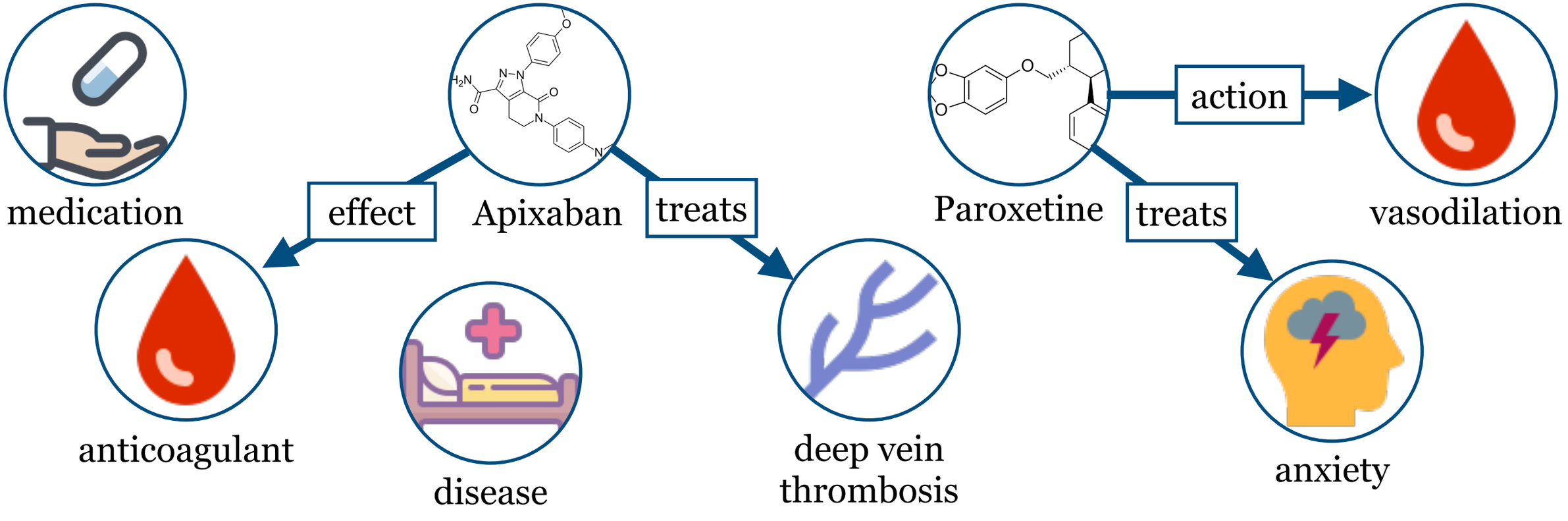
Complex Query Answering with Neural Link Predictors

