Trustworthy AI for Human and Science

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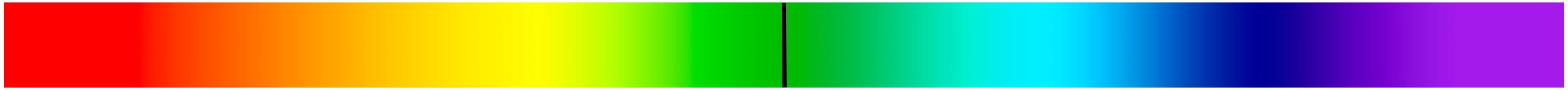
AI helps in many Research Areas

- A (very rough) spectrum of research discipline system

Human/Arts Nature/Science



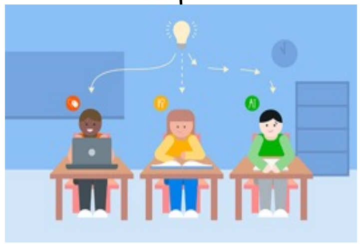
... Art Literature Sociology Education Economics CS/AI Engineering Biology Medical Chemistry Physics ...

AI Painting

WHAT STARTS OUT AS TRIUMPH SOON BECOMES MANIPULATED INTO A CACOPHONY OF FUTILITY, LEAVING ONLY A SENSE OF DREAD AND THE UNLIKELI-HOOD OF A NEW ORDER.

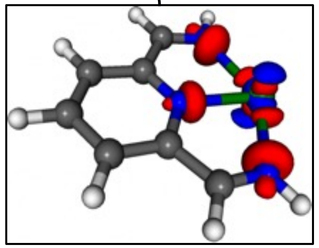
BY TEXT GENERATOR

AI-assisted writing



AI-assisted Learning

AI for Biology, AlphaFold

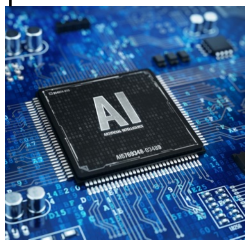


AI for Chemistry

AI and Arts

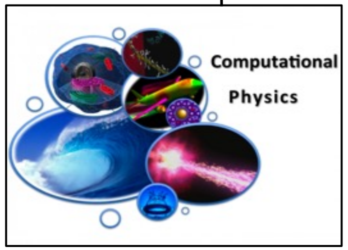
AI for Social Science

Computational Econ



AI for Chip Design

AI for Drug Discovery



AI for Physics

Trustworthy AI

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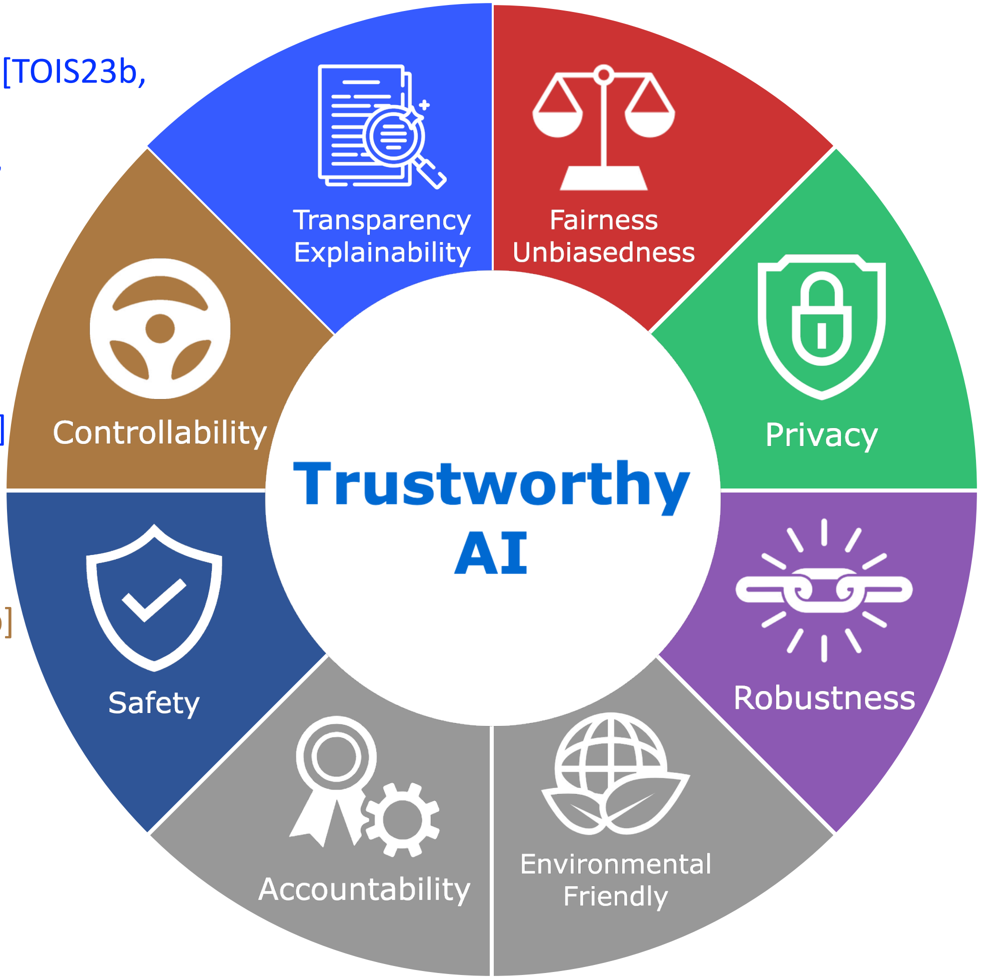
Our Research Landscape – Methodology

Counterfactual Explanation [SIGIR23, KDD23, ECAI23, WSDM23, WWW22a, CIKM21a]
Natural Language Explanation [CIKM23, EMNLP22b, ACL21, CIKM20c, COLING20, SIGIR14, AAAI19]
Visual Explanation [ICLR23, ACL22, SIGIR19b]
Large Language Model (LLM) based Explanation [TOIS23b, CIKM23, RecSys22a]
Neural-Symbolic Explanation [ICLM22, SIGIR22b, EMNLP22a, WSDM22a, CIKM22b, WWW21a, NAACL21, CIKM20a, CIKM20b]
Knowledge-based Explanation [WWW22b, RecSys21, SIGIR21c, SIGIR19a]
Explainable Model Debugging [TACL23, TOIS23a]
Evaluation of Explanations [WWW22c, SIGIR21d]

Controllable Text Generation [WWW20, ACL21, RecSys22a, TOIS23b, CIKM20c]
Controllable Image Generation [ACL22, SIGIR19b]
User Controllable Recommendation [ECAI23]
User Controllable Fairness [SIGIR21a]
White-box based Controllability [TOIS23a]

Counterfactual Attacking [SIGIR23]
Shilling Attack Detection [IJCAI15]



Counterfactual Fairness [SIGIR21a]
User-oriented Fairness [WWW21b]
Long-term Fairness [WSDM21]
Explainable Fairness [SIGIR22a, SIGIR20a]
Federated Fairness [RecSys22b]
Group-wise Fairness [RecSys17]
Fairness-Utility Relationship [WSDM22b]
Popularity Bias [CIKM21b]
Echo Chamber [SIGIR20b]
Bias and Fairness of LLMs [AACL22]

Federated Privacy [SIGIR21b, RecSys22b]
Adversarial Privacy [SIGIR21a]

Causal Robustness [CIKM22a, ICTIR23, TORS23, JCDL22]
Evaluation of Robustness [WSDM22c]

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Our Research Landscape – Application

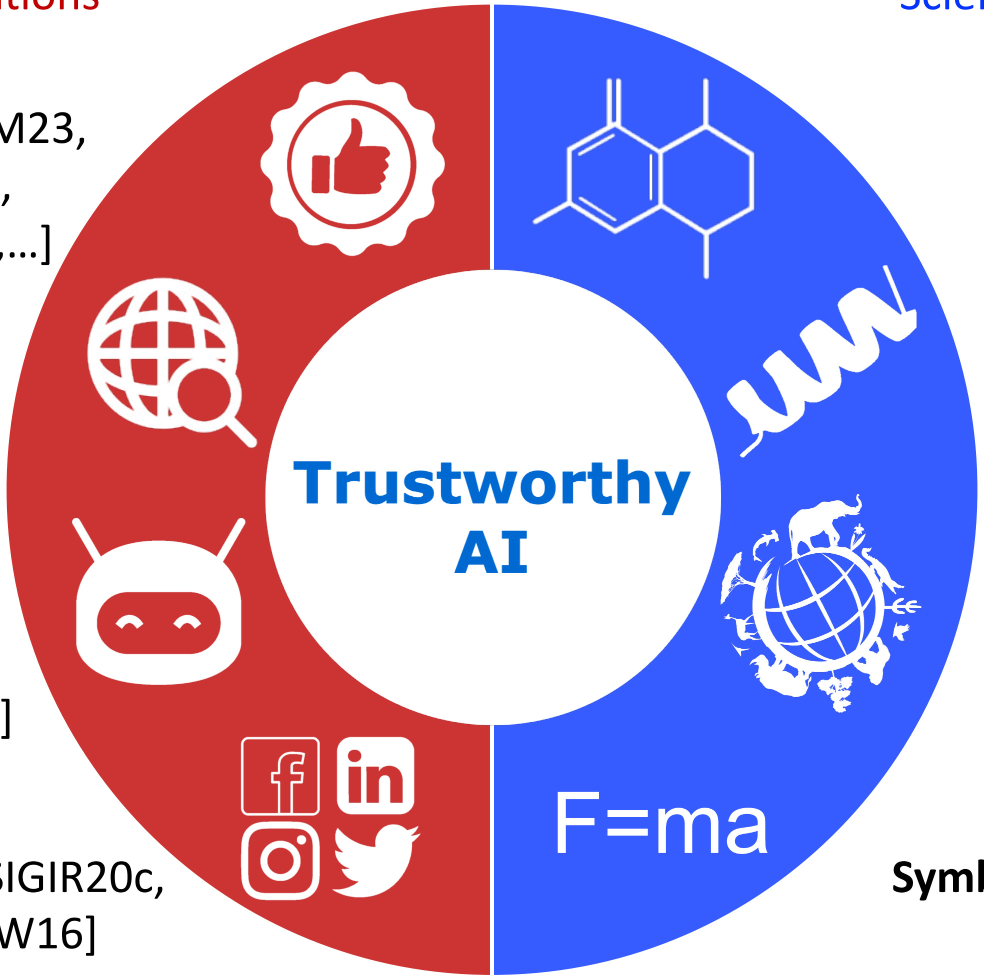
Human-oriented Applications

Recommender system [SIGIR23, WSDM23, CIKM23, WWW22b, RecSys22a, ACL22, WSDM22a-c, WWW21a-b, SIGIR21a-d,…]

Search engines [CIKM19a, TOIS19, CIKM18, SIGIR17]

QA and Dialog System [EMNLP22a, EMNLP22b, CIKM21b, SIGIR21c, SIGIR19c, CIKM19a, CIKM19b, CIKM18]

Economic and E-commerce Systems [SIGIR20c, WWW19a, WWW19b, WSDM17, WWW16]



Science-oriented Applications

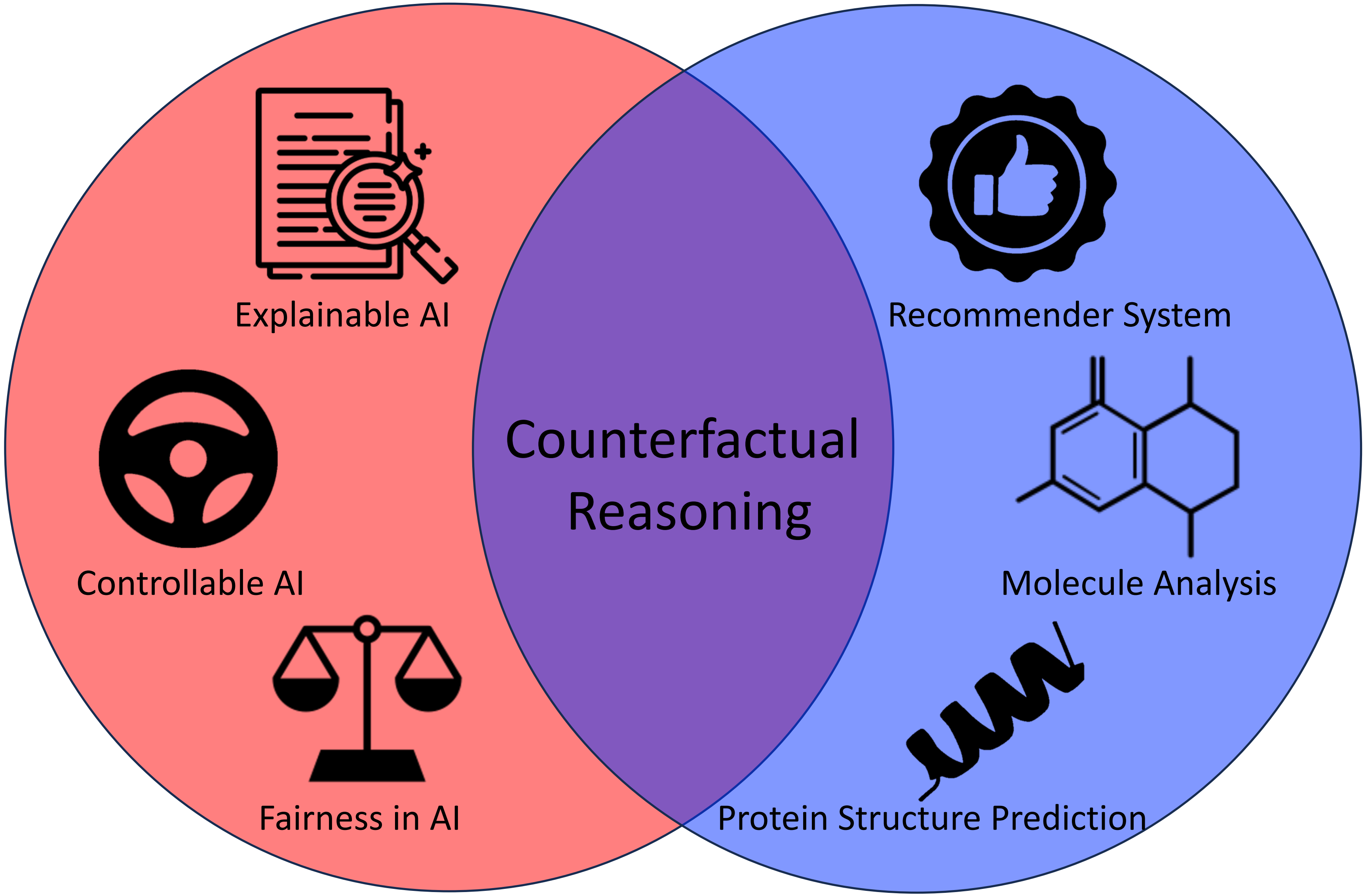
Molecule Analysis [WWW22a]

Protein Structure Prediction [KDD23]

Biodiversity Preservation [COLING20]

Symbolic Physical Rule Discovery [ICML22]

One Theme that Connects Many Dots



Multiple Trustworthy Perspectives **Multiple Application Domains**

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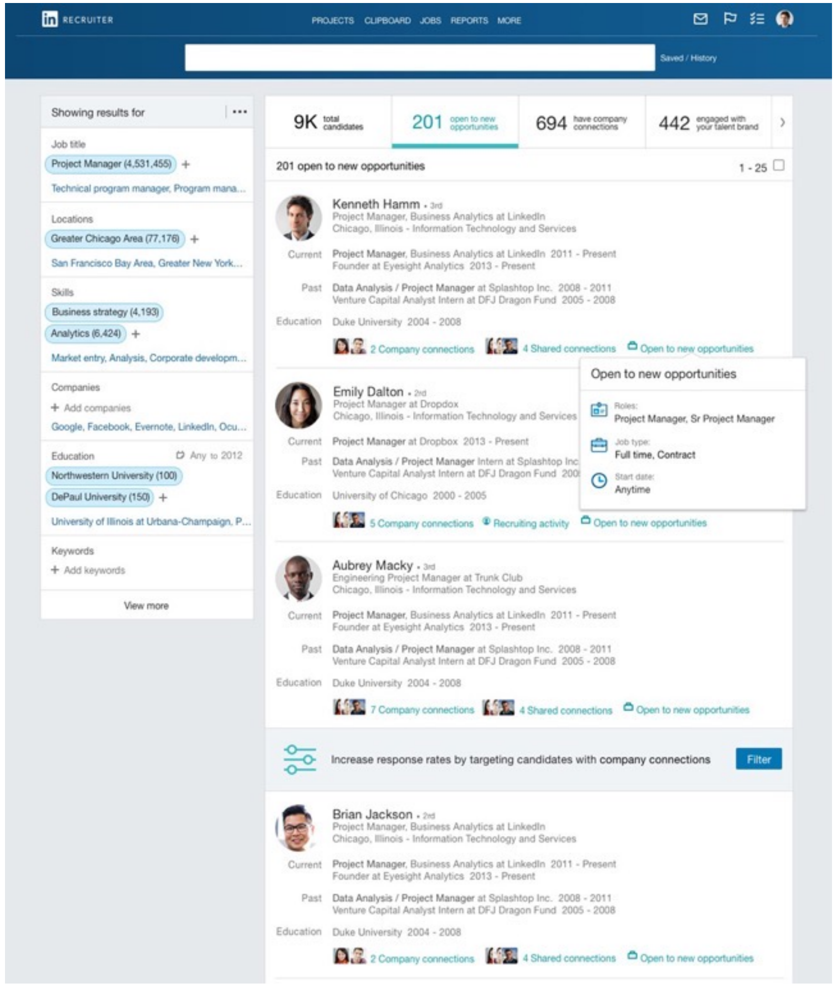
Why Trustworthy AI



Example of Human-oriented Application

Example of Science-oriented Application

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Example: Resume Ranking and Recommendation

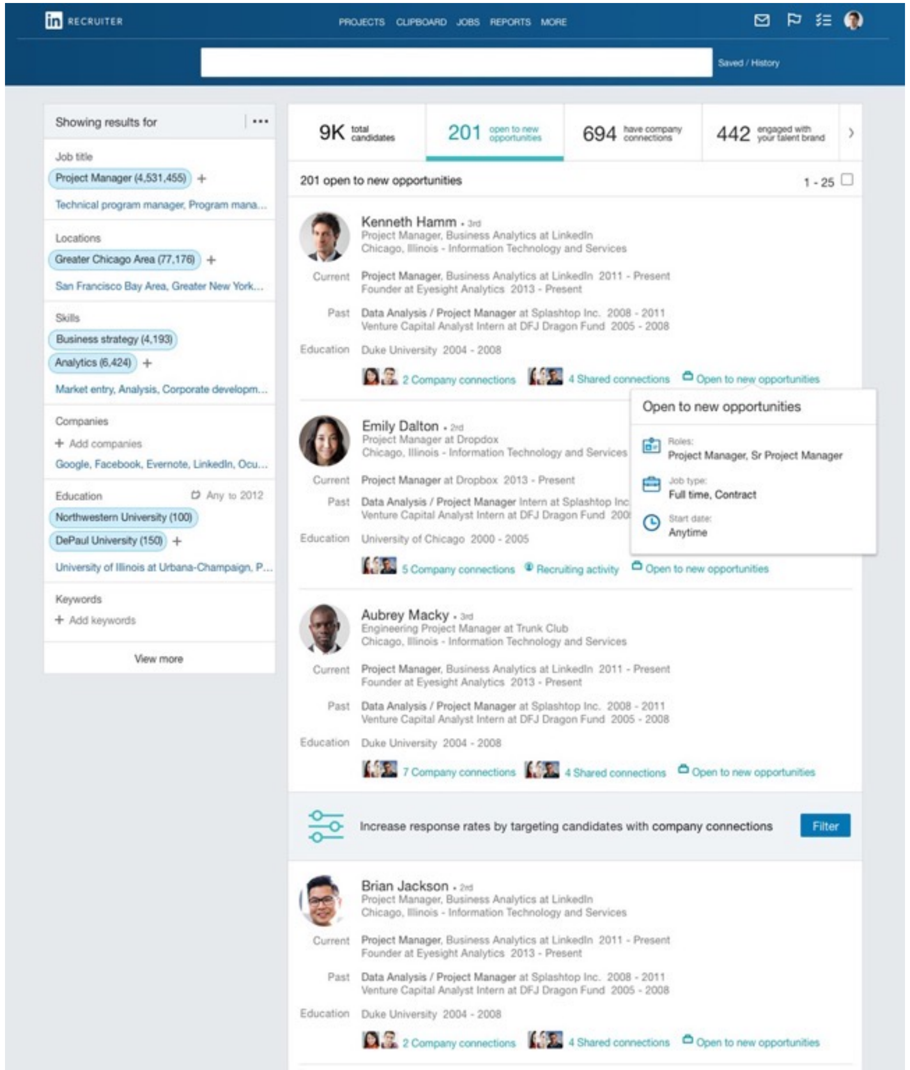

Figure 1: A (mocked) screenshot from the LinkedIn Recruiter (credit to [1])

Background: HR may use automated tools such as LinkedIn for ranking candidates due to too many applicants

Problem:
From recruiter's perspective:
Why this candidate is a better fit than another?

From applicant's perspective:
Why should I trust the algorithm?
Why should my career be decided by a machine?

To answer these **WHY** questions, we need Explainable AI

https://engineering.linkedin.com/blog/2019/04/ai-behind-linkedin-recruiter-search-and-recommendation-systems

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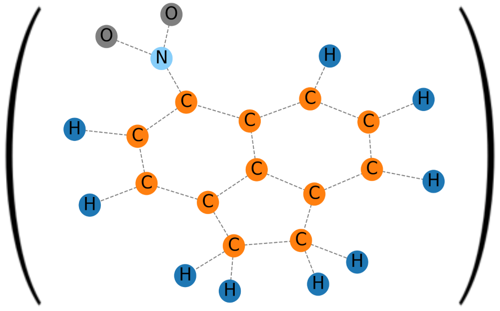
Example: Explainable AI for Science

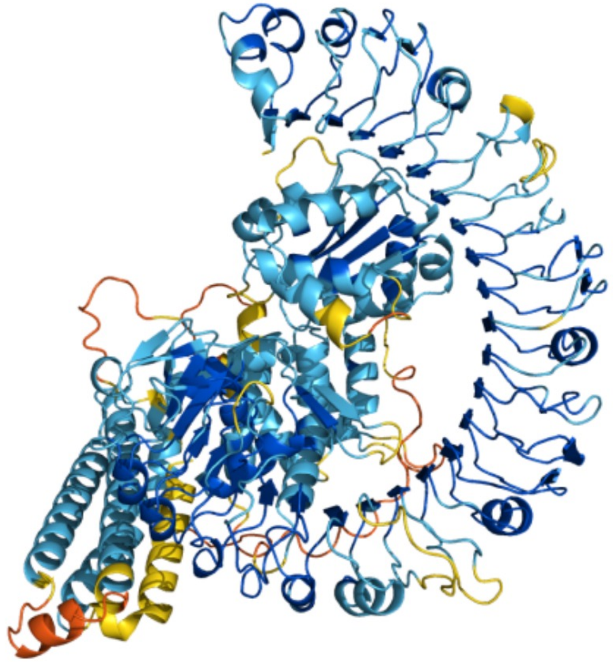
- AI for Drug Discovery
  - Molecule Property Prediction

NN  = Soluble? Toxic? Crosses the Blood Brain Barrier (BBB)?

