. 2, the results indicate that refinement with HNNs did not consistently improve prediction accuracy. This suggests that the scoring mechanism based solely on our empirical observations is already robust and effective, reducing the necessity for additional refinement in many cases.

G. Additional Results on "Q2. Speed and Scalability" (Supplementing Sect. VI-C)

We evaluated the running times of the considered methods and analyzed the scalability of HyperSearch by examining its runtime as a function of the number of predicted hyperedges across different datasets. The results, presented in Fig. 3 and Fig. 4, reveal the following key observations:

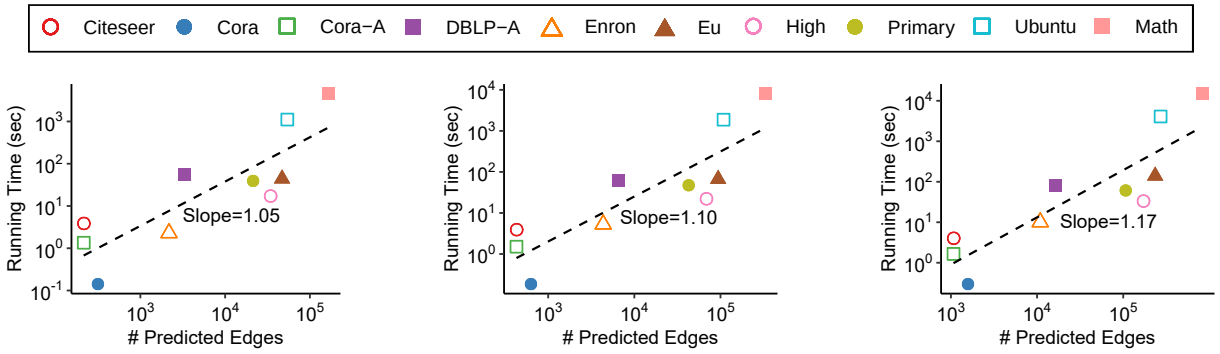
- HyperSearch runs faster than deep learning-based methods (highlighted in green in Fig. 3) in most cases, demonstrating its computational efficiency.
- The runtime of HyperSearch scales nearly linearly with the number of predicted hyperedges, with regression slopes



(a) Without timestamps ($\mathcal{K} = 1\times$) (b) Without timestamps ($\mathcal{K} = 2\times$) (c) Without timestamps ($\mathcal{K} = 5\times$)

(d) With timestamps ($\mathcal{K} = 1\times$) (e) With timestamps ($\mathcal{K} = 2\times$) (f) With timestamps ($\mathcal{K} = 5\times$)

Fig. 3. HyperSearch runs faster than deep learning-based methods (highlighted in green) in most cases, demonstrating its computational efficiency. This suggests that HyperSearch maintains efficient scalability as the prediction task size increases.



(a) 1× (b) 2× (c) 5×

Fig. 4. The runtime of HyperSearch scales nearly linearly with the number of predicted hyperedges, with a regression slope of 1.05 to 1.11, indicating its efficient scalability.

ranging from 1.05 to 1.17 (Fig. 4). This suggests that HyperSearch maintains efficient scalability as the prediction task size increases.

Scalability on Synthetic Hypergraphs. To further verify the scalability of HyperSearch in controlled large-scale settings, we conducted additional experiments using synthetic hypergraphs generated by HyperFF [3], a generative model that replicates structural properties observed in real-world hypergraphs. We generate synthetic datasets of increasing size and measure the runtime of HyperSearch while predicting the number of hyperedges equal to that of the input graph for each synthetic instance. As shown in Fig. 5, the runtime of HyperSearch increases with the number of predicted hyperedges, with a regression slope of 1.92. Although the trend is slightly super-linear, the runtime remains practical even at large scales, demonstrating that HyperSearch can efficiently scale to synthetic hypergraphs with millions of candidates.

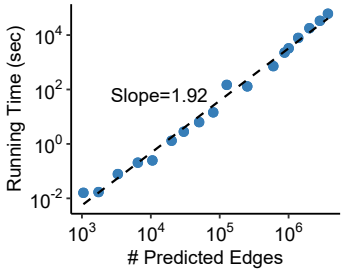


Fig. 5. The runtime of HyperSearch scales nearly linearly with the number of predicted hyperedges, with a regression slope of 1.92, indicating its practical scalability on synthetic datasets.

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[1] A. K. Poernomo and V. Gopalkrishnan, "Towards efficient mining of proportional fault-tolerant frequent itemsets," in *KDD*, 2009.

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[3] Y. Kook, J. Ko, and K. Shin, "Evolution of real-world hypergraphs: Patterns and models without oracles," in *ICDM*, 2020.