Erik Arakelyan* Daniel Daza* **Pasquale Minervini*** Michael Cochez

ICLR 2021

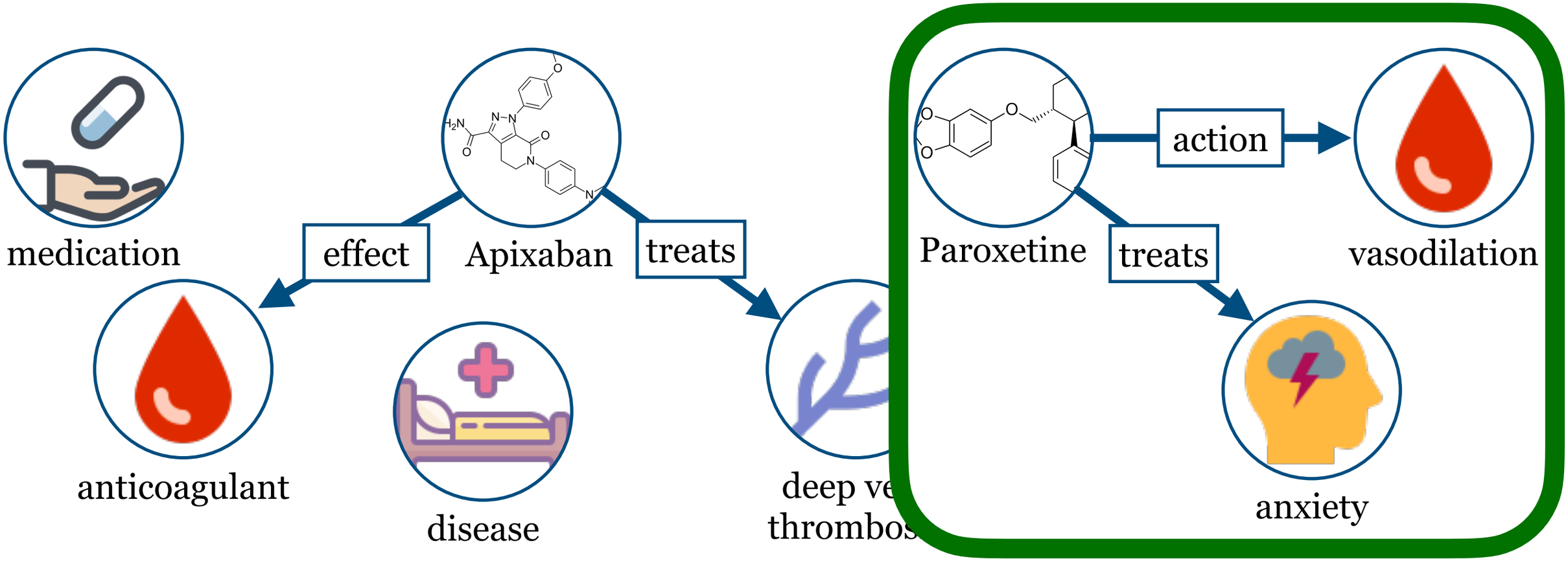
Knowledge Graphs

Knowledge Graph — graph-structured Knowledge Base, where knowledge about the world is encoded in the form of *relationships between entities*