- Protein Structure Prediction

```
MAGELVSFAVNKLWDLLSHEYTLFQGVEDQVAELKSDLNLLKSFLKDADAKKH
TSALVRYCVEEIKDIVYDAEDVLETFVQKEKLGTTSGIRKHIKRLTCIVPDRR
EIALYIGHVSKRITRVIRDMQSFGVQQMIVDDYMHPLRNREREIRRTFPKDNE
SGFVALEENVKKLVGYFVEEDNYQVVSITGMGGLGKTTLARQVFNHDMVTKKF
DKLAWVSVSQDFTLKNVWQNILGDLKPKEEETKEEEKKILEMTEYTLQRELYQ
LLEMSKSLIVLDDIWKKEDWEVIKPIFPPTKGWKLLLTSRNESIVAPTNTKYF
NFKPECLKTDDSWKLFQRIAFPINDASEFEIDEEMEKLGEKMIEHCGGLPLAI
KVLGGMLAEKYTSHDWRRLSENIGSHLVGGRTNFNDDNNNSCNYVLSLSFEEL
PSYLKHCFLYLAHFPEDYEIKVENLSYYWAAEEIFQPRHYDGEIIRDVGDVYI
EELVRRNMVISERDVKTSRFETCHLHDMMREVCLLKAKEENFLQITSNPPSTA
NFQSTVTSRRLVYQYPTTLHVEKDINNPKL…
```

AlphaFold



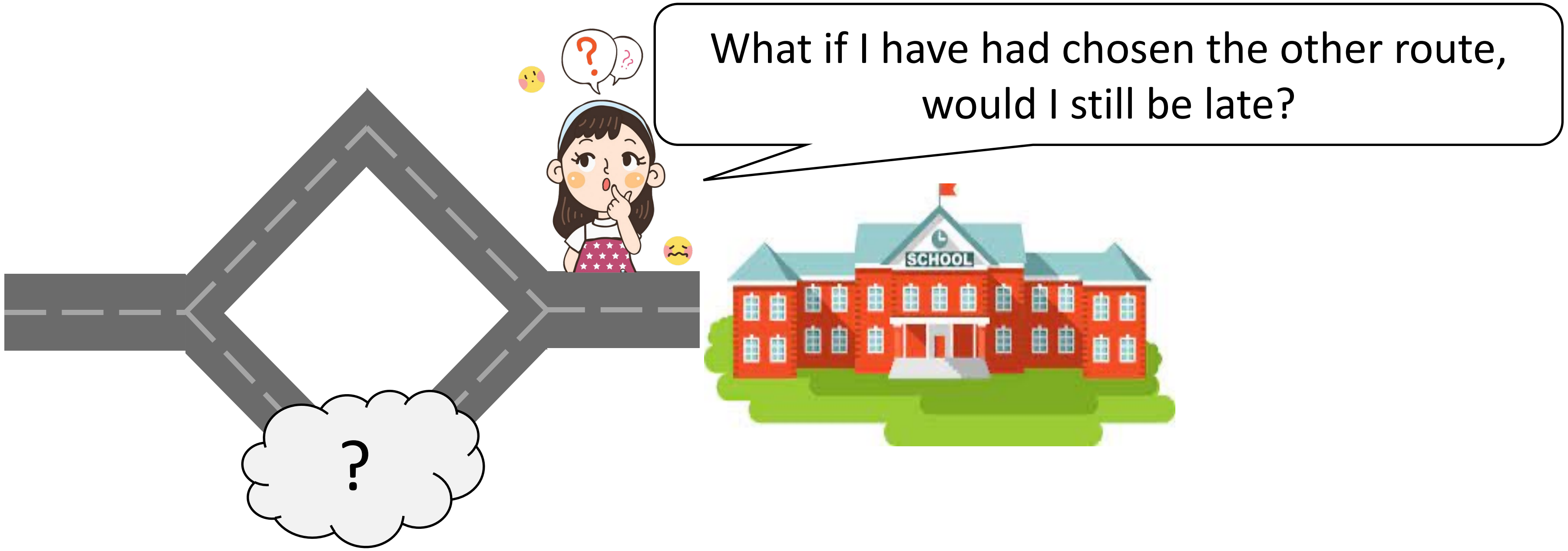
Trustworthy AI for Human

Counterfactual Reasoning and Counterfactual Explanation

[1] J Tan, S Xu, Y Ge, Y Li, X Chen, and **Y Zhang**. "Counterfactual explainable recommendation." In CIKM 2021.
[2] J Tan, Y Ge, Y Zhu, Y Xia, J Luo, J Ji, and **Y Zhang**. "User-Controllable Recommendation via Counterfactual Retrospective and Prospective Explanations." In ECAI 2023.
[3] Y Ge, J Tan, Y Zhu, Y Xia, J Luo, S Liu, Z Fu, S Geng, Z Li, and **Y Zhang**. "Explainable fairness in recommendation." In SIGIR 2022.

Counterfactual Reasoning

- Counterfactual Reasoning: the “What if” Question
  - What if something that did not happen happened?
  - What if something that happened did not happen?



- Counterfactual reasoning shows human’s pursuit of causal relationships

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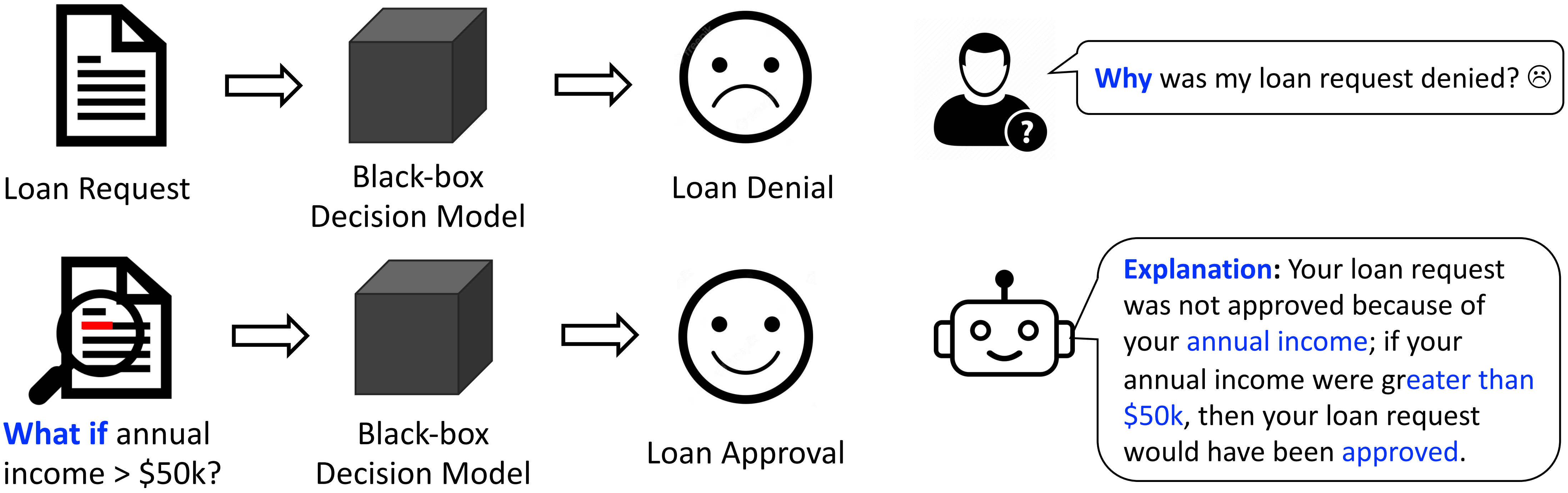
Counterfactual Explanation

- Explanations based on Counterfactual Reasoning



Associative Explanation vs. Causal Explanation

- Counterfactual Explanation is a type of Causal Explanation

	Recommended items		Not recommended items		
Screen: 4.0 Battery: 5.0 Price: 3.0	Screen: 4.5 Battery: 3.0 Price: 3.0	Screen: 4.5 Battery: 1.5 Price: 4.5	Screen: 5.0 Battery: 1.5 Price: 3.5	Screen: 5.0 Battery: 0.5 Price: 4.0	Screen: 5.0 Battery: 1.0 Price: 3.0
User	**Phone A** **Score:42.0**	**Phone B** **Score:39.0**	**Phone C** **Score:38.0**	**Phone D** **Score:34.5**	**Phone E** **Score:34.0**

[1] J Tan, S Xu, Y Ge, Y Li, X Chen, and **Y Zhang**. "Counterfactual explainable recommendation." In CIKM 2021.

Associative Explanation vs. Causal Explanation

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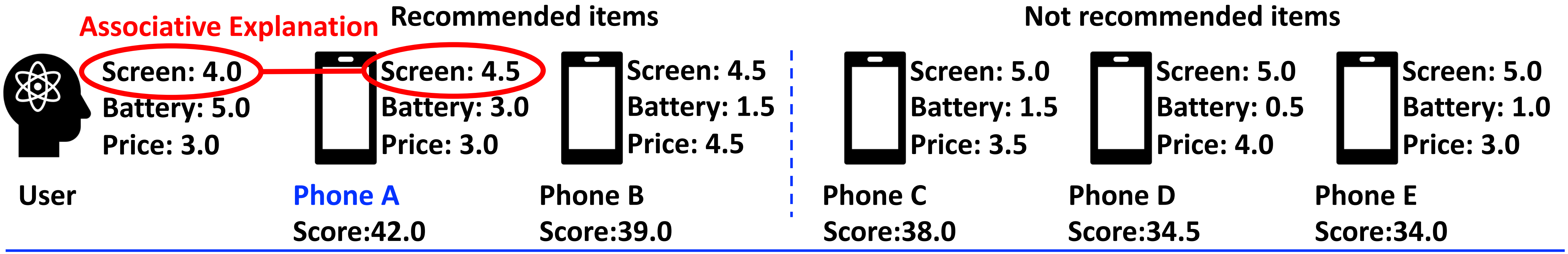

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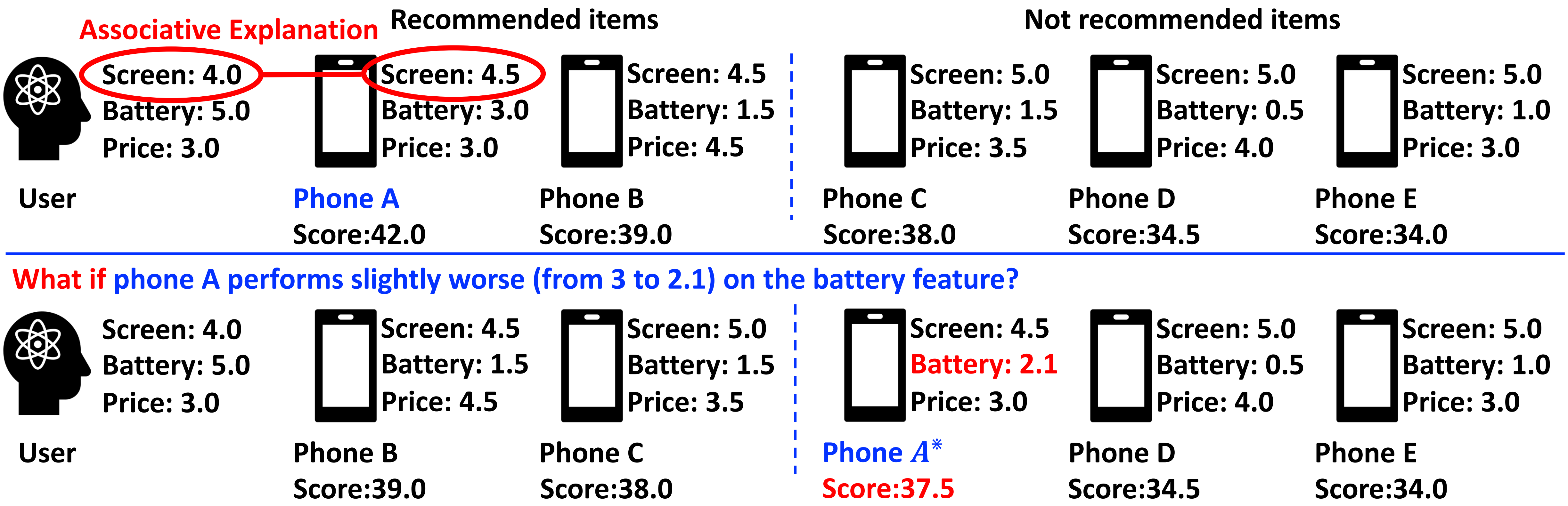

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Associative Explanation

	Recommended items		Not recommended items		
Screen: 4.0 Battery: 5.0 Price: 3.0	Screen: 4.5 Battery: 3.0 Price: 3.0	Screen: 4.5 Battery: 1.5 Price: 4.5	Screen: 5.0 Battery: 1.5 Price: 3.5	Screen: 5.0 Battery: 0.5 Price: 4.0	Screen: 5.0 Battery: 1.0 Price: 3.0
User	Phone A Score:42.0	Phone B Score:39.0	Phone C Score:38.0	Phone D Score:34.5	Phone E Score:34.0

What if phone A performs slightly worse (from 3 to 2.1) on the battery feature?

Screen: 4.0 Battery: 5.0 Price: 3.0	Screen: 4.5 Battery: 1.5 Price: 4.5	Screen: 5.0 Battery: 1.5 Price: 3.5	Screen: 4.5 Battery: 2.1 Price: 3.0	Screen: 5.0 Battery: 0.5 Price: 4.0	Screen: 5.0 Battery: 1.0 Price: 3.0
User	Phone B Score:39.0	Phone C Score:38.0	Phone A^* Score:37.5	Phone D Score:34.5	Phone E Score:34.0

Counterfactual Explanation

If the item had been slightly worse on [feature], then it would not have been recommended at all.

[1] J Tan, S Xu, Y Ge, Y Li, X Chen, and **Y Zhang**. "Counterfactual explainable recommendation." In CIKM 2021.

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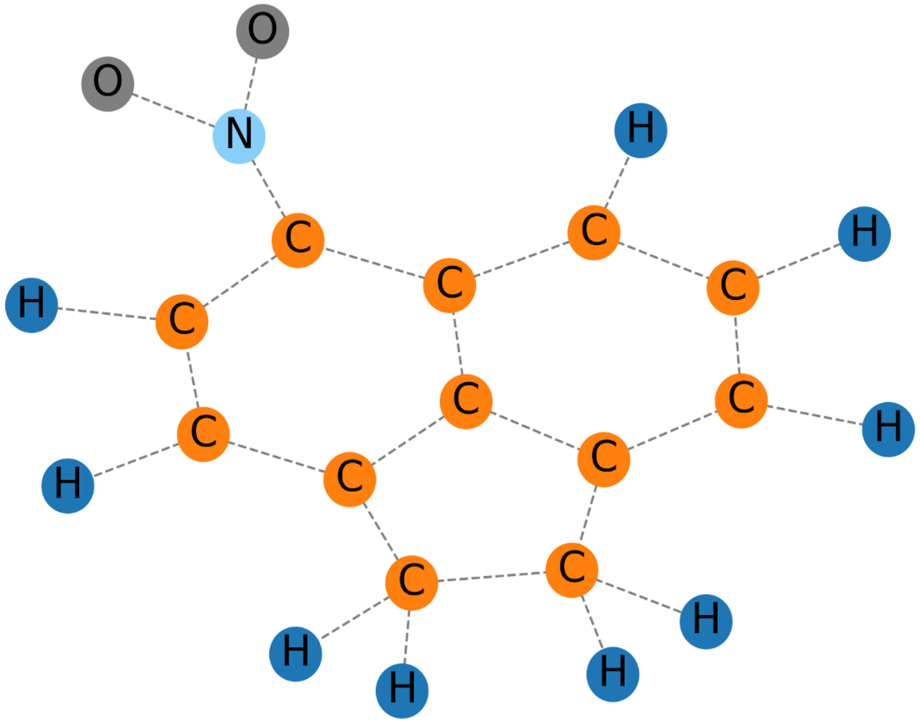
Counterfactual Explanation on Graphs



A mutagenic molecule

Why is this molecule toxic (mutagenic)?

[2] J Tan, S Geng, Z Fu, Y Ge, S Xu, Y Li, and **Y Zhang**. "Learning and evaluating graph neural network explanations based on counterfactual and factual reasoning." In WWW 2022.

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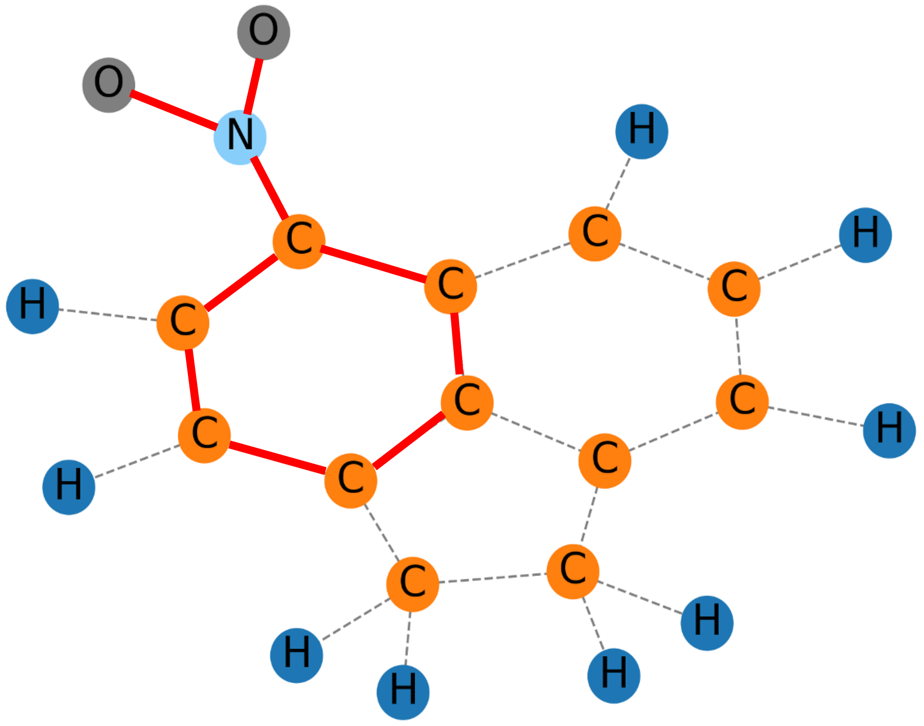
Counterfactual Explanation on Graphs



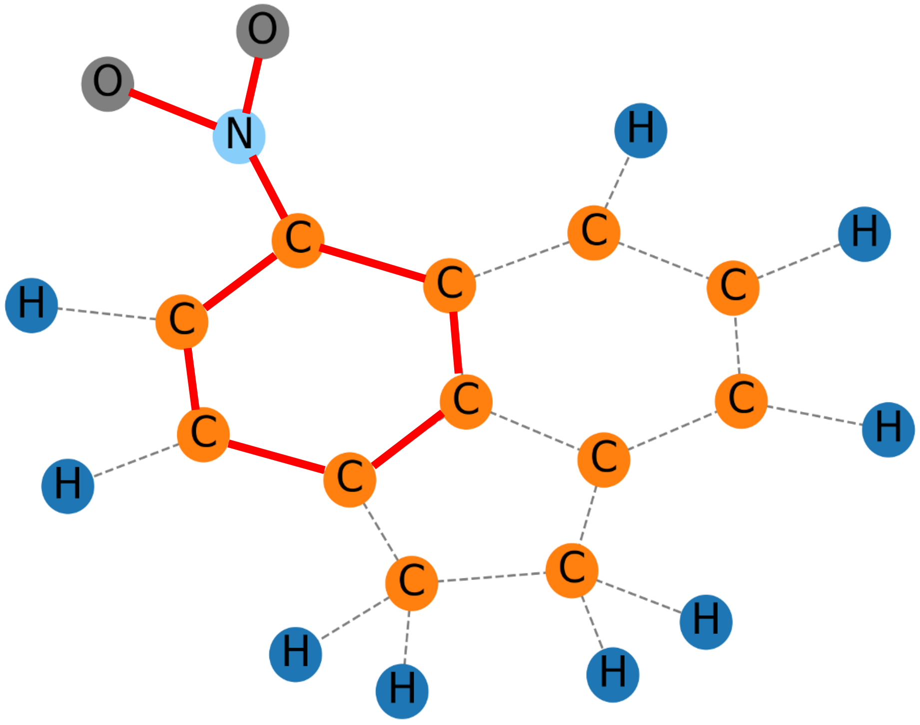
A mutagenic molecule

Why is this molecule toxic (mutagenic)?

Explanation: The **Nitrobenzene** structure

[2] J Tan, S Geng, Z Fu, Y Ge, S Xu, Y Li, and **Y Zhang**. "Learning and evaluating graph neural network explanations based on counterfactual and factual reasoning." In WWW 2022.

Counterfactual Explanation on Graphs

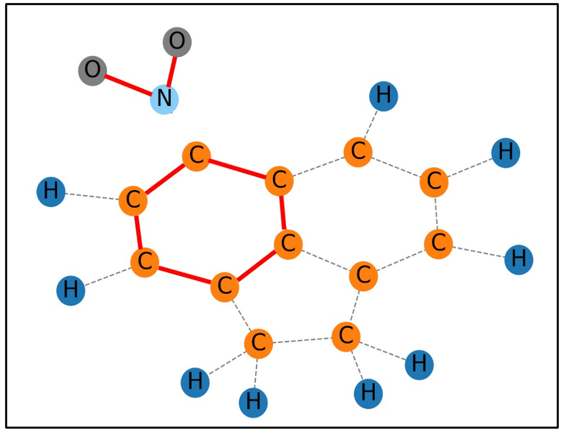


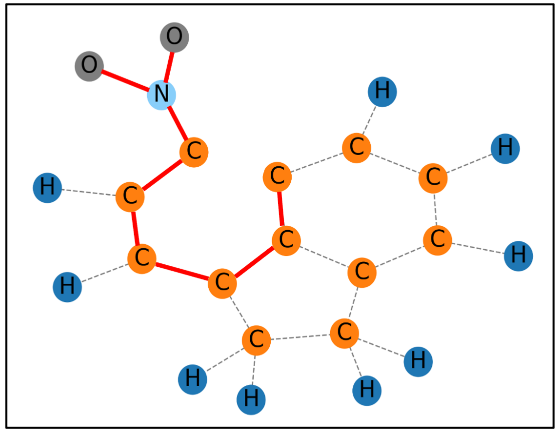
A mutagenic molecule

Why is this molecule toxic (mutagenic)?

Explanation: The **Nitrobenzene** structure.

If the Nitrobenzene structure were broken, then the molecule would not have been toxic at all.





[2] J Tan, S Geng, Z Fu, Y Ge, S Xu, Y Li, and **Y Zhang**. "Learning and evaluating graph neural network explanations based on counterfactual and factual reasoning." In WWW 2022.

Simple and Effective Explanations (CIKM’21)

What is a good explanation?

How to find the explanation?

How to evaluate the explanation?

[1] J Tan, S Xu, Y Ge, Y Li, X Chen, and **Y Zhang**. "Counterfactual explainable recommendation." In CIKM 2021.

What is a Good Explanation?

- A good explanation is Simple and Effective

Occam's Razor Principle for Explainable AI [1]:
When trying to explain a phenomenon, if two explanations are equally effective, then we prefer the simpler one.

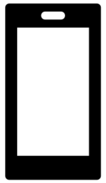
[1] J Tan, S Xu, Y Ge, Y Li, X Chen, and **Y Zhang**. "Counterfactual explainable recommendation." In CIKM 2021.

How to define Simplicity and Effectiveness?

- Counterfactual Explanation as Intervention Vector
  - Item Representation Vector

$Z =$

Screen	Battery	Price
4.5	3.0	3.0



Screen: 4.5
Battery: 3.0
Price: 3.0

  - Explanation as an Intervention Vector

$\Delta =$

Screen	Battery	Price
0	-0.9	0

  - Item Representation after Counterfactual Intervention

$$Z' = Z + \Delta$$

[1] J Tan, S Xu, Y Ge, Y Li, X Chen, and **Y Zhang**. "Counterfactual explainable recommendation." In CIKM 2021.

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How to define Simplicity and Effectiveness?

To define Simplicity:

Explanation Complexity

$$C(\Delta) = \underbrace{\gamma||\Delta||_0}_{} + \underbrace{||\Delta||_2^2}_{}$$

# of non-zeros in Δ, i.e., number of features we need to change

Square of Δ, i.e., the degree of change we need to apply on the features

To define Effectiveness:

Explanation Strength

$$S(\Delta) = \underbrace{s_{i,j} - s_{i,j_\Delta}}_{}$$

Change of the item's ranking score before and after applying the interventions

Simplicity means low complexity: change **as few features as possible** and the change should be **as small as possible**

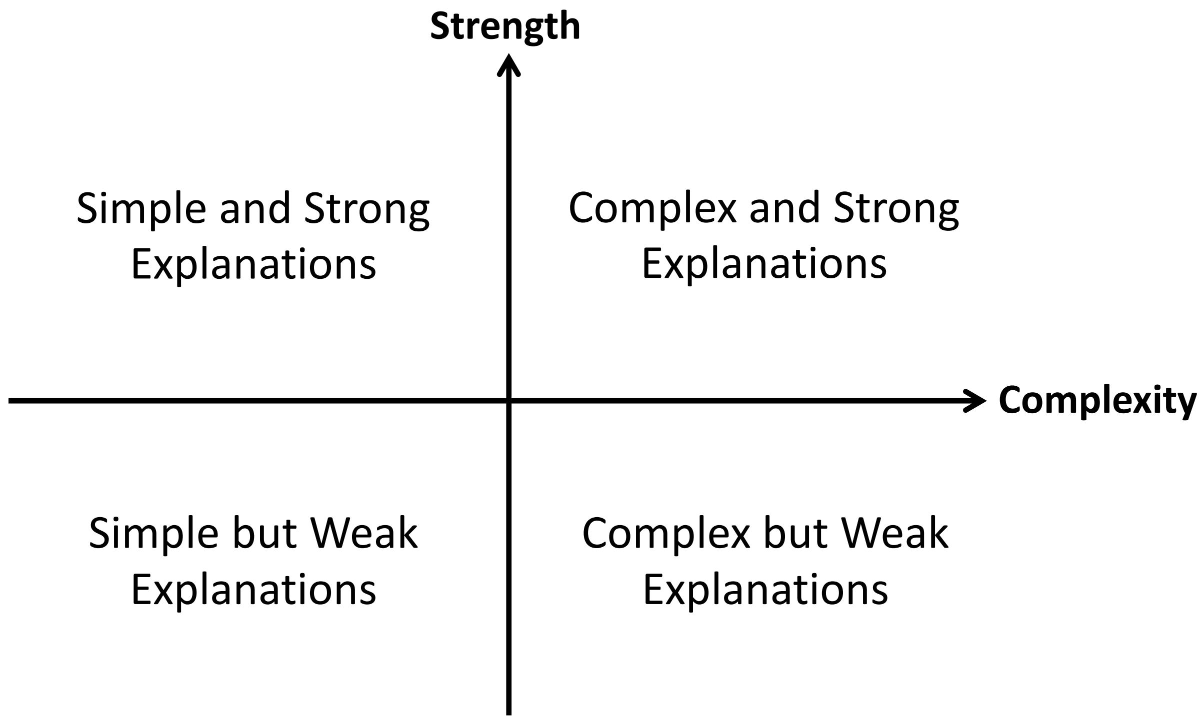
Effectiveness means high strength: item's ranking score should be reduced **large enough to be removed from the top-K list**

User	Phone B	Phone C	Phone A^*	Phone D	Phone E
Screen: 4.0	**Screen: 4.5**	**Screen: 5.0**	**Screen: 4.5**	**Screen: 5.0**	**Screen: 5.0**
Battery: 5.0	**Battery: 1.5**	**Battery: 1.5**	**Battery: 2.1**	**Battery: 0.5**	**Battery: 1.0**
Price: 3.0	**Price: 4.5**	**Price: 3.5**	**Price: 3.0**	**Price: 4.0**	**Price: 3.0**
	Score:39.0	**Score:38.0**	**Score:37.5**	**Score:34.5**	**Score:34.0**

Counterfactual Explanation: If the item had been slightly worse on [feature], then it would not have been recommended at all.

Complexity vs. Strength

- Two Orthogonal Dimensions
  - Complex explanations may not be strong, Simple explanations may not be weak
  - There exist complex but weak explanations, or simple and strong explanations



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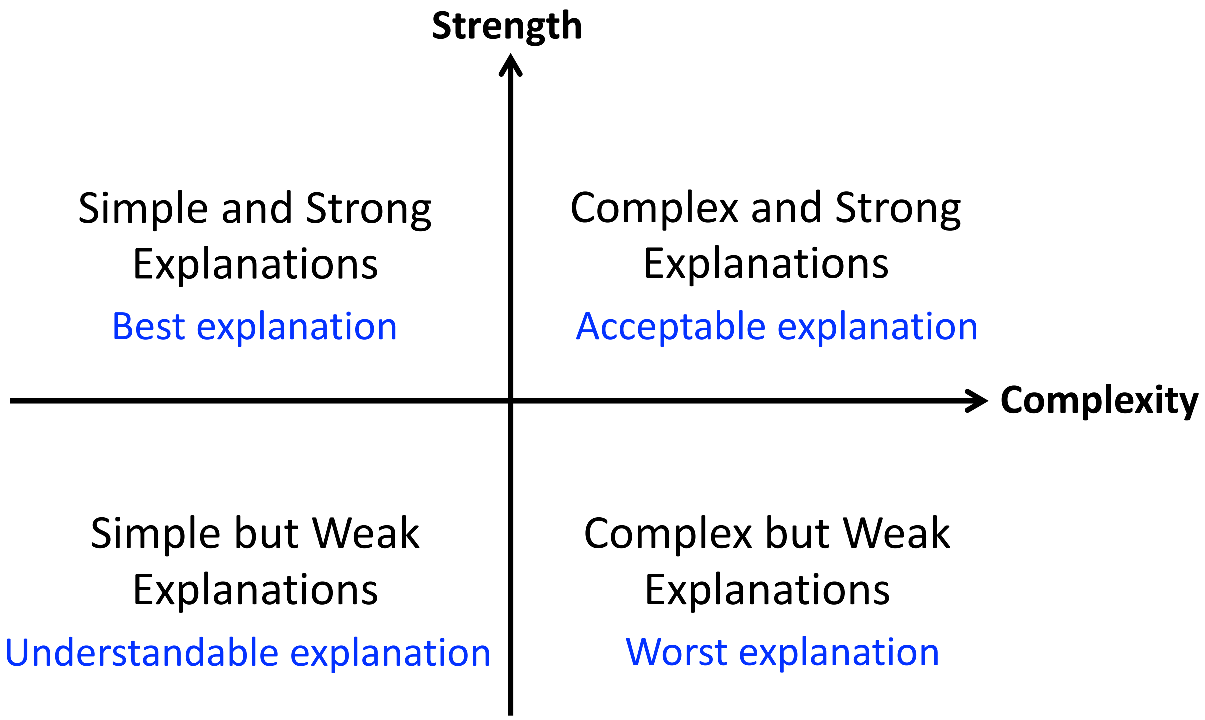

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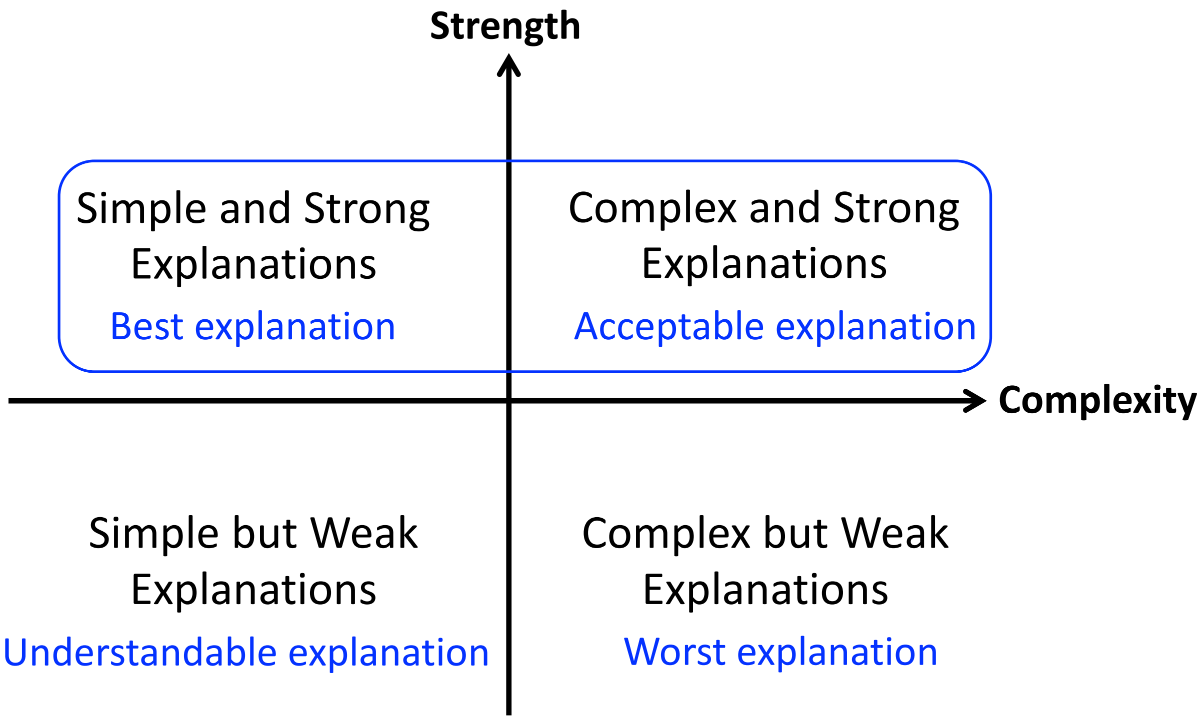

We need to guarantee the explanation is strong in the first place (High Strength)

Complexity vs. Strength

- Two Orthogonal Dimensions
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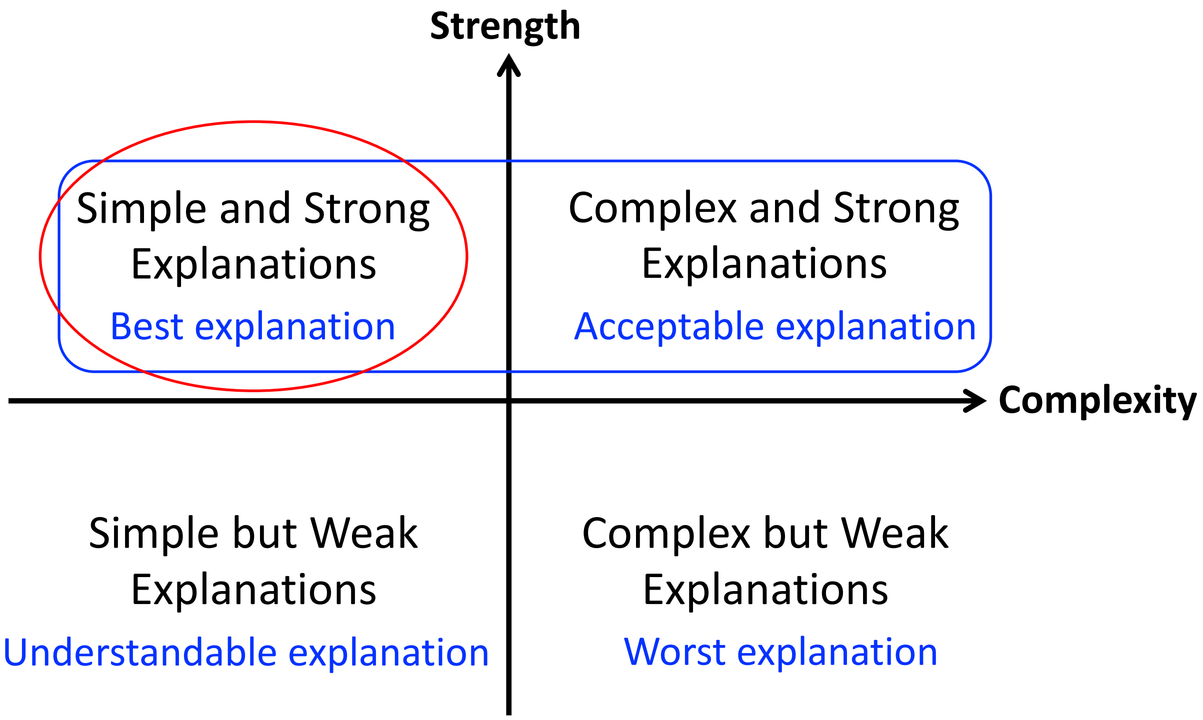

We need to guarantee the explanation is strong in the first place (High Strength)

Given that, seek for simple explanations (Low Complexity)

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How to Learn Counterfactual Explanations?

- A Counterfactual Constrained Learning Framework
  - Black-box Prediction Model $s_{ij} = f(Y_i, Z_j|\Theta)$
    - s_{ij}: algorithm's predicted score for user u_i on item v_j

$$\begin{aligned} &\text{minimize Explanation Complexity} \\ &\quad \text{s.t. Explanation is Strong Enough} \end{aligned} \quad \Rightarrow \quad \begin{aligned} &\underset{\Delta}{\text{minimize}} \ \|\Delta\|_2^2 + \gamma\|\Delta\|_0 \\ &\quad \text{s.t.} \ s_{i,j_\Delta} \le s_{i,j_{K+1}} \end{aligned}$$

Seek for simple (low complexity) explanations constrained on that the explanation is strong enough

- $s_{i,j_\Delta} = f\left(Y_i, Z_j + \Delta \middle| \Theta\right)$: score of item v_j after applying intervention vector Δ
- $s_{i,j_{K+1}} = f(Y_i, Z_{j_{K+1}}|\Theta)$: score of the item that was originally ranked at position $K+1$
- The framework can be applied on any black-box prediction model

How to Learn Counterfactual Explanations?

- A Counterfactual Constrained Learning Framework
  - Black-box Prediction Model $s_{ij} = f(Y_i, Z_j | \Theta)$
    - s_{ij}: algorithm's predicted score for user u_i on item v_j

$$\text{minimize Explanation Complexity} \quad \text{s.t. Explanation is Strong Enough}$$

$\Rightarrow$

$$\underset{\Delta}{\text{minimize}} \ \|\Delta\|_2^2 + \gamma\|\Delta\|_0 \quad \text{s.t.} \ s_{i,j_\Delta} \le s_{i,j_{K+1}}$$

Relaxed optimization with Lagrange multiplier:

$$\underset{\Delta}{\text{minimize}} \ \|\Delta\|_2^2 + \gamma\|\Delta\|_1 + \lambda L(s_{i,j_\Delta}, s_{i,j_{K+1}})$$

$$\text{where:} \quad L\left(s_{i,j_\Delta}, s_{i,j_{K+1}}\right) = \max(0, \alpha + s_{i,j_\Delta} - s_{i,j_{K+1}})$$

(0-norm $\|\Delta\|_0$ is replaced with 1-norm $\|\Delta\|_1$: optimizable and gives sparsity)

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How to Evaluate Counterfactual Explanations?

Sufficiency and Necessity:

$S \Rightarrow N$: S is a sufficient condition for N

$\neg N \Rightarrow \neg S$: N is a necessary condition for S

Two metrics for evaluating Counterfactual Explanations

Probability of Necessity (PN)

Probability of Sufficiency (PS)

Probability of Necessity (PN)

- Counterfactual Question:
  - If the explanation feature had not existed, would the item still be recommended?

Recommended items | **Not recommended items**

User	Phone A	Phone B	Phone C	Phone D	Phone E
Screen: 4.0	Screen: 4.5	Screen: 4.5	Screen: 5.0	Screen: 5.0	Screen: 5.0
~~Battery: 5.0~~	~~Battery: 3.0~~	~~Battery: 1.5~~	~~Battery: 1.5~~	~~Battery: 0.5~~	~~Battery: 1.0~~
Price: 3.0	Price: 3.0	Price: 4.5	Price: 3.5	Price: 4.0	Price: 3.0
	Score: 42.0	Score: 39.0	Score: 38.0	Score: 34.5	Score: 34.0

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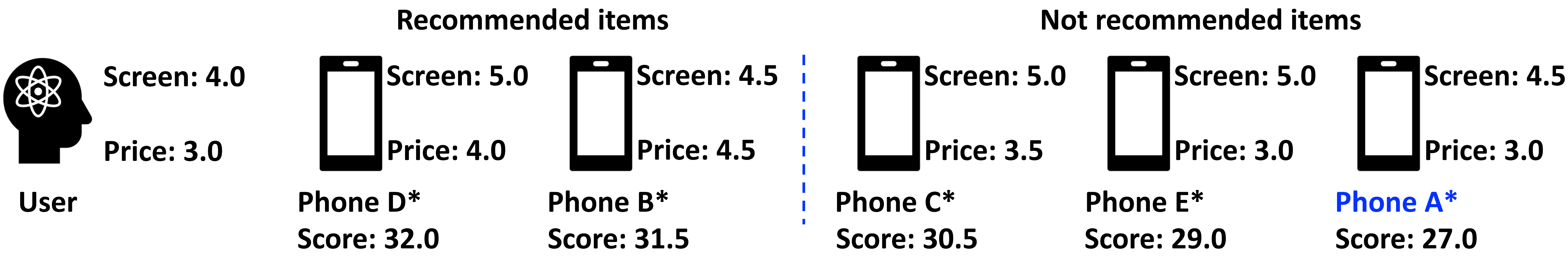
Probability of Necessity (PN)

- Counterfactual Question:
  - If the explanation feature had not existed, would the item still be recommended?
  - If the answer is NO, then it is a necessary explanation

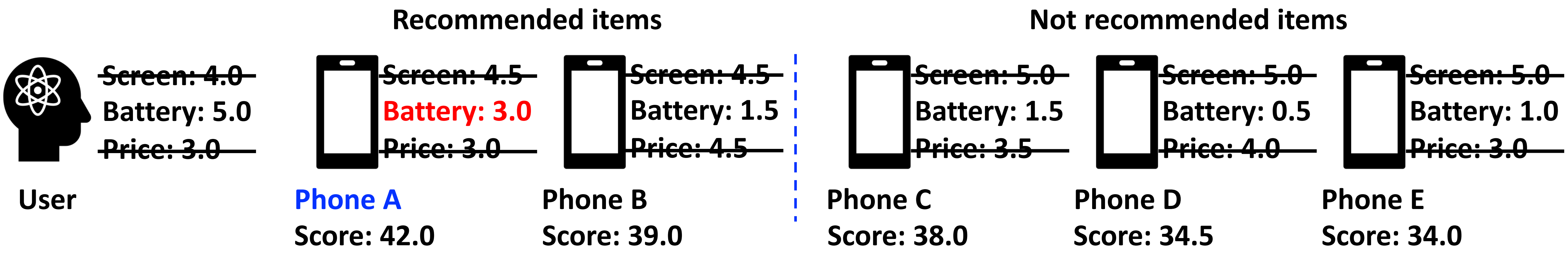


$$\mathrm{PN} = \frac{\sum_{u_i \in \mathcal{U}} \sum_{v_j \in R_{i,K}} \mathrm{PN}_{ij}}{\sum_{u_i \in \mathcal{U}} \sum_{v_j \in R_{i,K}} I(\mathcal{A}_{ij} \neq \emptyset)}, \text{ where } \mathrm{PN}_{ij} = \begin{cases} 1, & \text{if } v_j^* \notin R_{i,K}^* \\ 0, & \text{else} \end{cases}$$

PN: Percentage of explanation that satisfy the above necessity criterion

Probability of Sufficiency (PS)

- Counterfactual Question:
  - If the explanation feature were the only feature, would the item still be recommended?