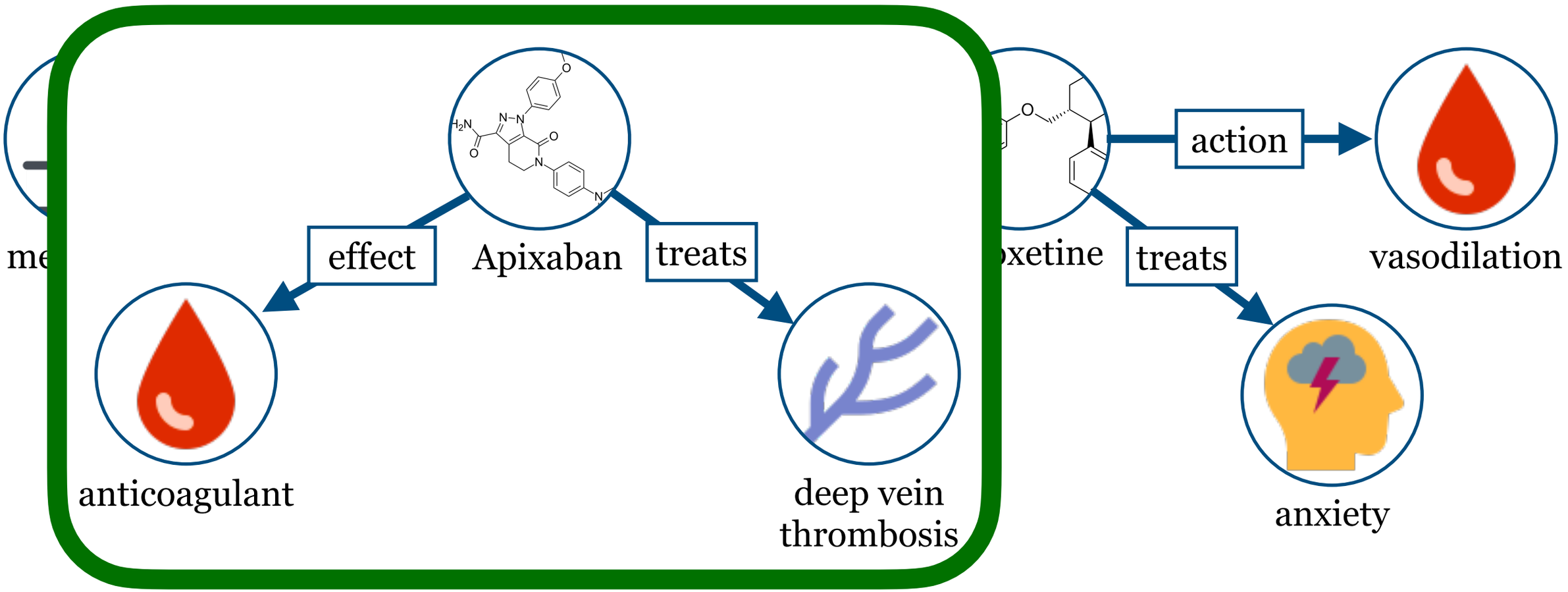
Knowledge Graphs

Knowledge Graph — graph-structured Knowledge Base, where knowledge about the world is encoded in the form of *relationships between entities*



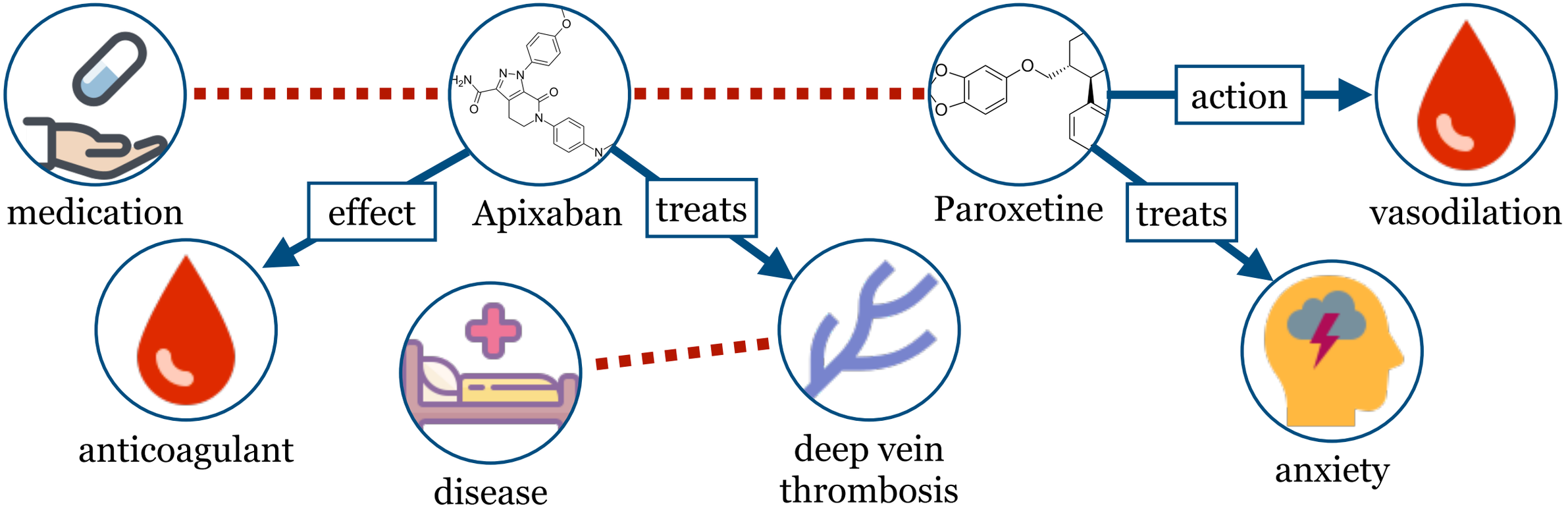
Knowledge Graphs

Knowledge Graph — graph-structured Knowledge Base, where knowledge about the world is encoded in the form of *relationships between entities*