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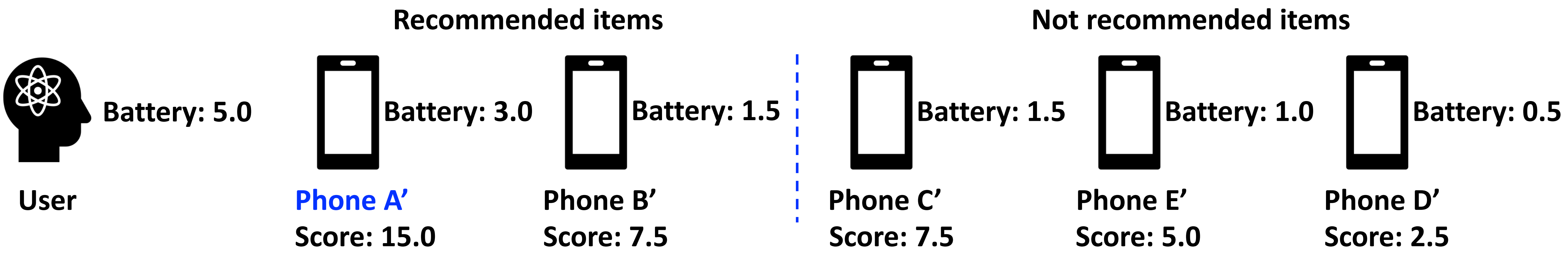
Probability of Sufficiency (PS)

- Counterfactual Question:
  - If the explanation feature were the only feature, would the item still be recommended?
  - If the answer is YES, then it is a sufficient explanation



$$\mathrm{PS} = \frac{\sum_{u_i \in \mathcal{U}} \sum_{v_j \in R_{i,K}} \mathrm{PS}_{ij}}{\sum_{u_i \in \mathcal{U}} \sum_{v_j \in R_{i,K}} I(\mathcal{A}_{ij} \neq \emptyset)}, \text{ where } \mathrm{PS}_{ij} = \begin{cases} 1, & \text{if } v'_j \in R'_{i,K} \\ 0, & \text{else} \end{cases}$$

PS: Percentage of explanation that satisfy the above sufficiency criterion

Evaluation of Counterfactual Explanation

- Counterfactual Explanations better than Associative Explanations

	Single Aspect Explanation														
	Electronic			Cell Phones			Kindle Store			CDs and Vinyl			Yelp		
	PN%	PS%	F_{NS}%	PN%	PS%	F_{NS}%	PN%	PS%	F_{NS}%	PN%	PS%	F_{NS}%	PN%	PS%	F_{NS}%
Random	2.05	2.10	2.07	3.39	3.50	3.44	3.16	2.75	2.94	1.58	2.03	1.78	7.52	10.68	8.82
EFM[50]	8.41	41.13	13.96	32.31	**82.09**	46.37	6.01	**73.84**	11.12	10.15	42.63	16.39	5.87	61.06	10.71
A2CF[9]	41.45	**77.60**	54.03	36.82	78.68	50.17	25.66	65.53	36.88	25.41	**84.51**	39.07	17.59	**96.92**	29.78
CountER	**65.54**	68.28	**66.83**	**74.03**	63.30	**68.25**	34.37	41.50	37.60	49.62	54.72	52.04	**65.26**	53.25	**58.64**

	Multiple Aspect Explanation														
	Electronic			Cell Phones			Kindle Store			CDs and Vinyl			Yelp		
	PN%	PS%	F_{NS}%	PN%	PS%	F_{NS}%	PN%	PS%	F_{NS}%	PN%	PS%	F_{NS}%	PN%	PS%	F_{NS}%
Random	2.24	4.90	3.08	6.25	10.13	7.73	5.80	7.80	6.65	3.22	7.65	4.53	13.84	12.92	13.36
EFM[50]	29.65	84.67	43.92	52.66	87.98	65.88	51.72	**96.42**	67.33	47.65	87.35	61.66	16.76	81.68	27.81
A2CF[9]	59.47	81.66	68.82	56.45	80.97	66.52	52.48	87.59	65.64	49.12	**91.52**	63.93	41.38	**98.28**	58.24
CountER	**97.08**	**96.24**	**96.66**	**99.52**	**98.48**	**99.00**	**64.00**	79.20	**70.79**	**80.89**	88.60	**84.57**	**99.91**	94.12	**96.93**

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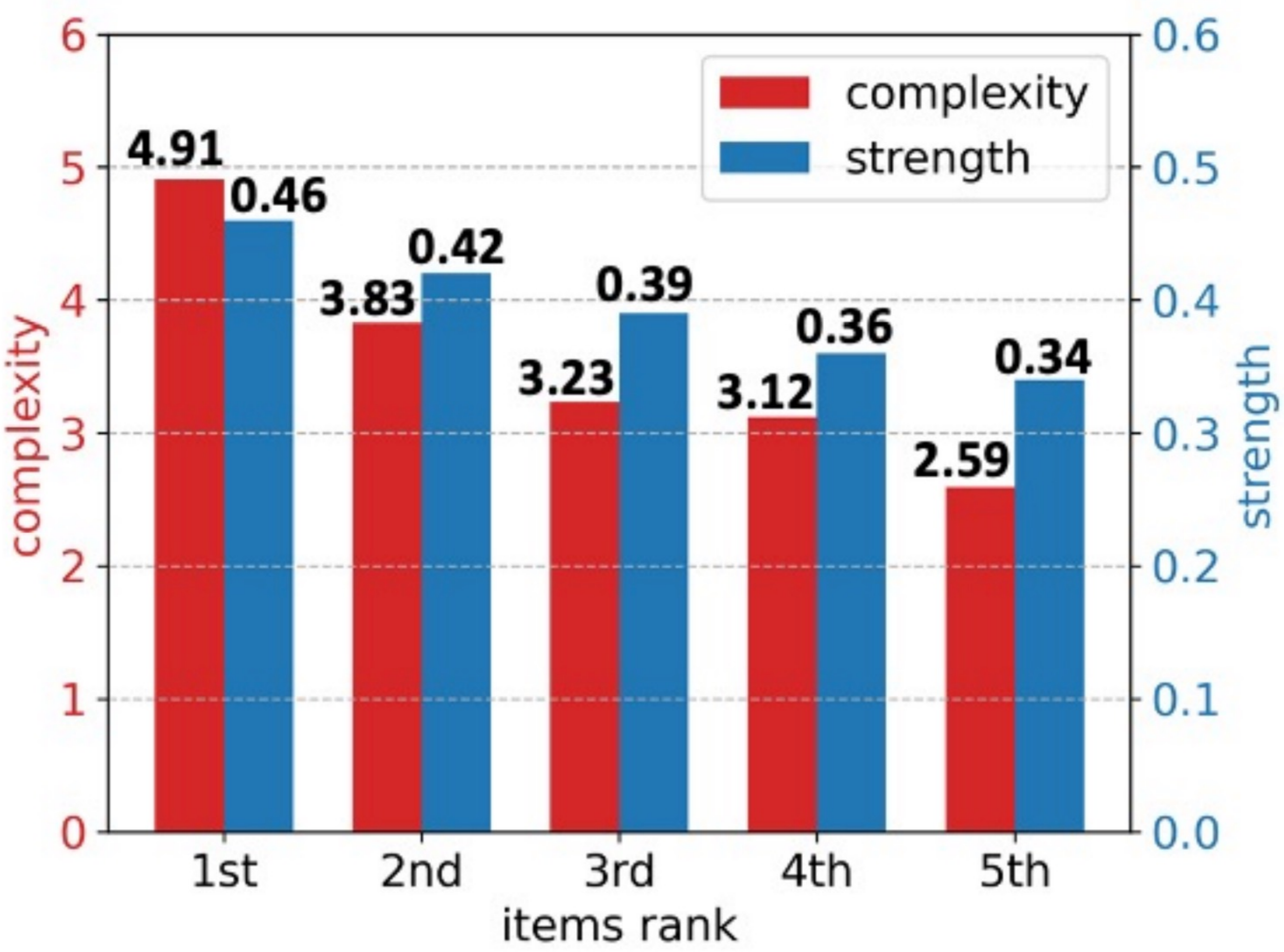
Interesting Observation

- Top-ranked items need to be backed by stronger and more complex explanations



User Controllable AI (ECAI’23)

[2] J Tan, Y Ge, Y Zhu, Y Xia, J Luo, J Ji, and **Y Zhang**. "User-Controllable Recommendation via Counterfactual Retrospective and Prospective Explanations." In ECAI 2023.

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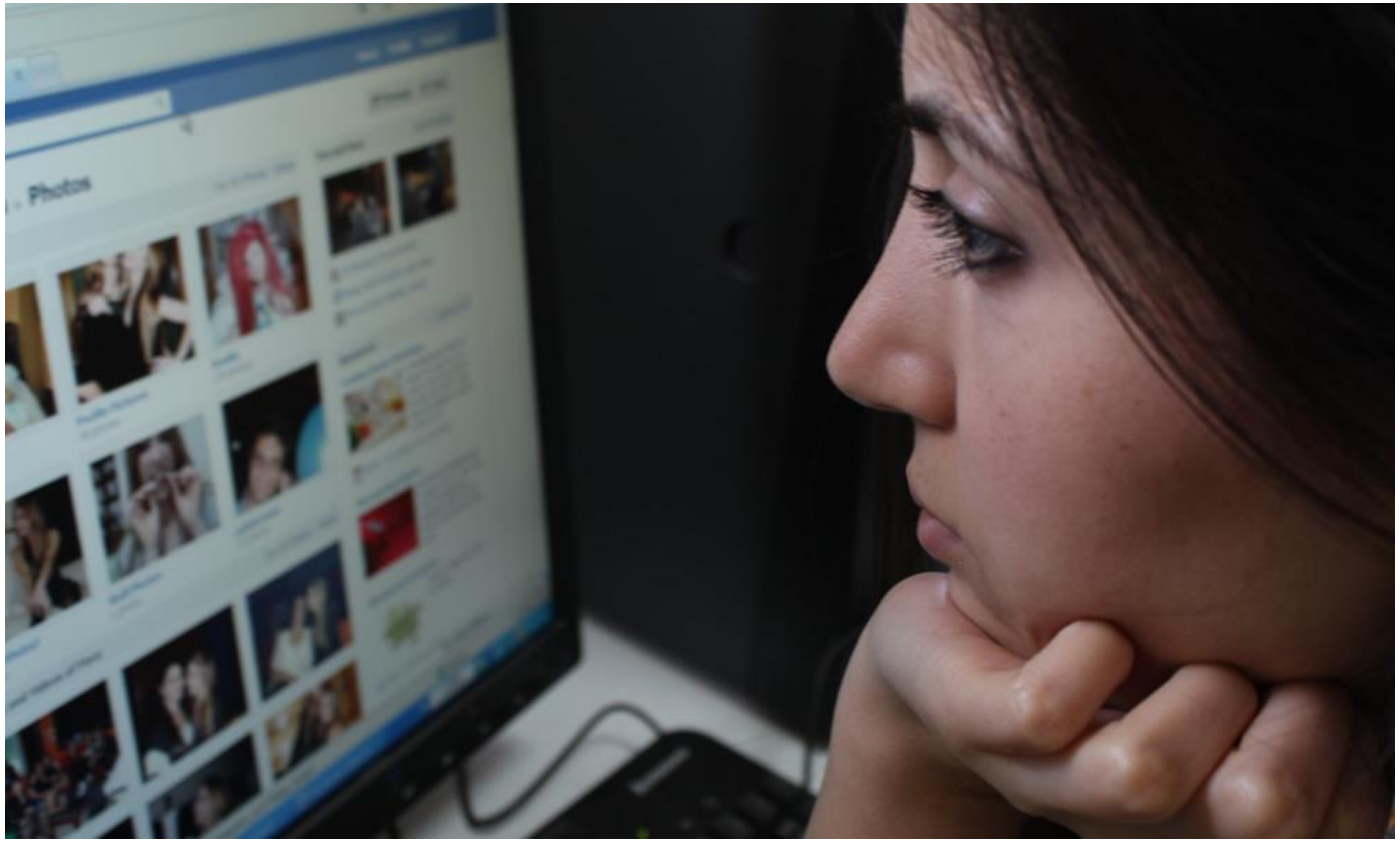
Towards User Controllable Recommender Systems

- Users almost have no control of their recommender system
  - They can only passively receive recommendations



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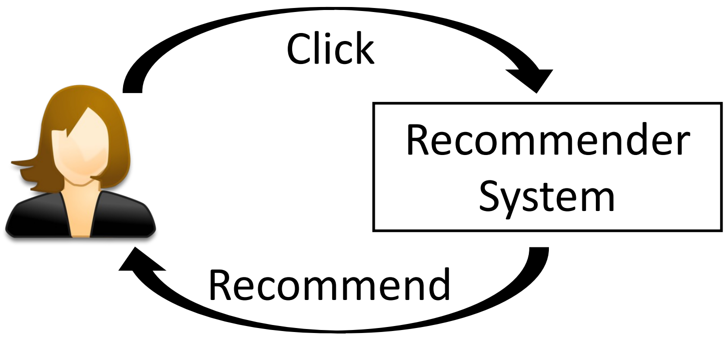
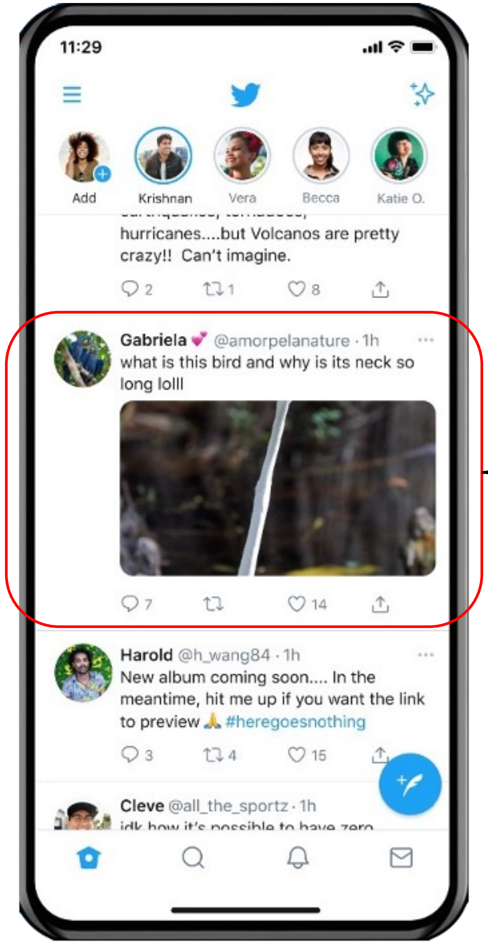
Towards User Controllable Recommender Systems

- Users almost have no control of their recommender system
  - They can only passively receive recommendations
- This causes many problems, e.g., echo chamber



The more you like something, the more RS will recommend similar things, and thus you like them even more.

User Control based on Counterfactual Explanations



Counterfactual Retrospective Explanation [3]

We recommend this video X because you previously ❤️videos A and B, if you did not ❤️ them, then we would not have recommended this video X.

Counterfactual Prospective Explanation [3]

If you ❤️ this video X, then we will recommend videos D and E in the future that otherwise would not be recommended.

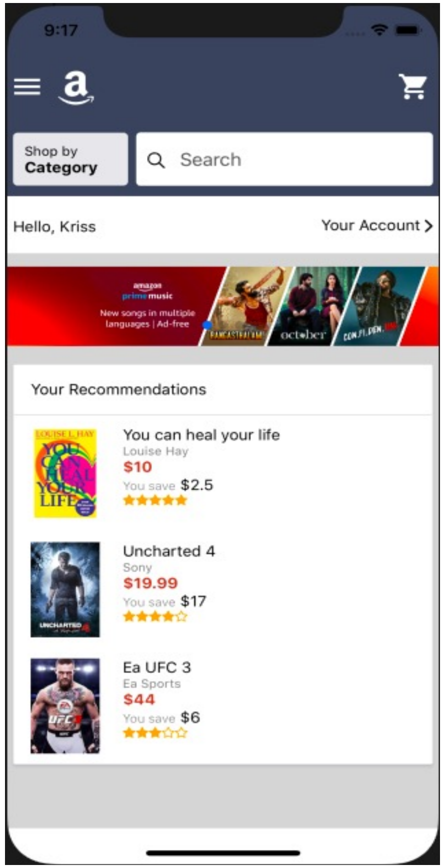
Help users know the consequences of their behaviors so that they can take informed actions.
Users can control their recommendation by invoking or revoking certain actions.

[2] J Tan, Y Ge, Y Zhu, Y Xia, J Luo, J Ji, and **Y Zhang**. "User-Controllable Recommendation via Counterfactual Retrospective and Prospective Explanations." In ECAI 2023.

Counterfactual Explainable Fairness (SIGIR'22)

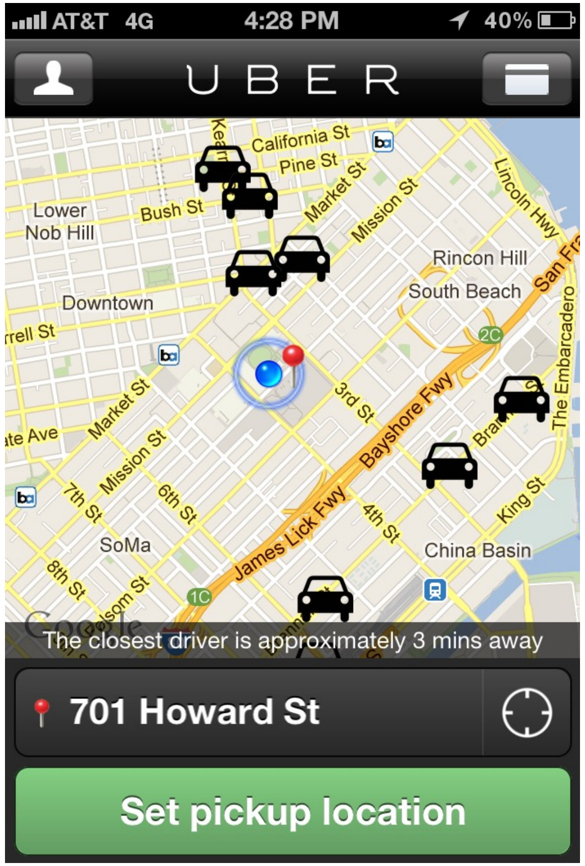
[3] Y Ge, J Tan, Y Zhu, Y Xia, J Luo, S Liu, Z Fu, S Geng, Z Li, and **Y Zhang**. "Explainable fairness in recommendation." In SIGIR 2022.

Why Fairness in RecSys? Resource is Limited

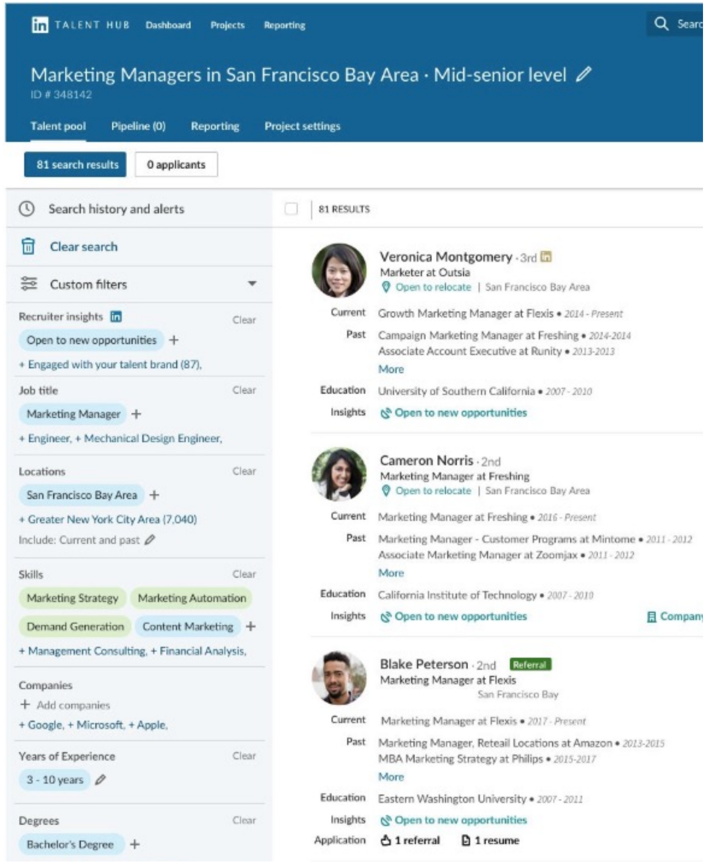


Recommendation slot positions are limited

User attention is a limited resource



Passengers are limited

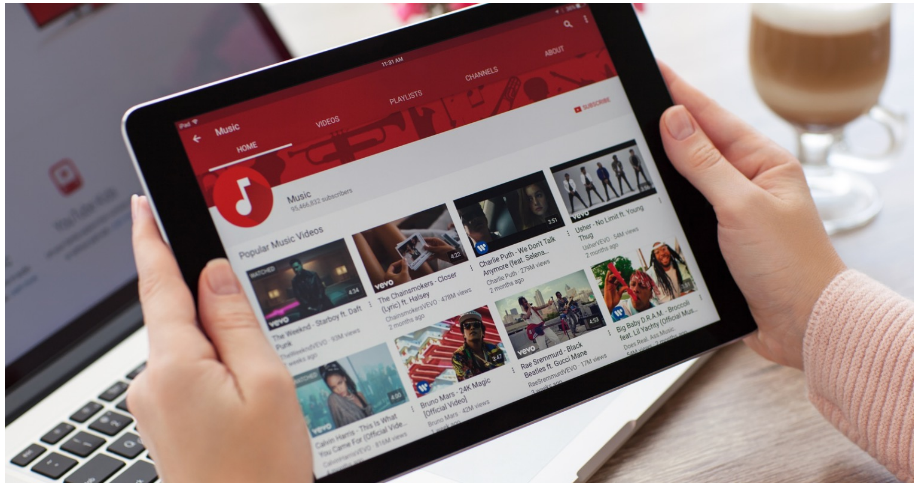


Interview opportunities are limited

Fairness and Sustainable Development

- RecSys platforms consider fairness for sustainable development

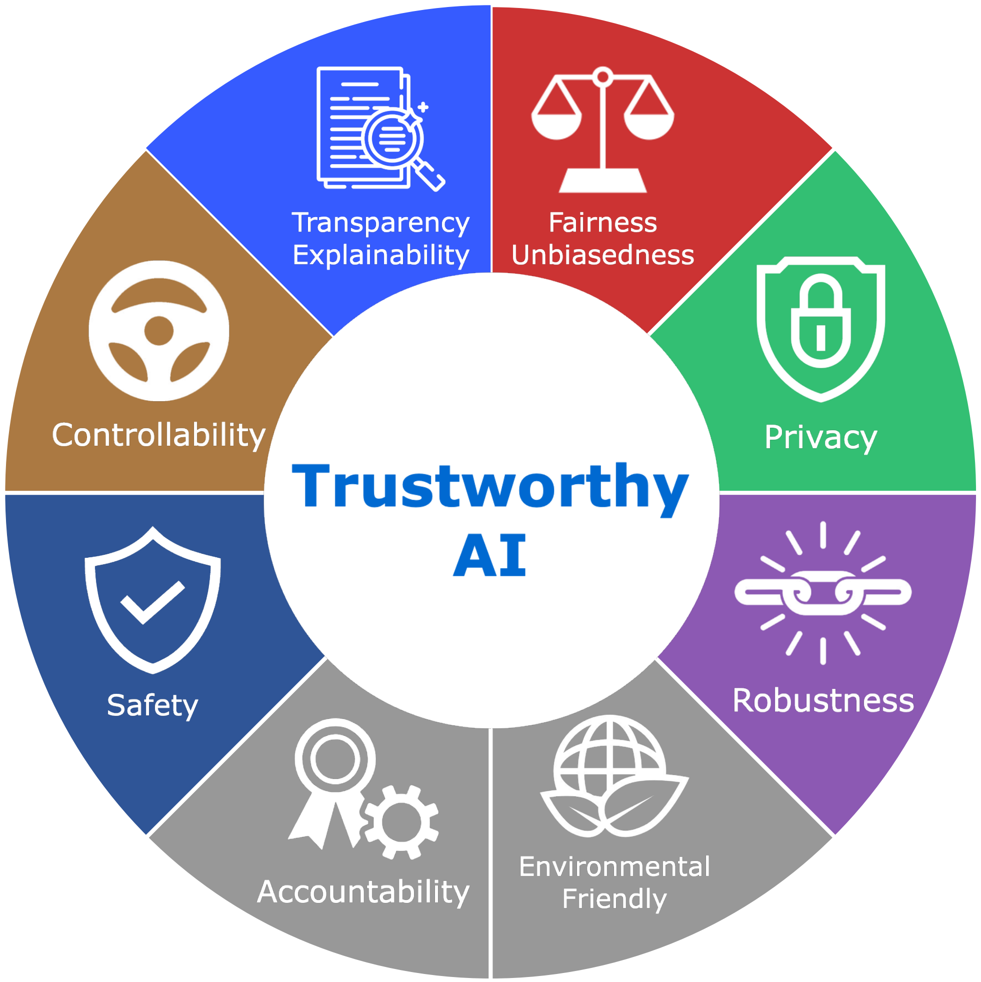
An e-commerce example
Big retailors vs. Small retailors



A social network example
Star accounts vs. Grassroot accounts

Various Types of Fairness Definitions

- Explainable Fairness based on Counterfactual Reasoning



Counterfactual Fairness [SIGIR21a]
User-oriented Fairness [WWW21b]
Long-term Fairness [WSDM21]
Explainable Fairness [SIGIR22a, SIGIR20a]
Federated Fairness [RecSys22b]
Group-wise Fairness [RecSys17]
Fairness-Utility Relationship [WSDM22b]
Popularity Bias [CIKM21b]
Echo Chamber [SIGIR20b]
Bias and Fairness of LLMs [AACL22]

Why Explainable Fairness?