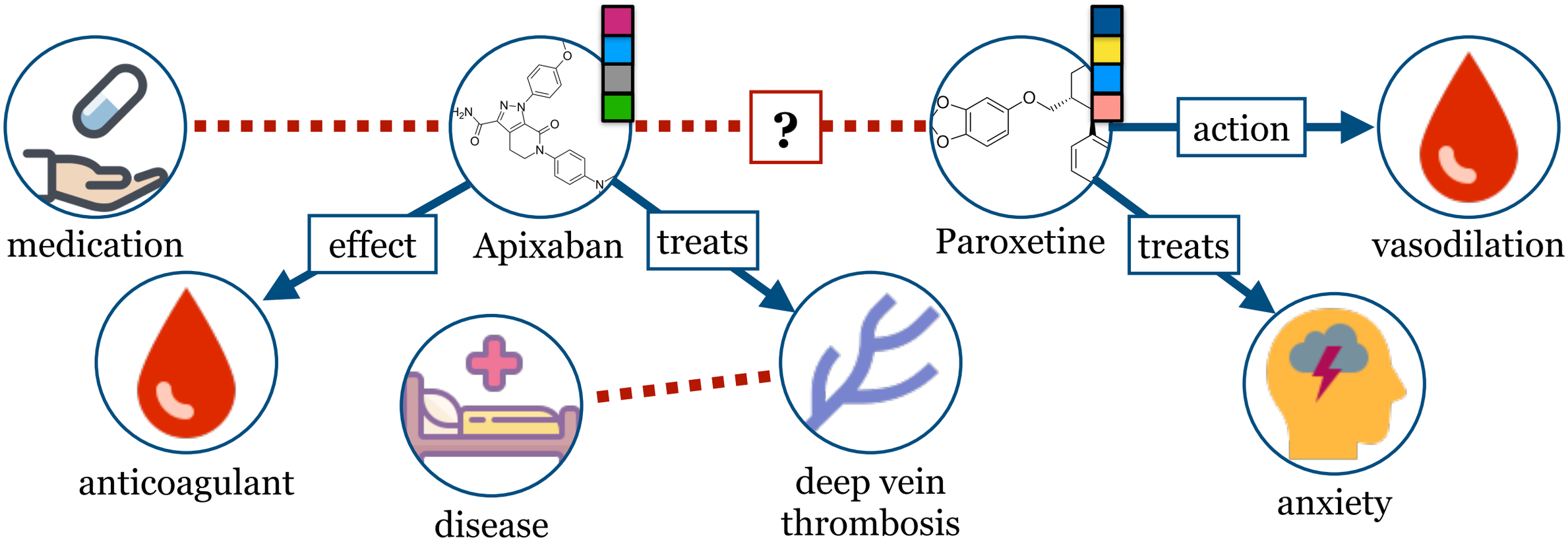


Knowledge Graphs

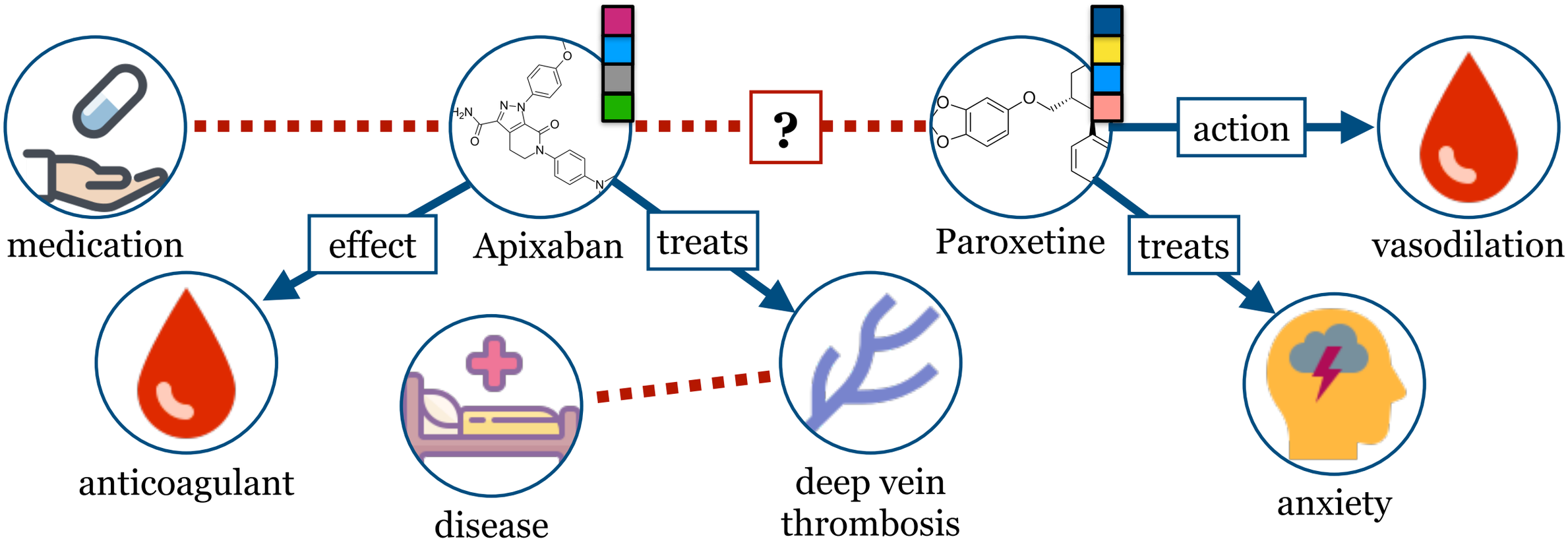
Knowledge Graph — graph-structured Knowledge Base, where knowledge about the world is encoded in the form of *relationships between entities*