- Explainable Fairness is important in Recommendation [4]
  - Hundreds, thousands or even more features
  - $y = f(F_u, F_v) = f(Lo, In, Ta, \dots, Ft, Ra, Pa, Wa, \dots)$

User ID	Item ID	Location	Income	Taste	Food Type	Rating	Parking	Waiting	Label
User_1	Restaurant_1	NJ	$500	Sweet	French	4.8	Yes	30min	1
User_1	Restaurant_2	NJ	$500	Sweet	Chinese	4.5	Yes	15min	1
User_2	Restaurant_3	NY	$600	Spicy	Mexico	4.5	Yes	20min	0
User_3	Restaurant_4	PA	$400	Salty	Fast food	3.8	No	5min	0

User Features   Item Features   Prediction

System designers: Difficult to know which feature(s) caused unfairness
Users: Difficult to know how to intervene unfair results

[3] Y Ge, J Tan, Y Zhu, Y Xia, J Luo, S Liu, Z Fu, S Geng, Z Li, and **Y Zhang**. "Explainable fairness in recommendation." In SIGIR 2022.

An Example of Yelp Recommendation

- Exposure Fairness as an Example

$$\frac{Exposure(G_0|R_{U,K})}{Exposure(G_1|R_{U,K})} = \frac{|G_0|}{|G_1|} \qquad Exposure(G_i|R_{U,K}) = \sum_{u\in U}\sum_{v\in R_{u,K}} I_{v\in G_i}$$

- Top-5 features that lead to exposure unfairness

Method	Feature-based Explanations
Pop-User	food, service, chicken, prices, hour
Pop-Item	food, service, prices, visit, hour
EFM-User	store, patio, dishes, dish, rice
EFM-Item	flavor, decor, dishes, inside, cheese
SV	server, size, pizza, food, restaurant
CEF	meal, cheese, dish, chicken, taste

[3] Y Ge, J Tan, Y Zhu, Y Xia, J Luo, S Liu, Z Fu, S Geng, Z Li, and **Y Zhang**. "Explainable fairness in recommendation." In SIGIR 2022.

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Counterfactual Explainable Fairness

- Explanation as a Feature Mask Vector $\Delta =$

Service	Price	Hour
1	0	0

- Simple and Effective Explanations

$$\begin{aligned}&\min.\ \text{Explanation Complexity}\\ &s.t.,\text{Model Unfairness } \leq \delta\end{aligned} \quad \Rightarrow \quad \begin{aligned}&\min.\ \|\Delta\|_1\\ &s.t.,\Psi \leq \delta\end{aligned}$$

- Ψ can be any fairness definition
  - Exposure fairness as an example

$$\frac{Exposure(G_0|R_{U,K})}{Exposure(G_1|R_{U,K})} = \frac{|G_0|}{|G_1|} \doteq \alpha \quad \Leftrightarrow \quad Exposure(G_0|R_{U,K}) = \alpha \cdot Exposure(G_1|R_{U,K})$$

$$\min_{\Delta}.\ \|\Delta\|_1 + \lambda|\Psi|$$

$$\text{where: } \Psi = Exposure(G_0|R_{U,K}) - \alpha \cdot Exposure(G_1|R_{U,K})$$

[3] Y Ge, J Tan, Y Zhu, Y Xia, J Luo, S Liu, Z Fu, S Geng, Z Li, and **Y Zhang**. "Explainable fairness in recommendation." In SIGIR 2022.

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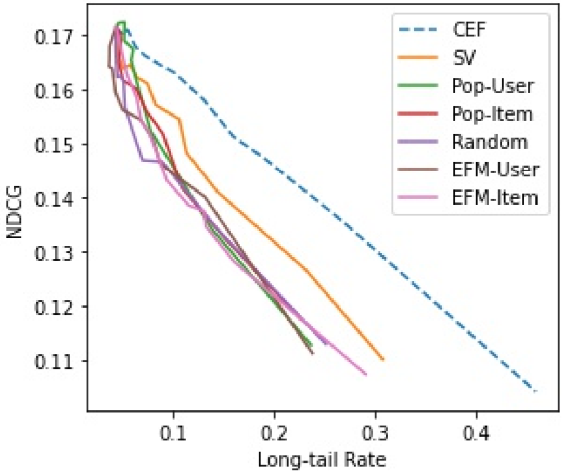
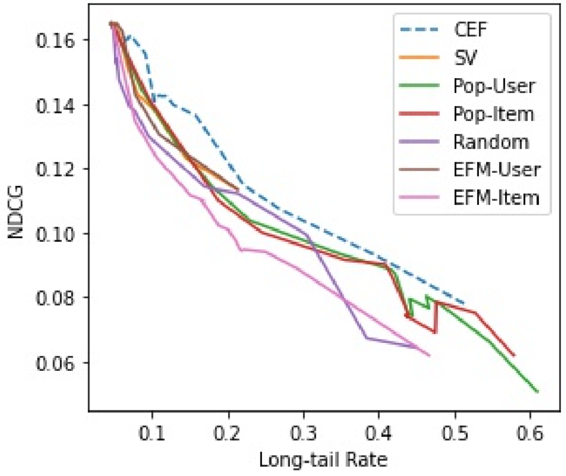
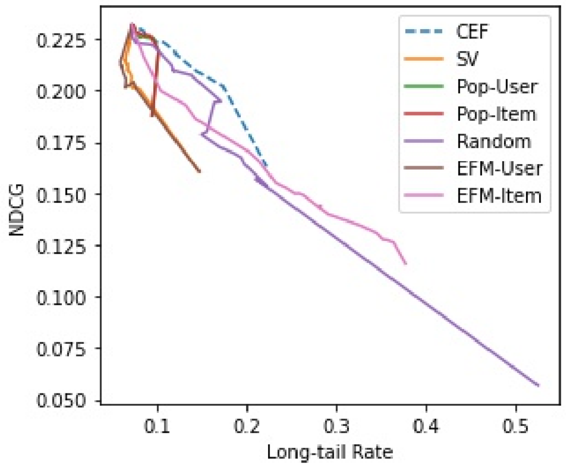
Better Fairness-Utility Trade-off



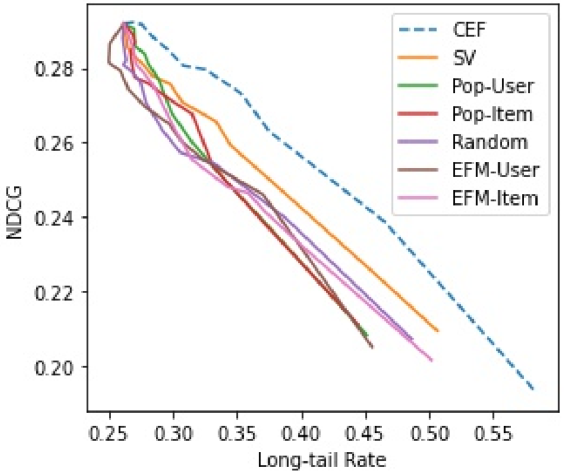
(a) NDCG@5 vs Long-tail Rate@5 on Yelp



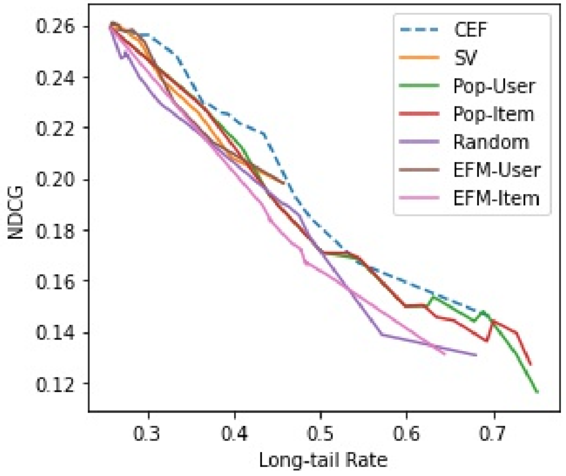
(b) NDCG@5 vs Long-tail Rate@5 on Electronics



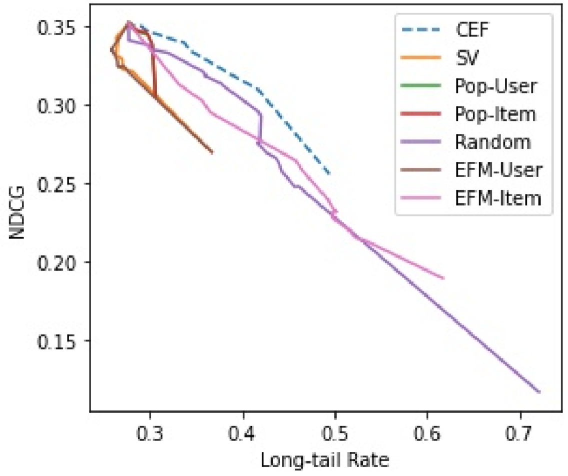
(c) NDCG@5 vs Long-tail Rate@5 on CDs&Vinyl



(d) NDCG@20 vs Long-tail Rate@20 on Yelp



(e) NDCG@20 vs Long-tail Rate@20 on Electronics



(f) NDCG@20 vs Long-tail Rate@20 on CDs&Vinyl

Trustworthy AI for Science

(ICML22, WWW22, KDD23)

[4] Z Li, J Ji, and **Y Zhang**. "From Kepler to Newton: Explainable AI for Science Discovery." In ICML AI for Science. 2022.
[5] J Tan, S Geng, Z Fu, Y Ge, S Xu, Y Li, and **Y Zhang**. "Learning and evaluating graph neural network explanations based on counterfactual and factual reasoning." In WWW 2022.
[6] J Tan and **Y Zhang**. "ExplainableFold: Understanding AlphaFold Prediction with Explainable AI." In KDD 2023.

Science is not only about understanding the "what" and "how", but also, and perhaps more importantly, the *"why"*.

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The Conquest of “Why” in Science

- The conquest of why has always been the key theme of science in human history
- A Legend Example
  - The Kepler’s Laws of Planetary Motion
  - The Newton’s Law of Universal Gravitation

Tycho Brahe (1546-1610) Johannes Kepler (1571-1630) Isaac Newton (1643-1727)

[4] Z Li, J Ji, and **Y Zhang**. "From Kepler to Newton: Explainable AI for Science Discovery." In ICML AI for Science. 2022.

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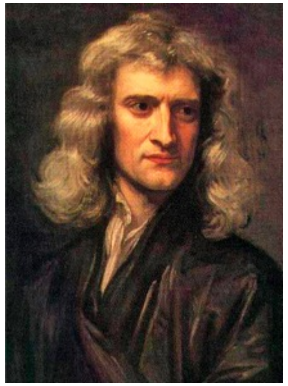
Three Key Roles in the Scientific Discovery Process

Tycho Brahe (1546-1610)

Johannes Kepler (1571-1630)



Isaac Newton (1643-1727)

Observation	Analyzation	Explanation

Time	Position
1	(a,b)
2	(c,d)
3	(e,f)

$$\frac{\tau^2}{r^3} = K$$

$$F = G\frac{m_1 m_2}{r^2}$$

Data Collection
Almost automated

Model Learning
Many available methods

Model Interpretation (XAI)
Still needs much exploration

[4] Z Li, J Ji, and **Y Zhang**. "From Kepler to Newton: Explainable AI for Science Discovery." In ICML AI for Science. 2022.

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Explainable Graph Neural Networks (WWW'22)

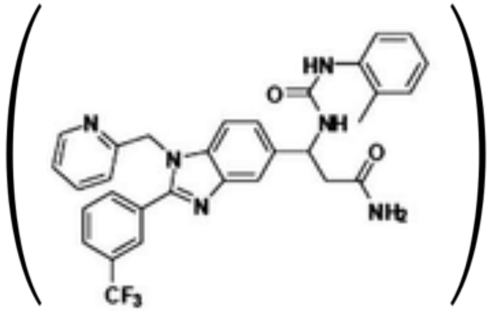
Molecule Analysis

[5] J Tan, S Geng, Z Fu, Y Ge, S Xu, Y Li, and **Y Zhang**. "Learning and evaluating graph neural network explanations based on counterfactual and factual reasoning." In WWW 2022.

The Molecule Classification Problem

- Predict the property of molecules
  - E.g., If a molecule is soluble, toxic, or can pass the Blood-Brain Barrier
  - A fundamental problem in many tasks, e.g., drug discovery
- Molecule is a graph
  - Current approaches use Graph Neural Networks (GNN) for prediction
  - E.g., A binary classification problem

GNN



= Yes / No

- However, we want to know **why** the model produce such results

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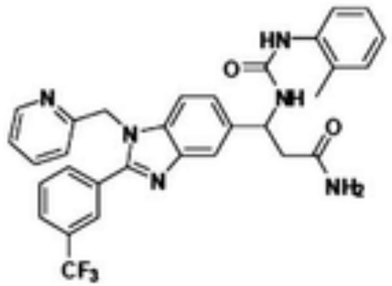
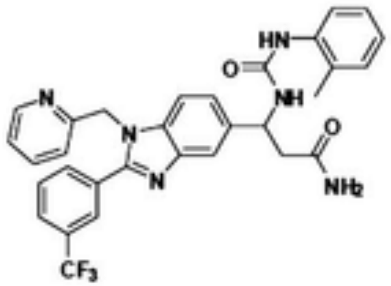
Explainable Graph Neural Networks

GNN 

= Yes / No

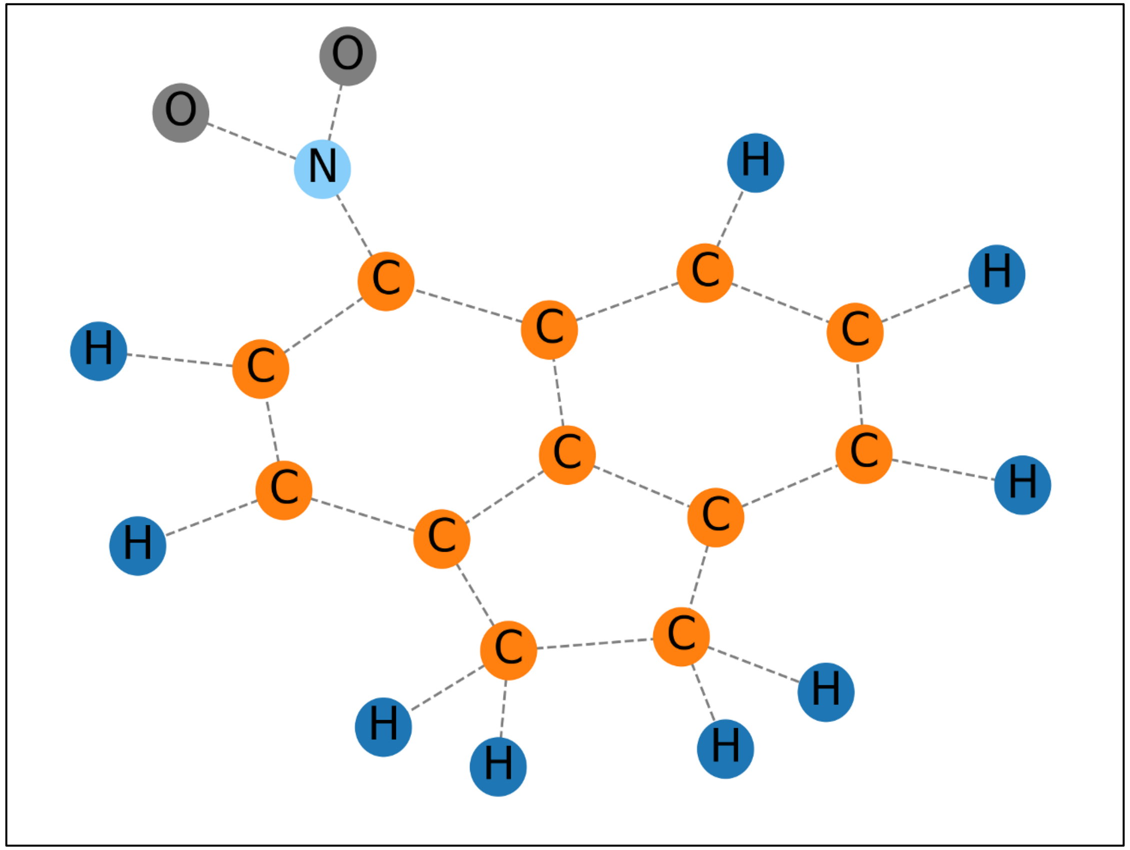
⇩

XGNN 

= Yes / No + Explanation

Factual and Counterfactual Explanations

- Example: Molecule toxicity (mutagenetic) prediction [2]
  - If the GNN model predicts the molecule as toxic, why?



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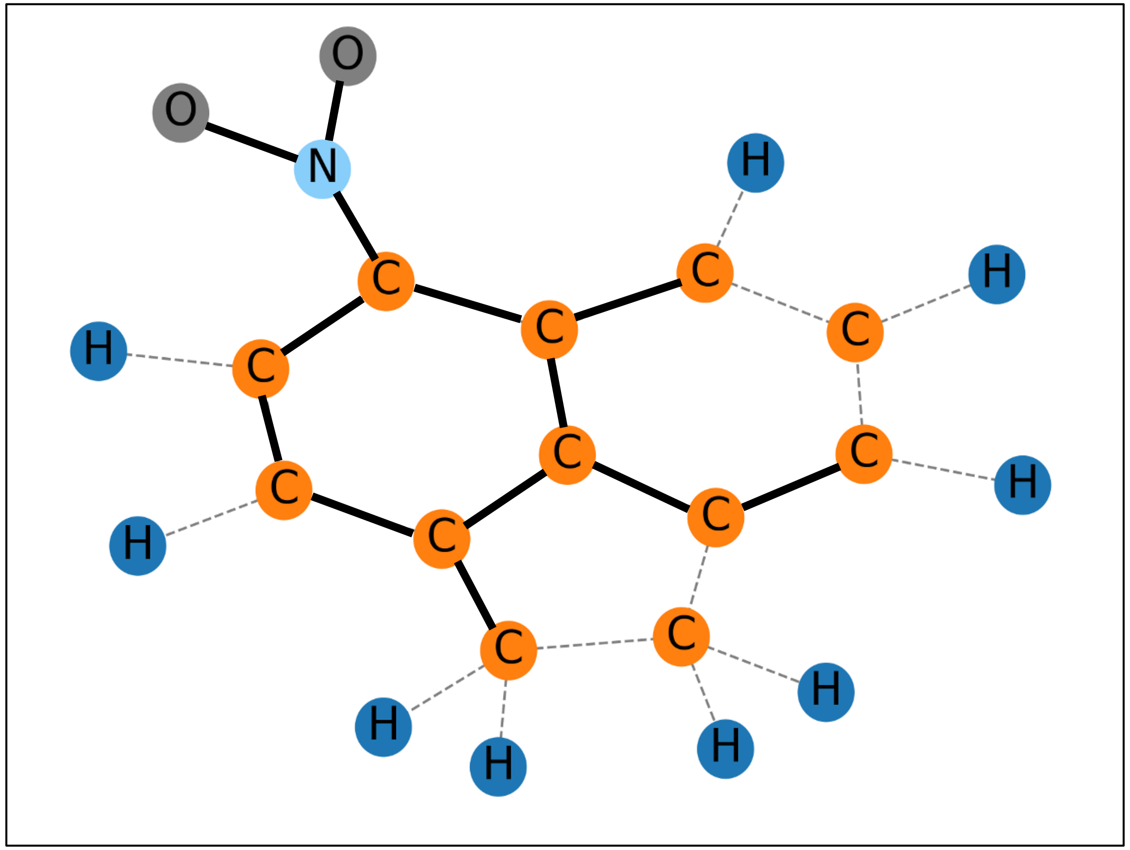
Factual and Counterfactual Explanations

- Factual explanation seeks a sufficient condition
  - The molecule would be toxic with the highlighted bonds



[5] J Tan, S Geng, Z Fu, Y Ge, S Xu, Y Li, and **Y Zhang**. "Learning and evaluating graph neural network explanations based on counterfactual and factual reasoning." In WWW 2022.

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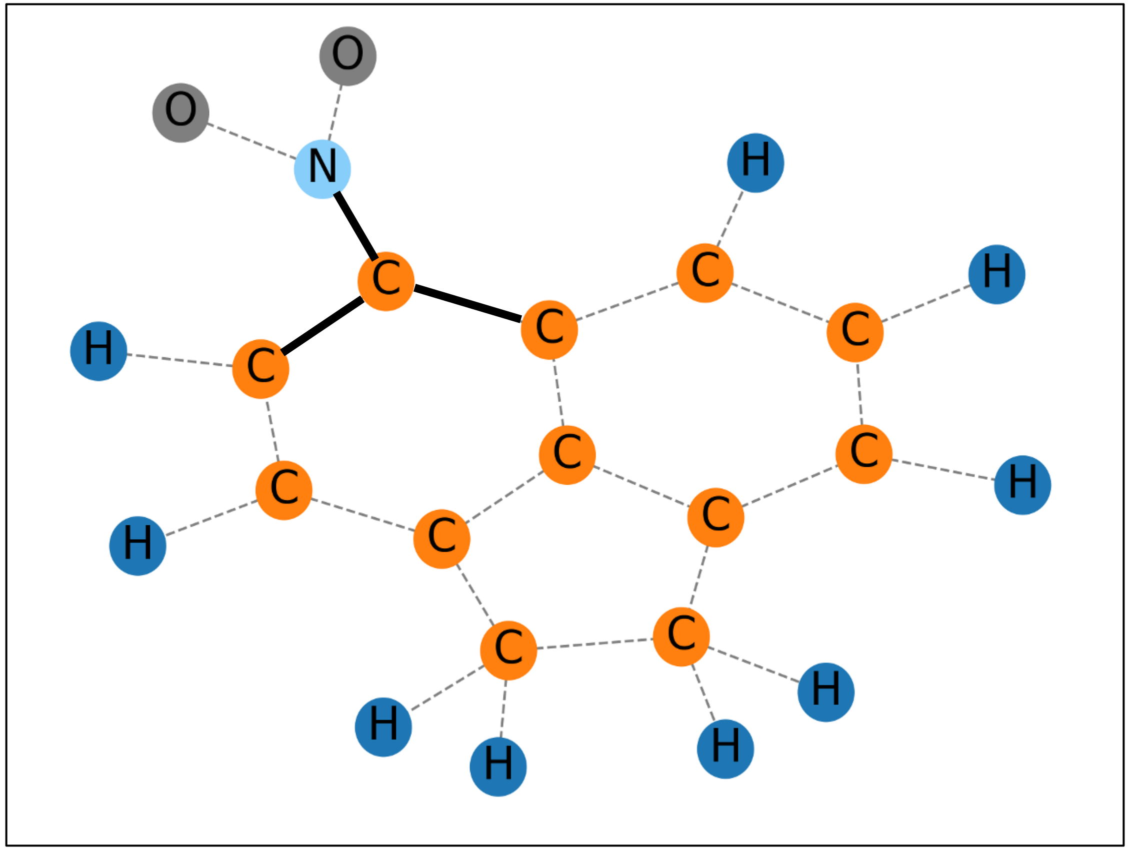
Factual and Counterfactual Explanations

- Counterfactual explanation seeks a necessary condition
  - The molecule would not be toxic without the highlighted bonds



[5] J Tan, S Geng, Z Fu, Y Ge, S Xu, Y Li, and **Y Zhang**. "Learning and evaluating graph neural network explanations based on counterfactual and factual reasoning." In WWW 2022.

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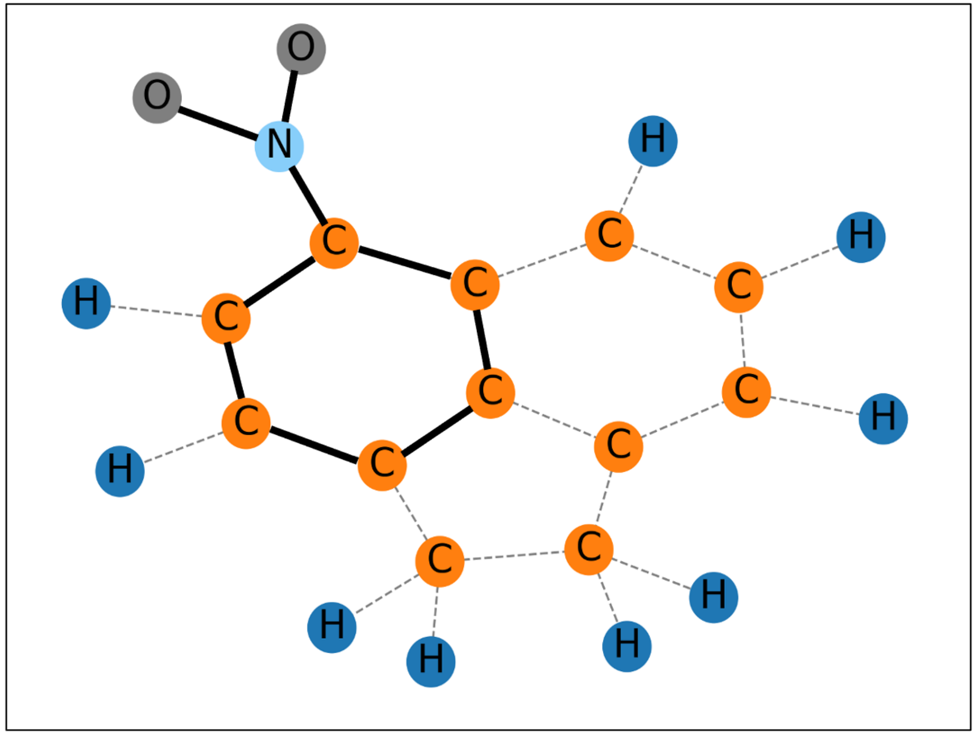
Factual and Counterfactual Explanations

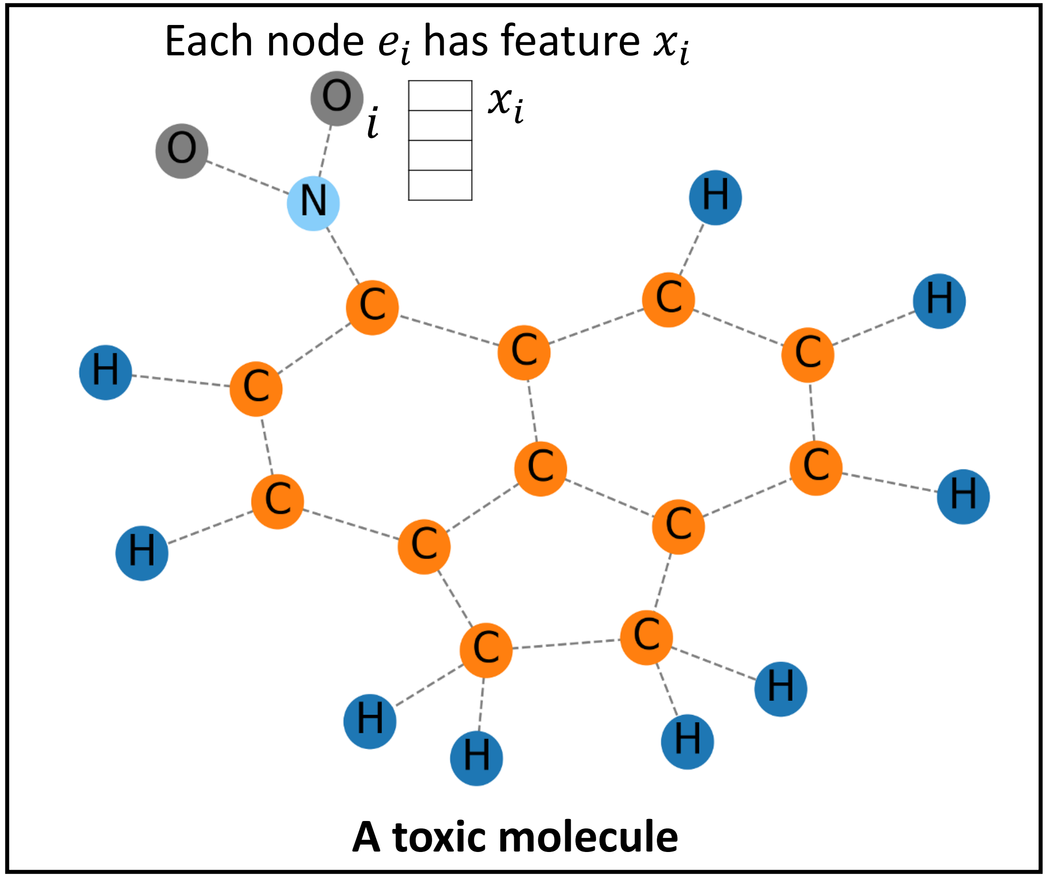
- Factual and Counterfactual explanation seeks a compact (both sufficient and necessary) condition
  - The molecule would be toxic with the highlighted bonds
  - The molecule would not be toxic without the highlighted bonds
  - No more, no less, just enough

The Nitro-Benzene Structure



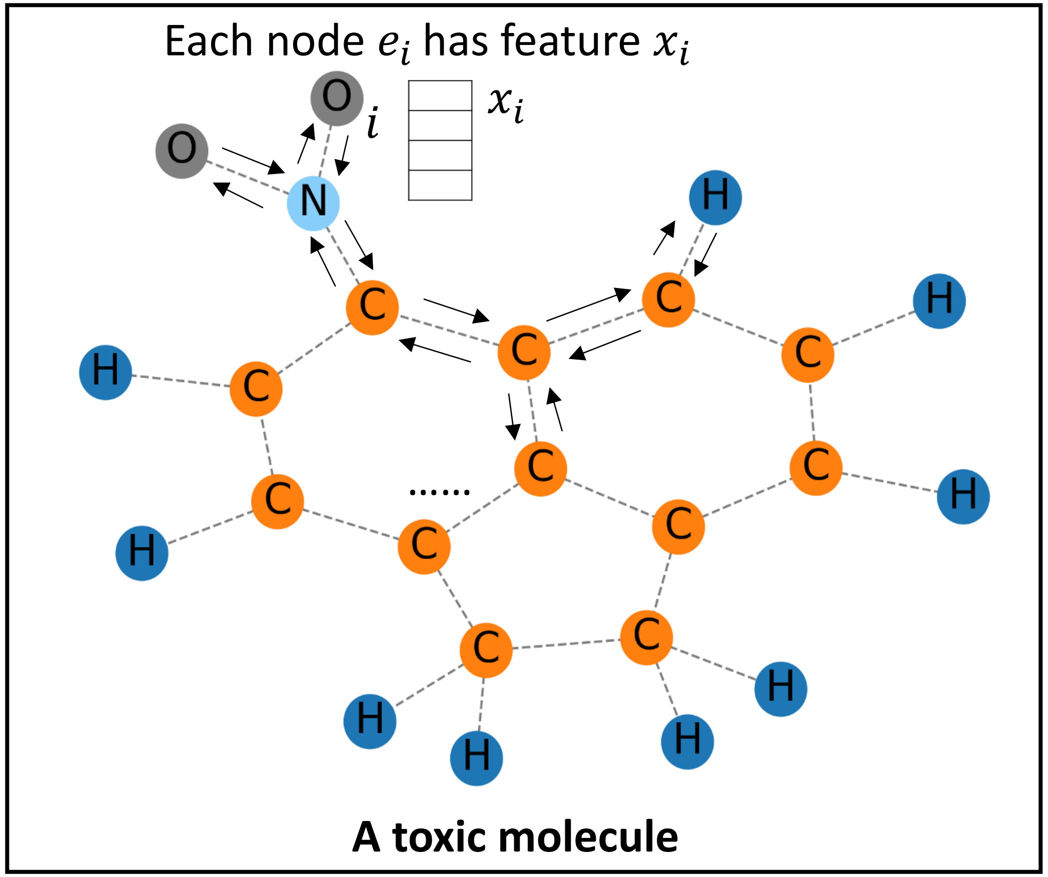
[5] J Tan, S Geng, Z Fu, Y Ge, S Xu, Y Li, and **Y Zhang**. "Learning and evaluating graph neural network explanations based on counterfactual and factual reasoning." In WWW 2022.

GNN Basics



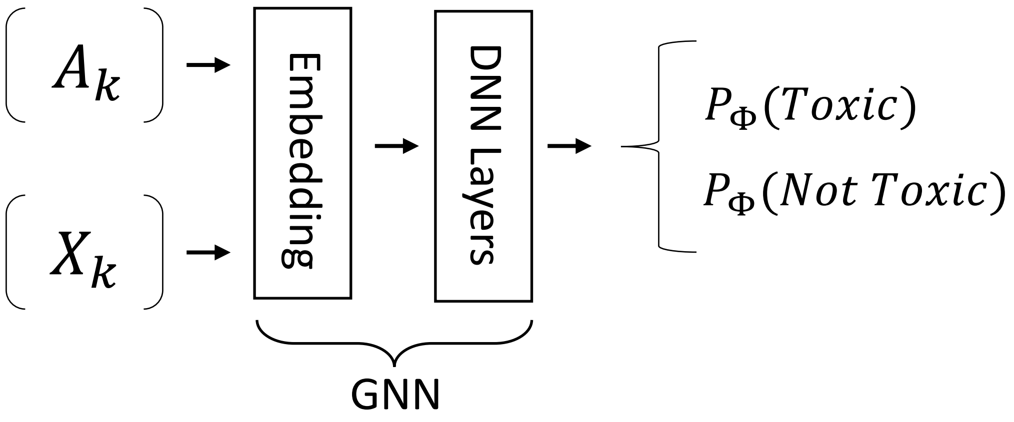
- A graph $G_k = \{\mathcal{V}_k, \mathcal{E}_k\}$
  - Adjacency matrix $A_k \in \{0,1\}^{|\mathcal{V}_k| \times |\mathcal{V}_k|}$
  - Node feature matrix $X_k \in \mathbb{R}^{|\mathcal{V}_k| \times d}$

GNN Basics



Information propagate through the graph to get graph embedding

- A graph $G_k = \{\mathcal{V}_k, \mathcal{E}_k\}$
  - Adjacency matrix $A_k \in \{0,1\}^{|\mathcal{V}_k| \times |\mathcal{V}_k|}$
  - Node feature matrix $X_k \in \mathbb{R}^{|\mathcal{V}_k| \times d}$



- GNN predicts the label $\hat{y}_k$ for G_k by:

$$\hat{y}_k = \arg\max_{c \in C} P_\Phi(c \mid A_k, X_k)$$

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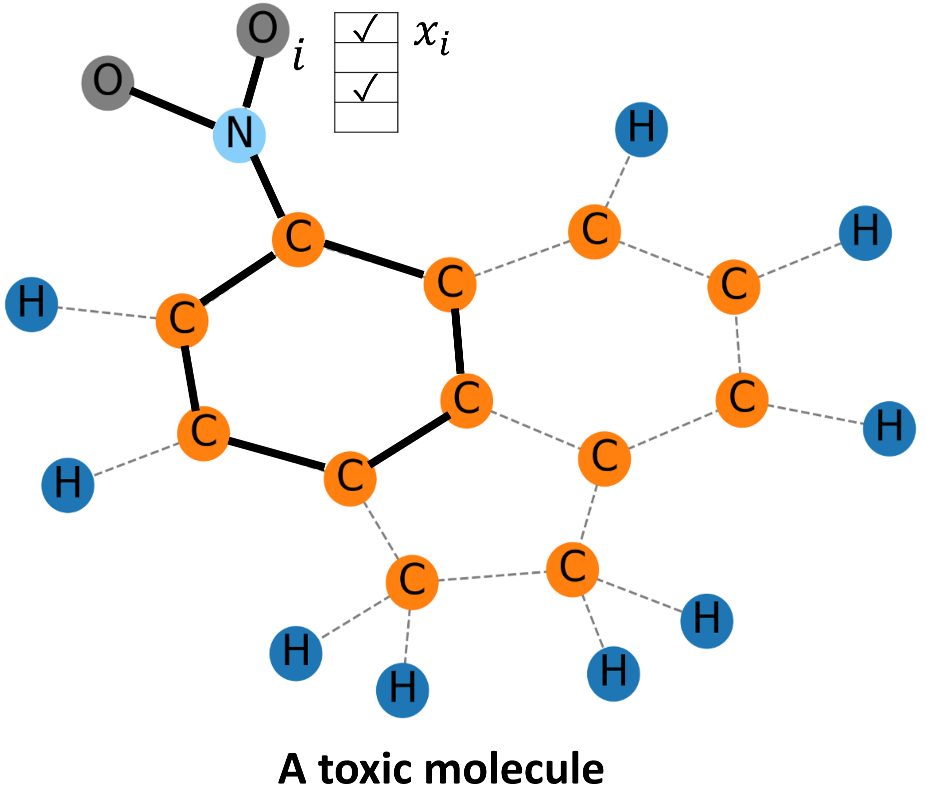
GNN Explanation as Sub-Graph Mask Vector

Each node e_i has feature x_i



Explanation Sub-Graph

- A graph $G_k = \{\mathcal{V}_k, \mathcal{E}_k\}$
  - Adjacency matrix $A_k \in \{0,1\}^{|\mathcal{V}_k| \times |\mathcal{V}_k|}$
  - Node feature matrix $X_k \in \mathbb{R}^{|\mathcal{V}_k| \times d}$
- Edge mask $M_k \in \{0, 1\}^{|\mathcal{V}_k| \times |\mathcal{V}_k|}$
- Feature mask $F_k \in \{0, 1\}^{|\mathcal{V}_k| \times d}$
- Sub-Graph as Explanation
  - Sub-Edges $A_k \odot M_k$
  - Sub-Features $X_k \odot F_k$

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How to Find the Explanation?

- Factual Reasoning: Given A already happened, will B happen?
  - Factual Condition:

$$\arg\max_{c \in C} P_{\Phi}(c \mid \underbrace{A_k \odot M_k, X_k \odot F_k}_{\text{With only the explanation sub-graph}}) = \hat{y}_k$$

- Counterfactual Reasoning: If A did not happen, would B still happen?
  - Counterfactual Condition:

$$\arg\max_{c \in C} P_{\Phi}(c \mid \underbrace{A_k - A_k \odot M_k, X_k - X_k \odot F_k}_{\text{Without the explanation sub-graph}}) \neq \hat{y}_k$$

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What are Good Explanations? Simple and Effective (again!)

Occam's Razor Principle for Explainable AI:
When trying to explain a phenomenon, if two explanations are equally effective, then we prefer the simpler one.

- To quantify Simplicity
  - Explanation Complexity

$$C(M, F) = \|M\|_0 + \|F\|_0$$

How many **edges** are included in the explanation

How many **features** are included in the explanation

- To quantify Effectiveness
  - Factual Explanation Strength

$$S_f(M, F) = P_\Phi(\hat{y}_k \mid A_k \odot M_k, X_k \odot F_k)$$

  - Counterfactual Explanation Strength

$$S_c(M, F) = -P_\Phi(\hat{y}_k \mid A_k - A_k \odot M_k, X_k - X_k \odot F_k)$$

Both should be large enough to satisfy the conditions

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Counterfactual Learning and Reasoning

- Seek simple and effective explanations

$$\text{minimize} \;\; \text{Explanation Complexity}$$
$$\text{s.t.,} \;\; \text{Explanation is Strong Enough}$$

⇩

$$\text{minimize} \;\; C(M_k, F_k)$$
$$\text{s.t.,} \;\; S_f(M_k, F_k) > P_\Phi(\hat{y}_{k,s} \mid A_k \odot M_k, X_k \odot F_k),$$
$$S_c(M_k, F_k) > -P_\Phi(\hat{y}_{k,s} \mid A_k - A_k \odot M_k, X_k - X_k \odot F_k)$$

- $\hat{y}_{k,s}$ is the label of the second largest prediction probability
- Idea: Find minimal components of a molecule which is both sufficient and necessary

Evaluation of Counterfactual Explanations

Sufficiency and Necessity:

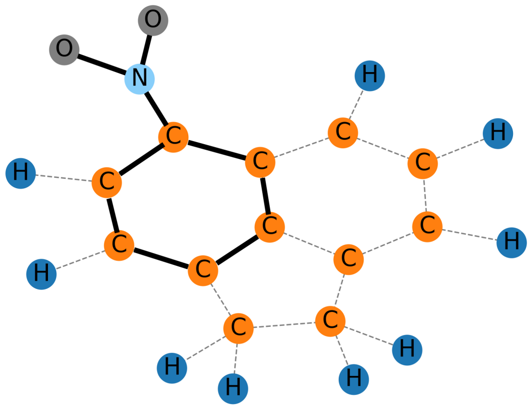
S ⇒ N: S is a sufficient condition for N

¬N ⇒ ¬S: N is a necessary condition for S

- Probability of Sufficient (PS)
  - If we only keep the explanation sub-graph, the prediction result is the same, then the explanation is sufficient
  - PS: Percentage of molecules whose explanation sub-graph is Sufficient

$$\mathrm{PS} = \frac{\sum_{G_k \in \mathcal{G}} \mathrm{ps}_k}{|\mathcal{G}|}, \text{ where } \mathrm{ps}_k = \begin{cases} 1, & \text{if } \hat{y}'_k = \hat{y}_k \\ 0, & \text{else} \end{cases}$$

$$\text{where } \hat{y}'_k = \arg\max_{c \in C} P_\Phi(c \mid A_k \odot M_k, X_k \odot F_k)$$



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Evaluation of Counterfactual Explanations

Sufficiency and Necessity:

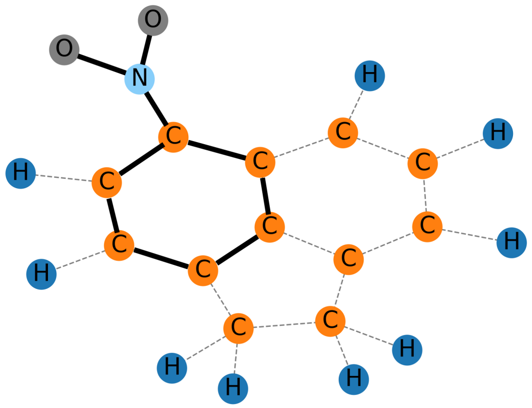
S ⇒ N: S is a sufficient condition for N

¬N ⇒ ¬S: N is a necessary condition for S

- Probability of Necessity (PN)
  - If we remove the explanation sub-graph, the prediction result will change, then the explanation is necessary
  - PN: Percentage of molecules whose explanation sub-graph is Necessary

$$\mathrm{PN} = \frac{\sum_{G_k \in \mathcal{G}} \mathrm{pn}_k}{|\mathcal{G}|}, \text{ where } \mathrm{pn}_k = \begin{cases} 1, & \text{if } \hat{y}'_k \neq \hat{y}_k \\ 0, & \text{else} \end{cases}$$

$$\text{where } \hat{y}'_k = \arg\max_{c \in C} P_\Phi(c \mid A_k - A_k \odot M_k, X_k - X_k \odot F_k)$$