Neural Link Prediction

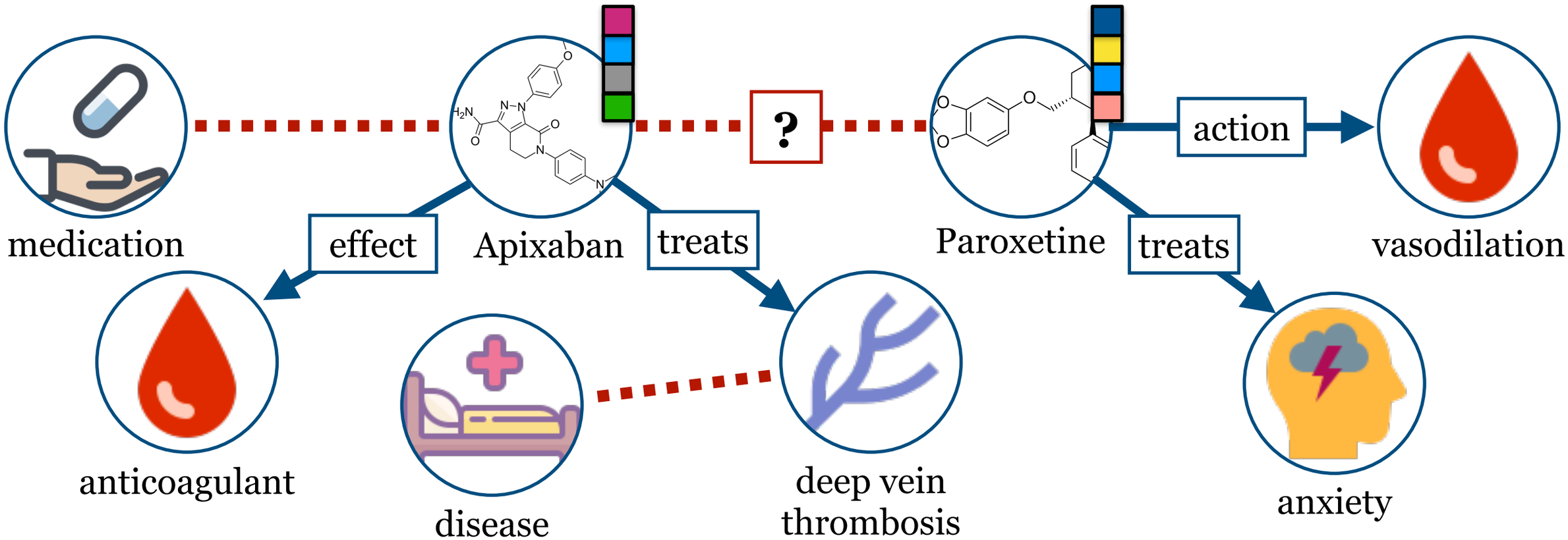


Neural Link Prediction



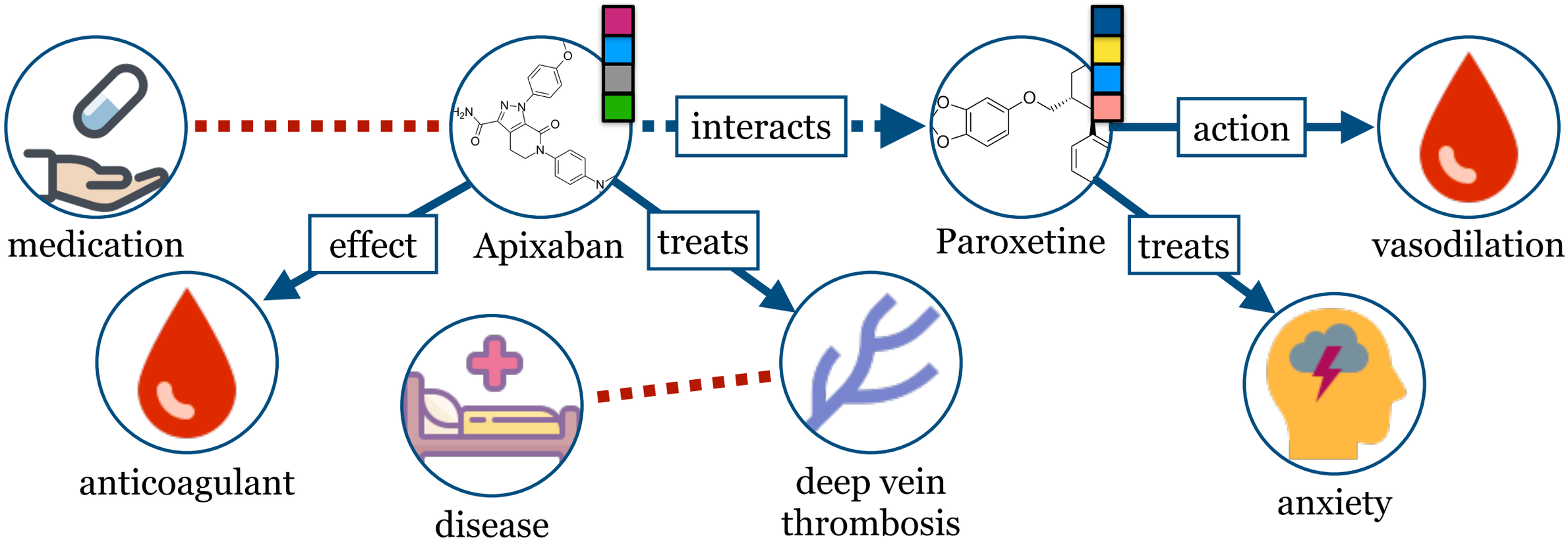
$$P(\text{Apixaban} \xrightarrow{\text{interacts}} \text{Paroxetine}) \propto$$

Neural Link Prediction



$$P(\text{Apixaban} \xrightarrow{\text{interacts}} \text{Paroxetine}) \propto \phi_{\text{interacts}}\left(\text{Apixaban}, \text{Paroxetine} \right)$$

Neural Link Prediction



$$P(\text{Apixaban} \xrightarrow{\text{interacts}} \text{Paroxetine}) \propto \phi_{\text{interacts}}\left(\text{Apixaban}, \text{Paroxetine} \right)$$

Complex Queries on Incomplete Graphs

Query: Which medications have side-effects when taken with drugs for treating Anxiety?

Complex Queries on Incomplete Graphs

Query: Which medications have side-effects when taken with drugs for treating Anxiety?

$$?M$$

Complex Queries on Incomplete Graphs

Query: Which medications have side-effects when taken with drugs for treating Anxiety?

$$?M : \exists D$$

Complex Queries on Incomplete Graphs

Query: Which medications have side-effects when taken with drugs for treating Anxiety?

$$?M : \exists D \,.\, \text{interacts}\,(M, D)$$

Complex Queries on Incomplete Graphs

Query: Which medications have side-effects when taken with drugs for treating Anxiety?

$$?M : \exists D \,.\, \text{interacts}\,(M, D) \wedge \text{treats}\,\big(D, \text{anxiety}\big)$$