Datasets for Evaluation

Dataset	#graph	#ave n	#ave e	#class	#feat	task	gt
BA-Shapes	1	700	4100	4	-	node	✓
Tree-Cycles	1	871	1950	2	-	node	✓
Mutag	4337	30.32	30.77	2	14	graph	
$Mutag_0$	2301	31.74	32.54	2	14	graph	✓
NCI1	4110	29.87	32.30	2	37	graph	
CiteSeer	1	3312	4732	6	3703	node	

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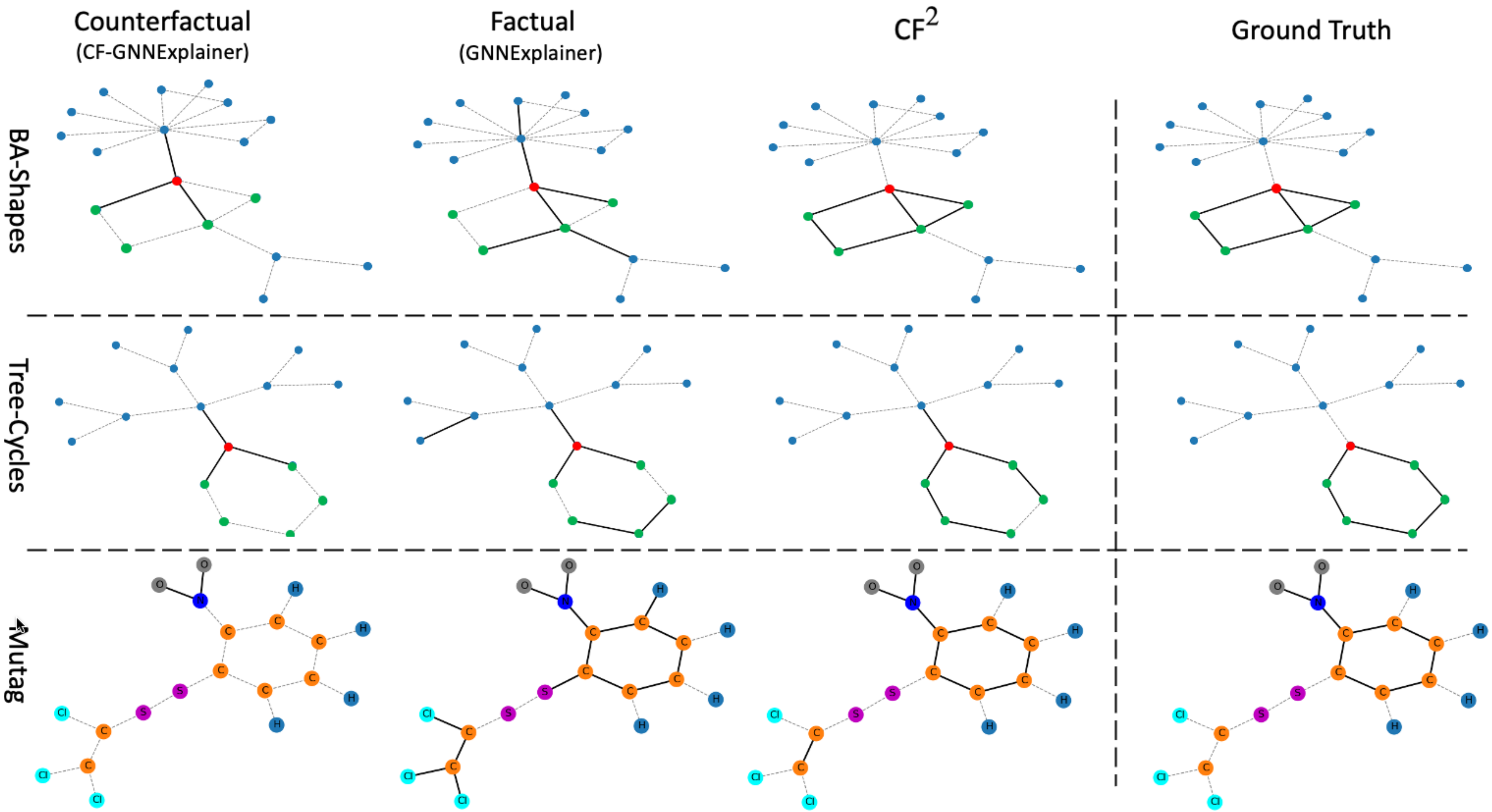
Qualitative Case Study



Evaluation with PN, PS

- This evaluation does not need ground-truth explanation

Models	BA-Shapes				Tree-Cycles				Mutag$_0$			
	PN%	PS%	F_{NS}%	#exp	PN%	PS%	F_{NS}%	#exp	PN%	PS%	F_{NS}%	#exp
GNNExplainer†	72.19	45.62	55.91	6.00	100.00	59.72	74.78	6.00	71.79	97.44	82.67	15.00
CF-GNNExplainer	75.34	41.10	53.18	5.79	100.00	31.94	48.42	3.44	96.26	7.48	13.88	7.72
Gem†	61.36	52.27	56.45	6.00	100.00	29.89	46.02	6.00	83.01	76.42	79.58	15.00
CF^2	76.73	68.22	**72.07**	6.21	100.00	81.94	**90.08**	5.81	97.44	100.00	**98.70**	14.95

Models	NCI1				CiteSeer (edge)				CiteSeer (feature)			
	PN%	PS%	F_{NS}%	#exp	PN%	PS%	F_{NS}%	#exp	PN%	PS%	F_{NS}%	#exp
GNNExplainer†	92.13	62.16	74.24	15.00	66.67	90.05	76.61	5.00	71.64	99.50	72.79	60.00
CF-GNNExplainer	97.14	31.43	47.49	7.75	69.50	82.00	75.23	2.58	72.14	92.54	81.07	72.91
Gem†	99.03	52.15	68.32	15.00	61.05	72.67	66.36	5.00	-	-	-	-
CF^2	100.00	63.81	**77.91**	17.70	71.00	94.50	**81.08**	3.18	74.63	95.02	**83.60**	62.73

Evaluate with Accuracy

- This evaluation needs ground-truth explanation

Models	BA-Shapes				Tree-Cycles				Mutag_0			
	Acc%	Pr%	Re%	F_1%	Acc%	Pr%	Re%	F_1%	Acc%	Pr%	Re%	F_1%
GNNExplainer†	95.25	60.08	60.08	60.08	92.78	68.06	68.06	68.06	96.96	59.71	85.17	68.85
CF-GNNExplainer	94.39	67.19	54.11	56.79	90.27	87.40	47.45	59.10	96.91	66.09	39.46	47.39
Gem†	**96.97**	64.16	64.16	64.16	89.88	57.23	57.23	57.23	96.43	63.12	47.11	54.68
CF^2	96.37	73.15	68.18	**66.61**	**93.26**	84.92	73.84	**75.69**	**97.34**	65.28	88.59	**72.56**

Kendall's τ and Spearman's ρ correlation between Accuracy and PN, PS

Models	BA-Shapes		Tree-Cycles		Mutag_0	
	$\tau\uparrow$	$\rho\uparrow$	$\tau\uparrow$	$\rho\uparrow$	$\tau\uparrow$	$\rho\uparrow$
F_{NS} & F_1	1.00	1.00	1.00	1.00	1.00	1.00
F_{NS} & Acc	0.66	0.79	1.00	1.00	0.66	0.79

$$Pr = \frac{TP}{TP+FP} \quad Re = \frac{TP}{TP+FN} \quad Acc = \frac{TP+TN}{ALL}$$

$$F_1 = \frac{2Pr \cdot Re}{Pr + Re} \quad F_{NS} = \frac{2PN \cdot PS}{PN + PS}$$

PN/PS-based evaluation is highly correlated with ground-truth-based evaluation.

We can use PN/PS to evaluate explanations when ground-truth is not available

Rutgers

ExplainableFold (KDD'23)

Understanding AlphaFold Prediction with Explainable AI

[6] J Tan and **Y Zhang**. "ExplainableFold: Understanding AlphaFold Prediction with Explainable AI." In KDD 2023.

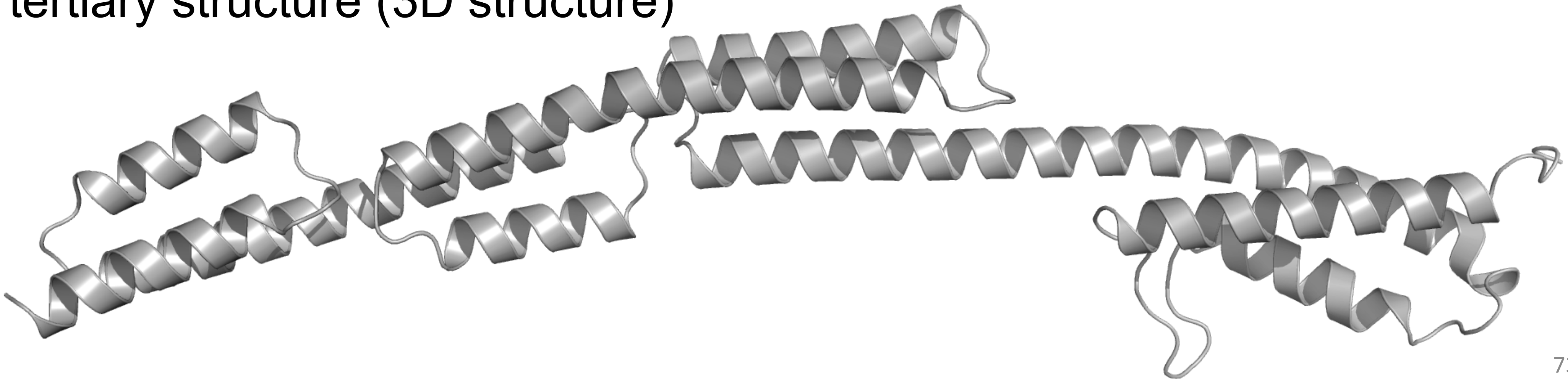
The Protein Folding Problem

From primary structure (amino acid sequence)

D Q E L G K Q S R R S Q D I I K S L …… D L T R G T K E D

Cryo-Electron Microscopy
(Cryo-EM)

To tertiary structure (3D structure)



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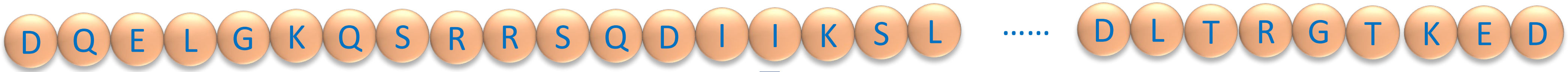
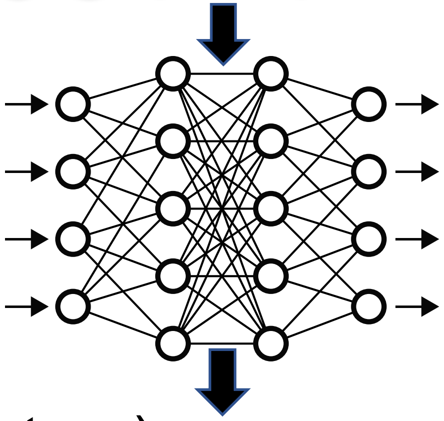
The Protein Folding Problem

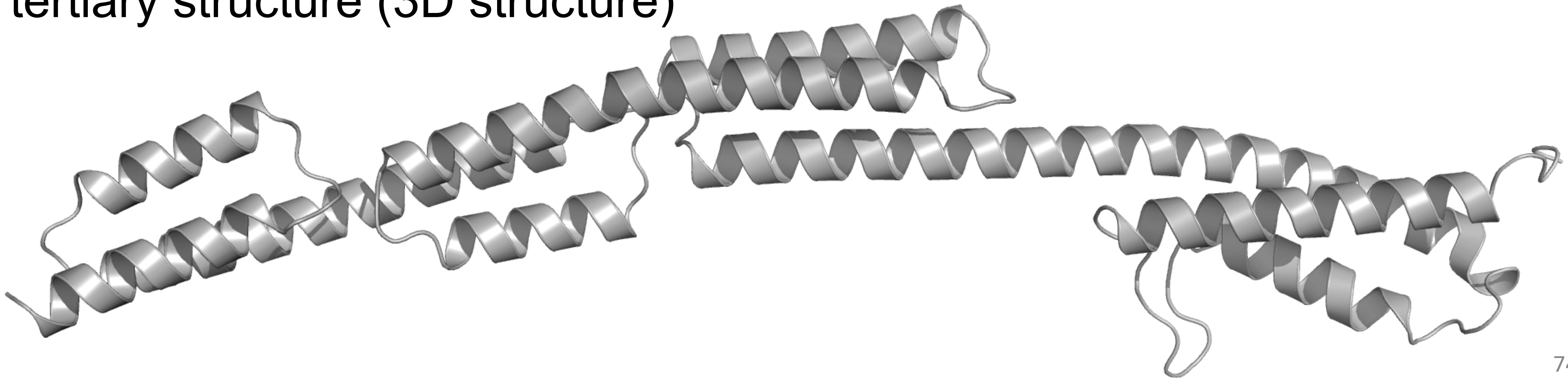
From primary structure (amino acid sequence)





AlphaFold revolutionizes Protein Structure Prediction

To tertiary structure (3D structure)



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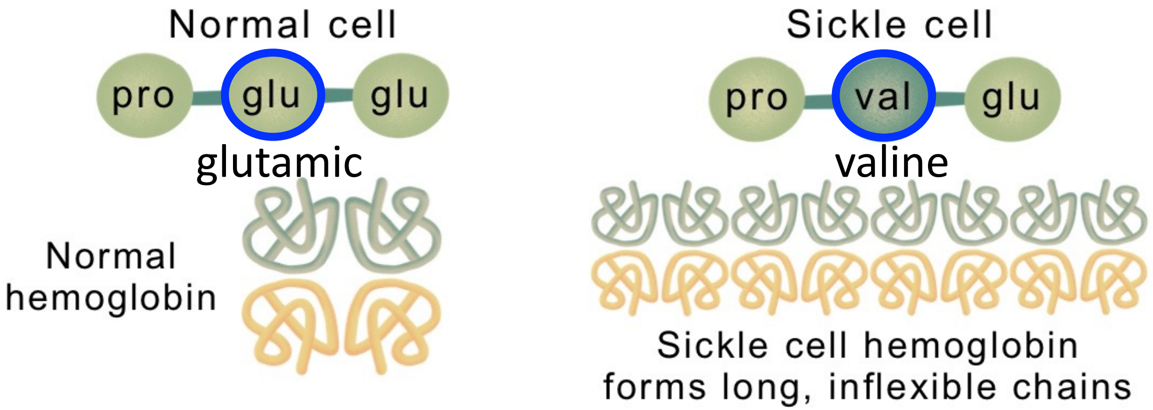
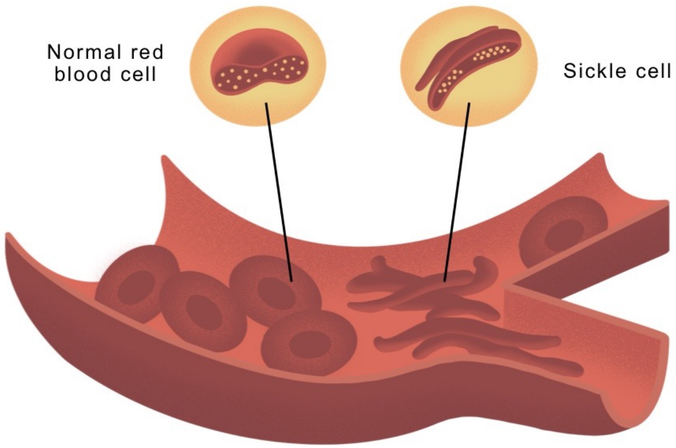
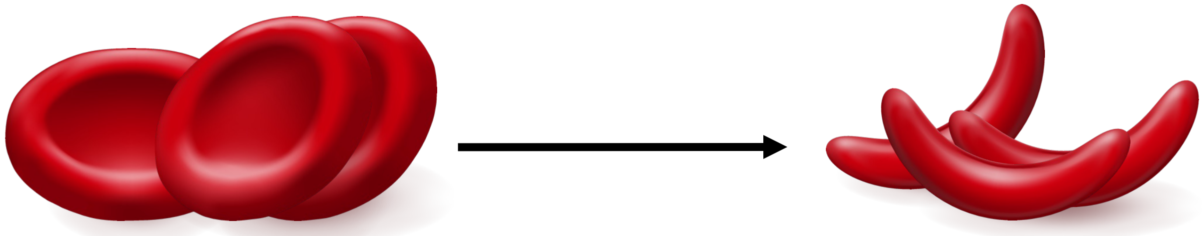
Science is not
only about understanding the “what” and “how”,
but also, and perhaps more importantly, the
“why”.

Explanation Provides Important Insights for Scientists

- Cause-effect explanation between amino-acid and protein structure
  - One single substitution in the HBB gene can significantly change the structure of hemoglobin, causing the sickle-cell anemia







Certain amino acids play significant roles in the protein folding process!

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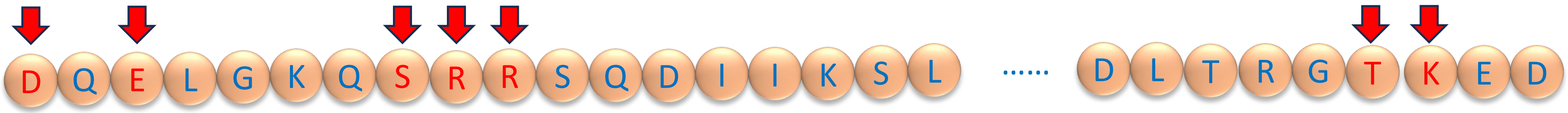
ExplainableFold Problem Definition

Identify the most crucial residues that cause the proteins to fold into the structures they are [6].



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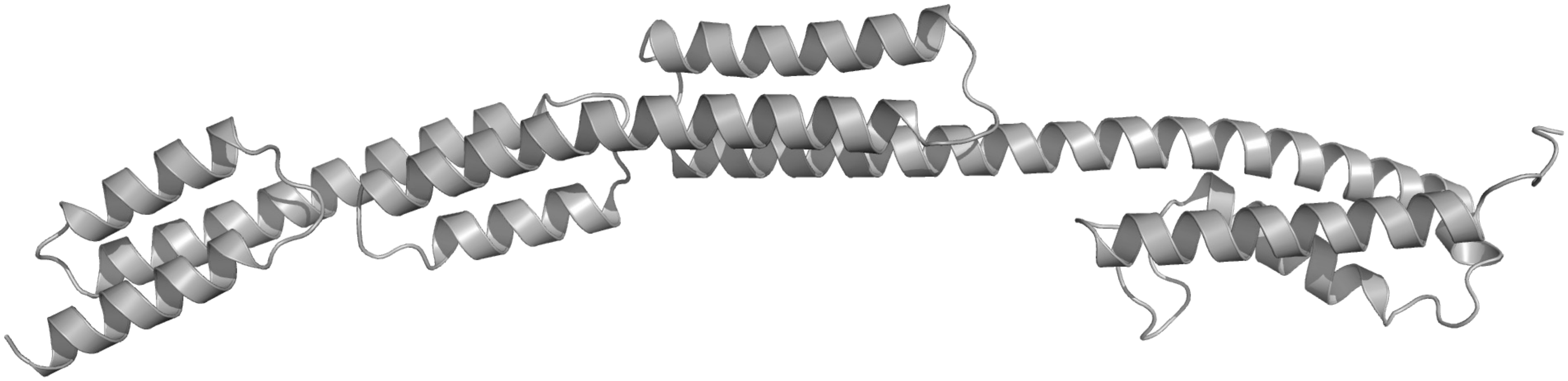
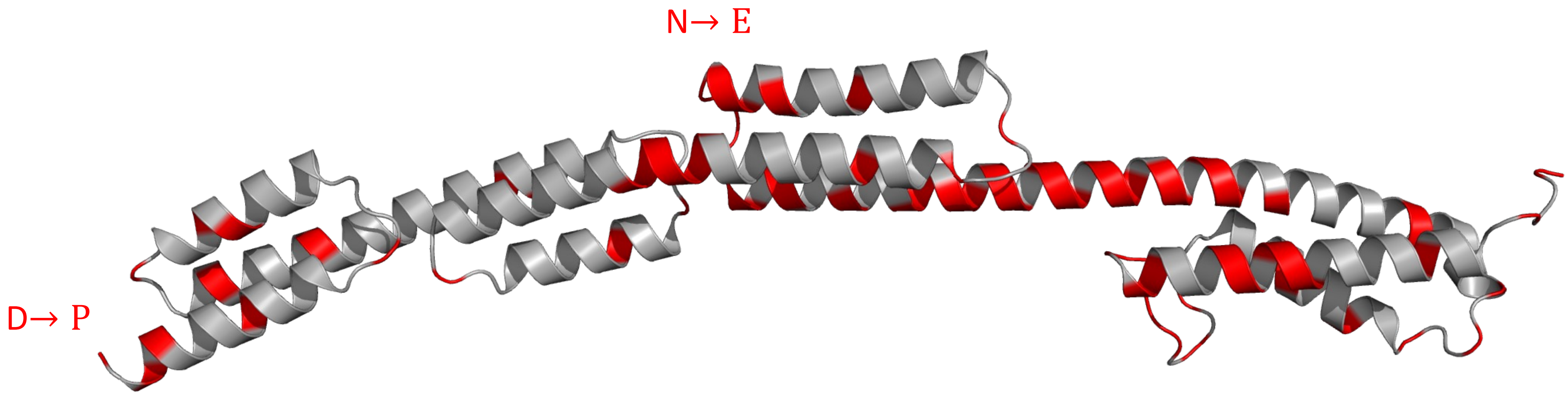
ExplainableFold Problem Definition



ExplainableFold Problem Definition



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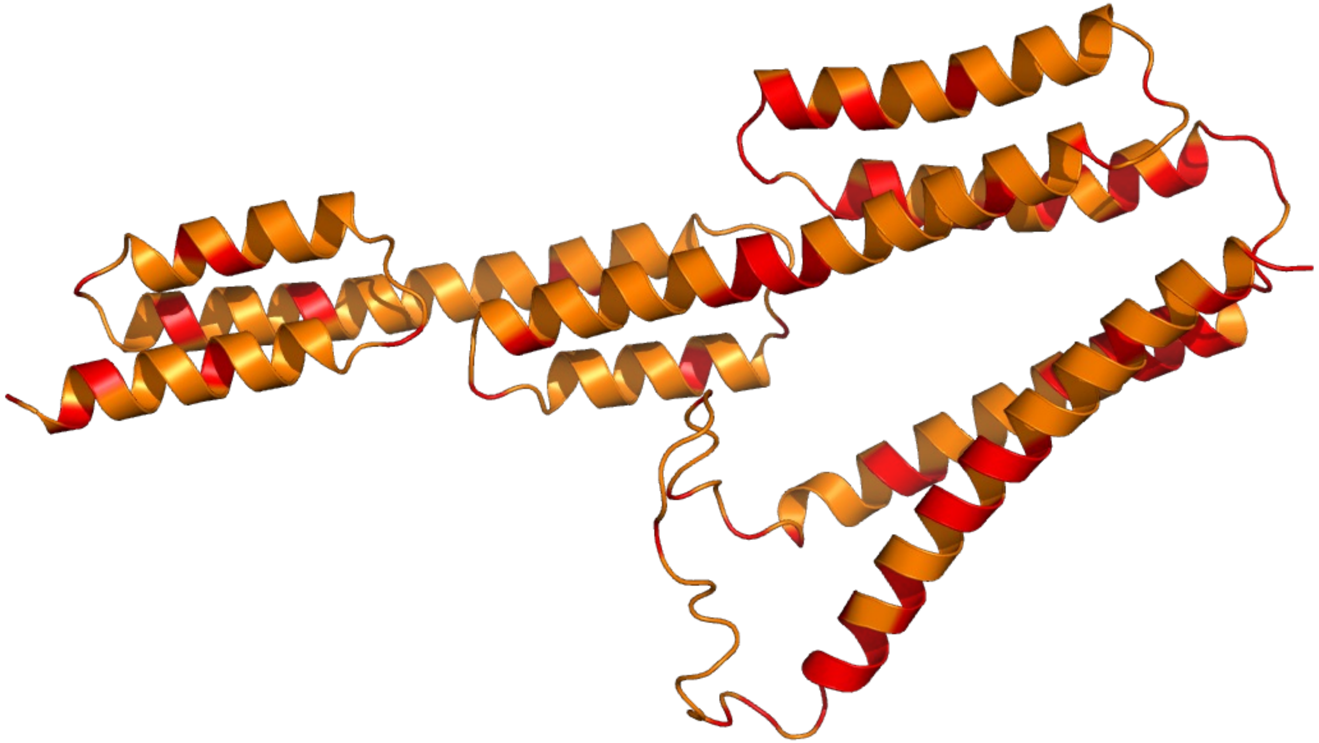
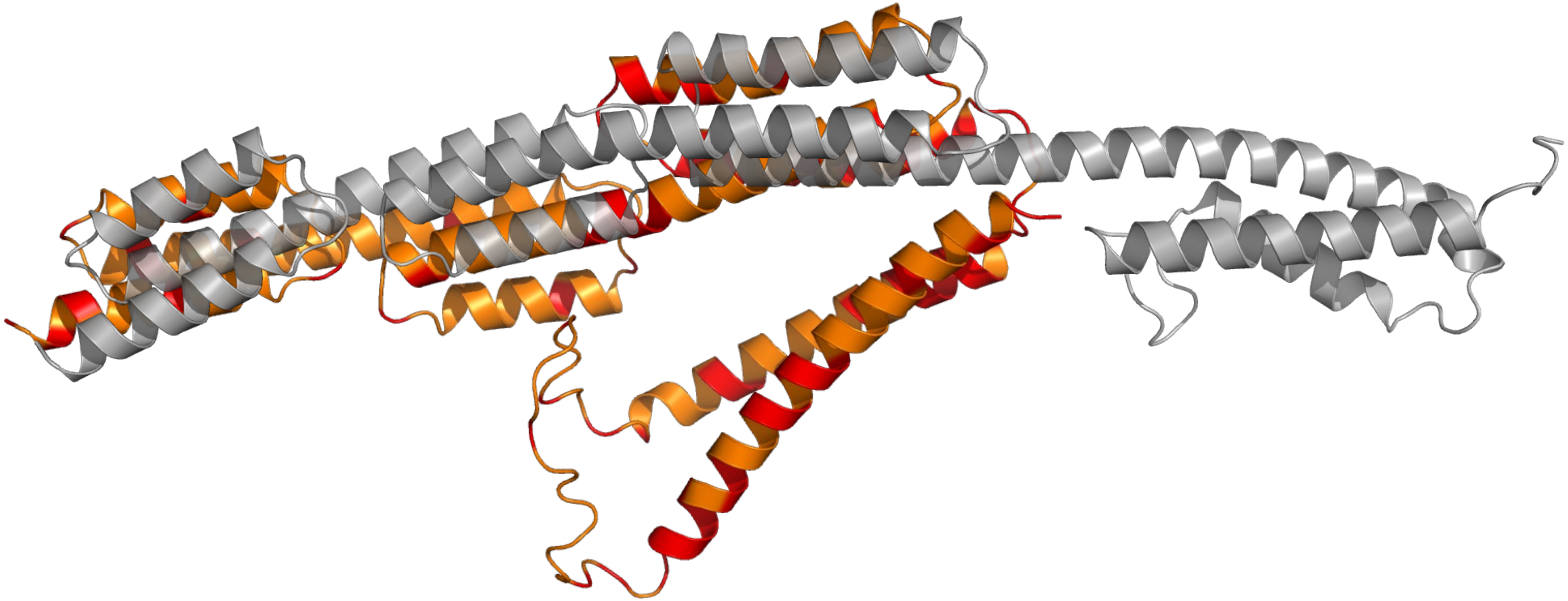
ExplainableFold Problem Definition



ExplainableFold Problem Definition

TM-score: 0.44 (TM<0.5 means different folding structure [7,8])

TM-score = Template Modeling score



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What are Good Explanations? Simple and Effective (again!)

Occam's Razor Principle for Explainable AI:
When trying to explain a phenomenon, if two explanations are equally effective, then we prefer the simpler one.

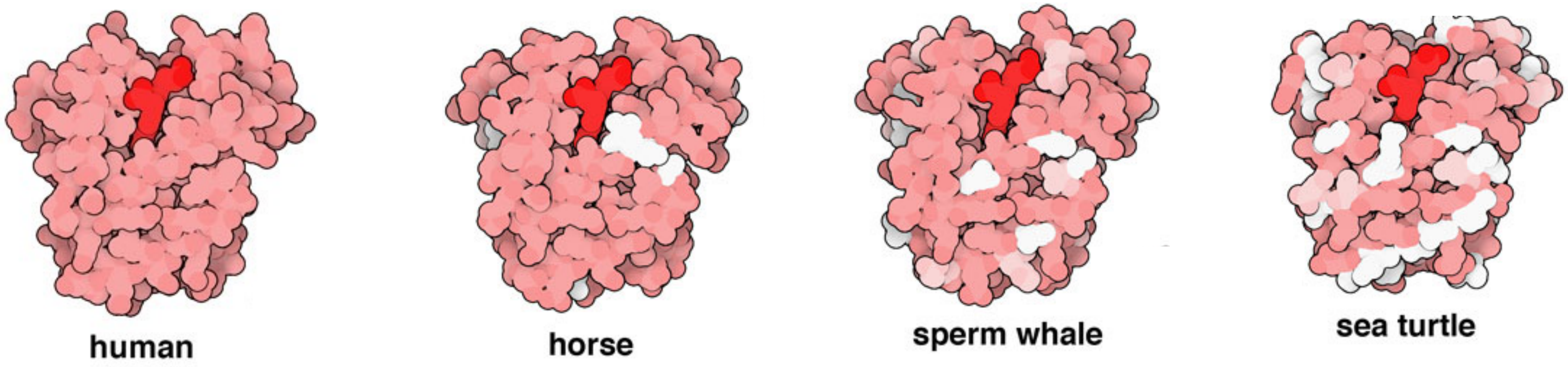
- For a target protein $\boldsymbol{P}$, $\boldsymbol{P} \in \{0,1\}^{21\times l}$, MSA $\boldsymbol{M}(\boldsymbol{P}) \in \{0,1\}^{m\times 21\times l}$
- We learn a counterfactual protein embedding $\boldsymbol{P}'$

$$\begin{aligned} &\text{minimize} \;\; \text{Explanation Complexity} \\ &\text{s.t.,} \;\; \text{Explanation is Strong Enough} \end{aligned} \Rightarrow \begin{aligned} &\text{minimize } ||\boldsymbol{P} - \boldsymbol{P}'||_0 && \text{Simple} \\ &\text{s.t. } \mathrm{TM}(\boldsymbol{S}, \boldsymbol{S}') \le 0.5, \;\; \boldsymbol{P}' \in \{0,1\}^{21\times l} && \text{Effective} \\ &\text{where } \boldsymbol{S}' = f_\theta\big(\boldsymbol{P}', \boldsymbol{M}(\boldsymbol{P}')\big) && \text{Blackbox (AlphaFold)} \end{aligned}$$

Evaluation

- CASP-14 Dataset (same as AlphaFold): 152 target proteins

	Ave Explanation Size ($\lvert\mathcal{E}\rvert$) ↓	Ave Complexity ($\lvert\mathcal{E}\rvert/l$) ↓	Ave TM-score $TM(S, S^*)$ ↓	PN score↑
Random	85.22	0.33	0.83	0.07
Evolutionary [40]	88.42	0.33	0.77	0.16
ExplainableFold	**83.33**	**0.31**	**0.59**	**0.40**



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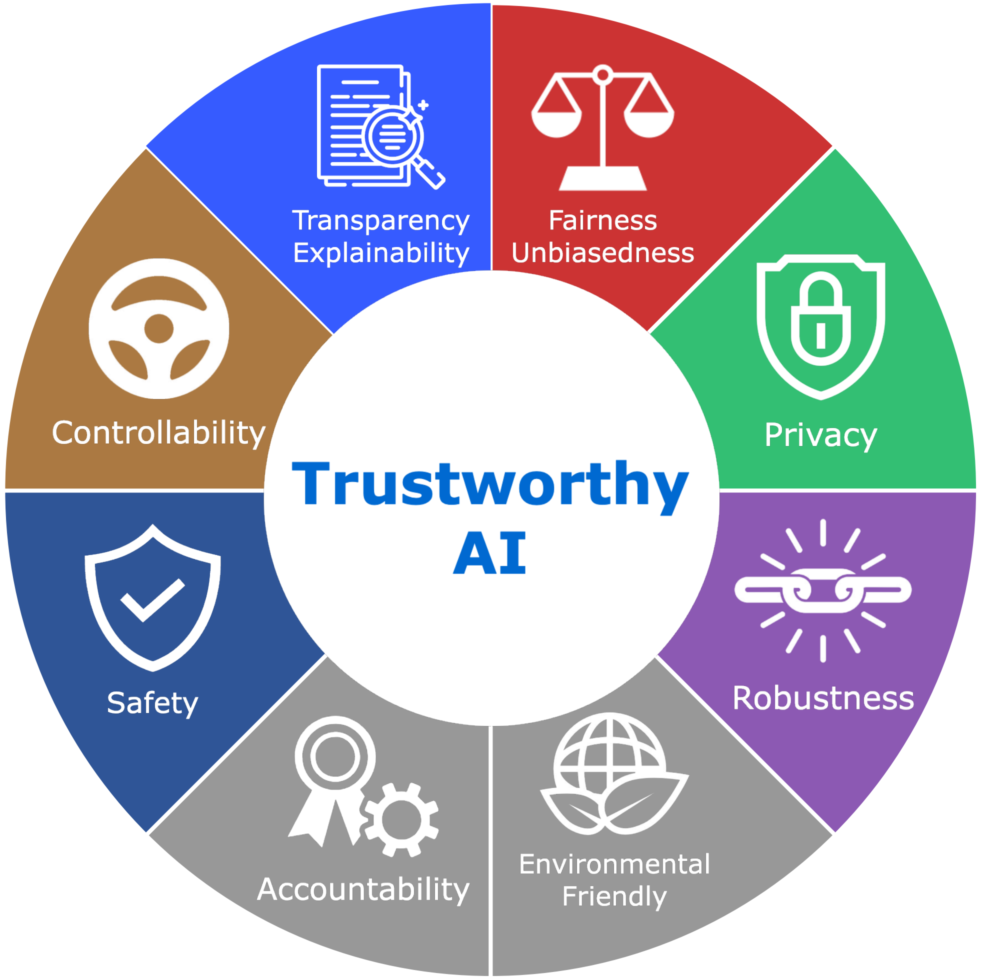
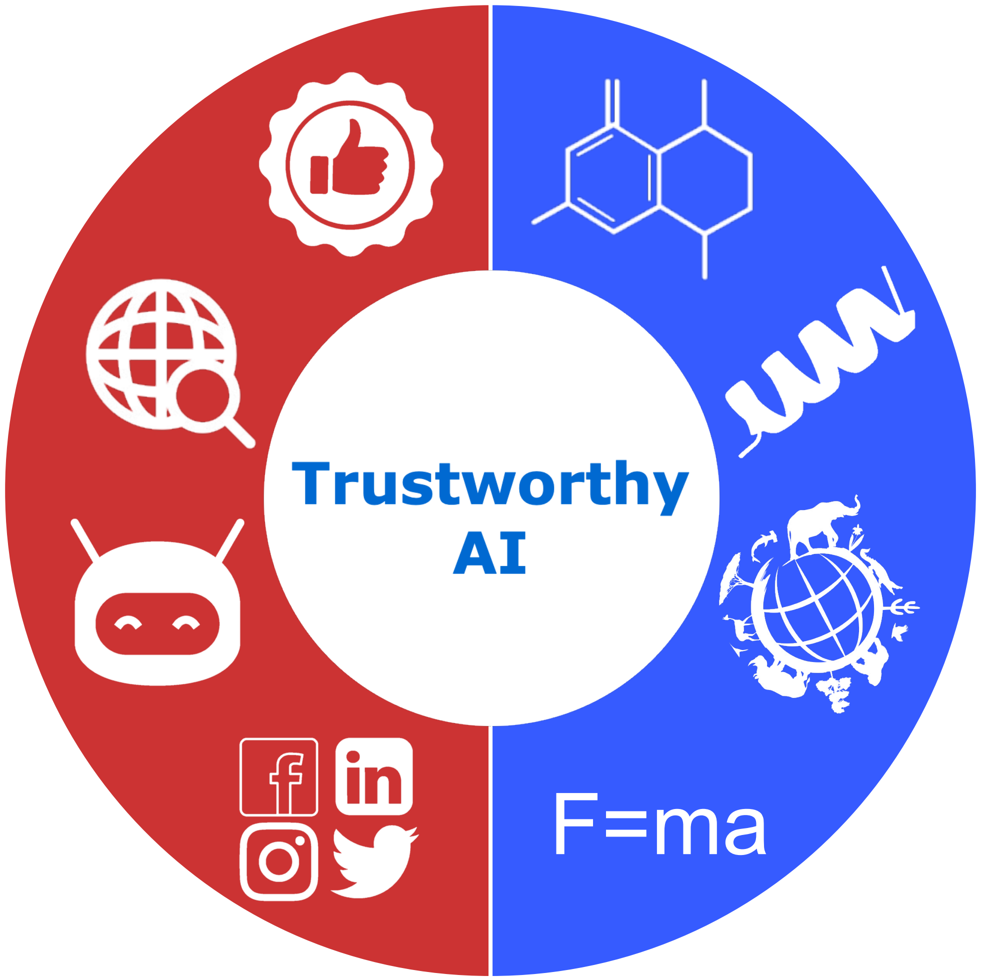
Summary



Methodology



Applications

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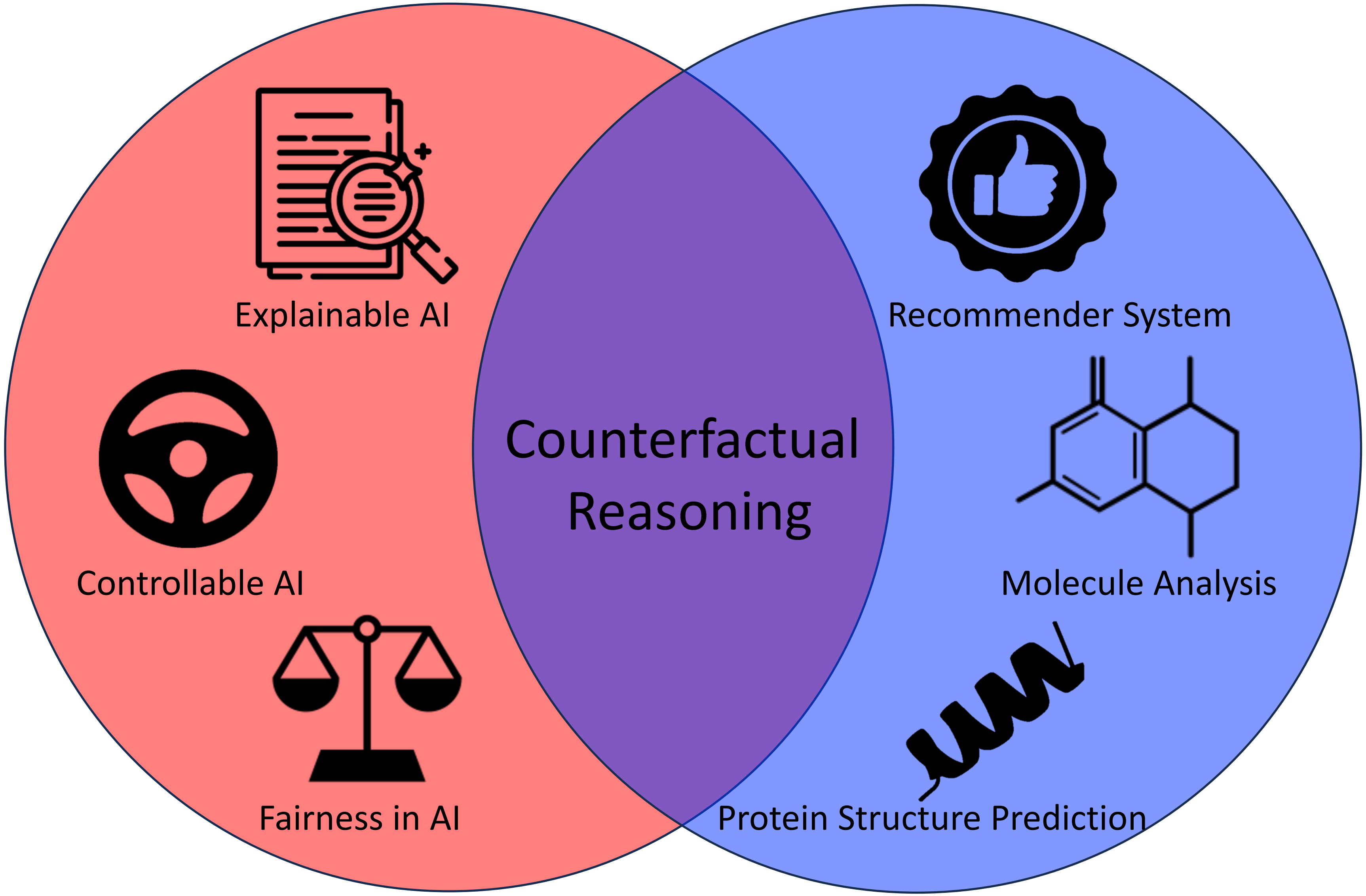
Summary



Multiple Trustworthy Perspectives **Multiple Application Domains**

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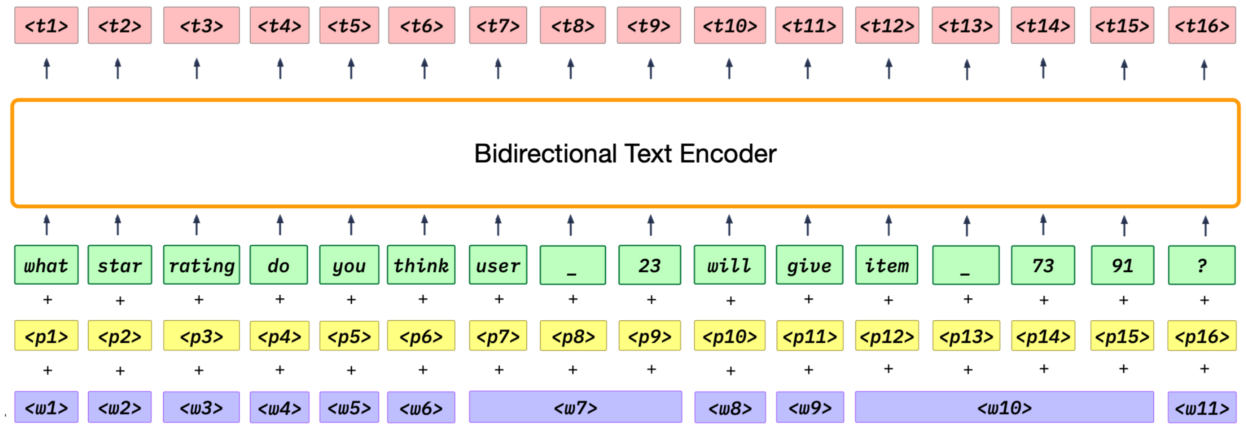
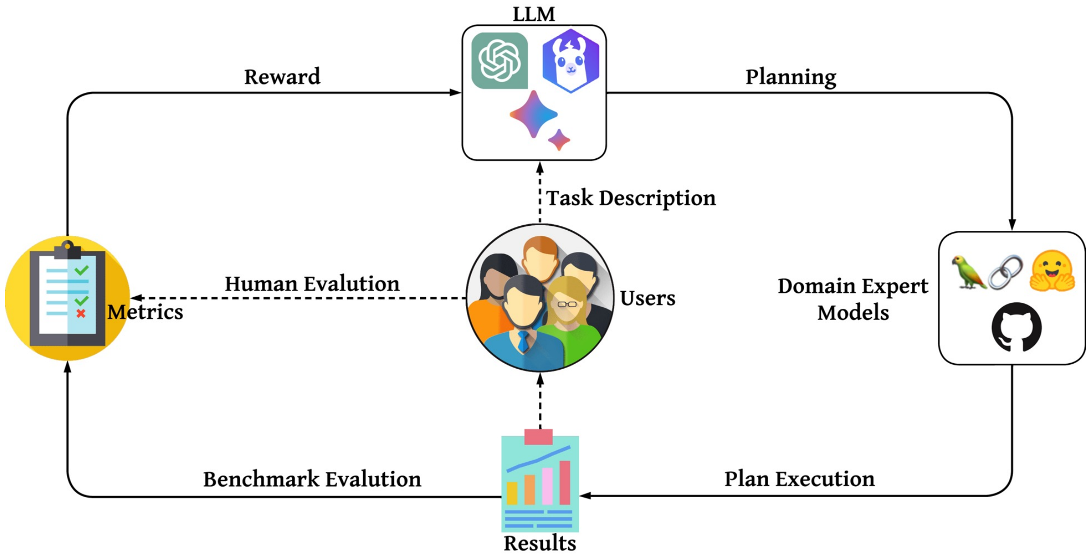
Future Research



Trustworthy Large Language Models (LLMs) [9]



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