Complex Queries on Incomplete Graphs

Query: Which medications have side-effects when taken with drugs for treating Anxiety?

$$?M : \exists D \,.\, \text{interacts}\,(M, D) \wedge \text{treats}\,\big(D, \text{anxiety}\big)$$

BetaE — Ren et al. [ICLR 2020]

Q2B — Ren et al. [NeurIPS 2020]

GQE — Hamilton et al. [NeurIPS 2018]

Process

Complex Queries on Incomplete Graphs

Query: Which medications have side-effects when taken with drugs for treating Anxiety?

$$?M : \exists D \,.\, \text{interacts}\,(M, D) \wedge \text{treats}\,\big(D, \text{anxiety}\big)$$

BetaE — Ren et al. [ICLR 2020]

Q2B — Ren et al. [NeurIPS 2020]

GQE — Hamilton et al. [NeurIPS 2018]

Process

1. Generate *millions* of complex query-answer pairs

Complex Queries on Incomplete Graphs

Query: Which medications have side-effects when taken with drugs for treating Anxiety?

$$?M : \exists D \,.\, \text{interacts}\,(M, D) \wedge \text{treats}\,\big(D, \text{anxiety}\big)$$

BetaE — Ren et al. [ICLR 2020]

Q2B — Ren et al. [NeurIPS 2020]

GQE — Hamilton et al. [NeurIPS 2018]

Process

1. Generate *millions* of complex query-answer pairs
2. Train a deep neural model to answer complex queries

Complex Queries on Incomplete Graphs

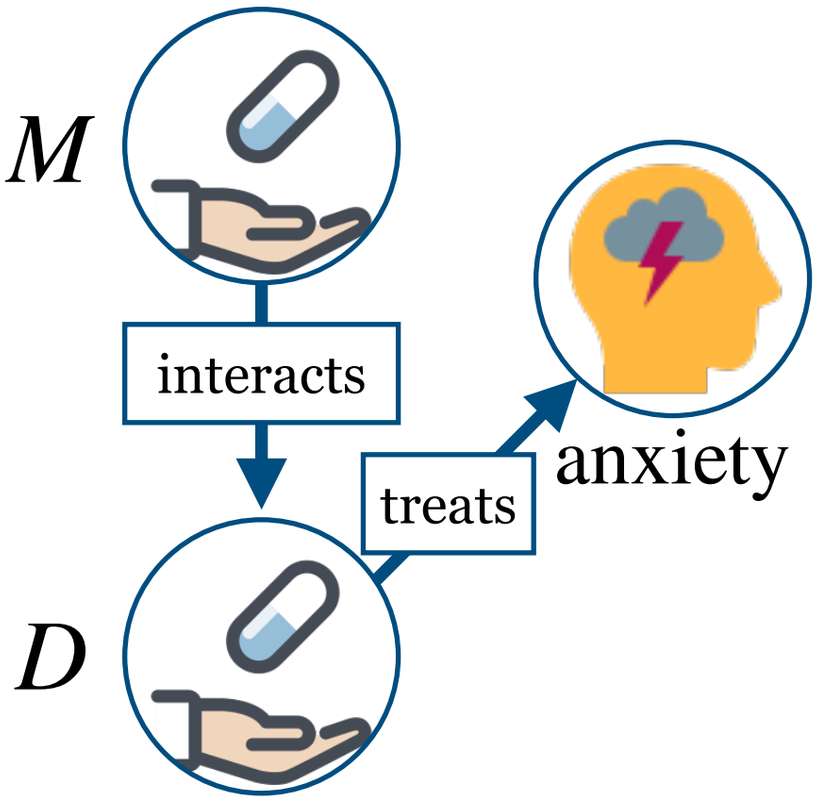
Query: Which medications have side-effects when taken with drugs for treating Anxiety?

$$?M : \exists D \,.\, \text{interacts}\,(M, D) \wedge \text{treats}\,\big(D, \text{anxiety}\big)$$

BetaE — Ren et al. [ICLR 2020]

Q2B — Ren et al. [NeurIPS 2020]

GQE — Hamilton et al. [NeurIPS 2018]



Complex Queries on Incomplete Graphs

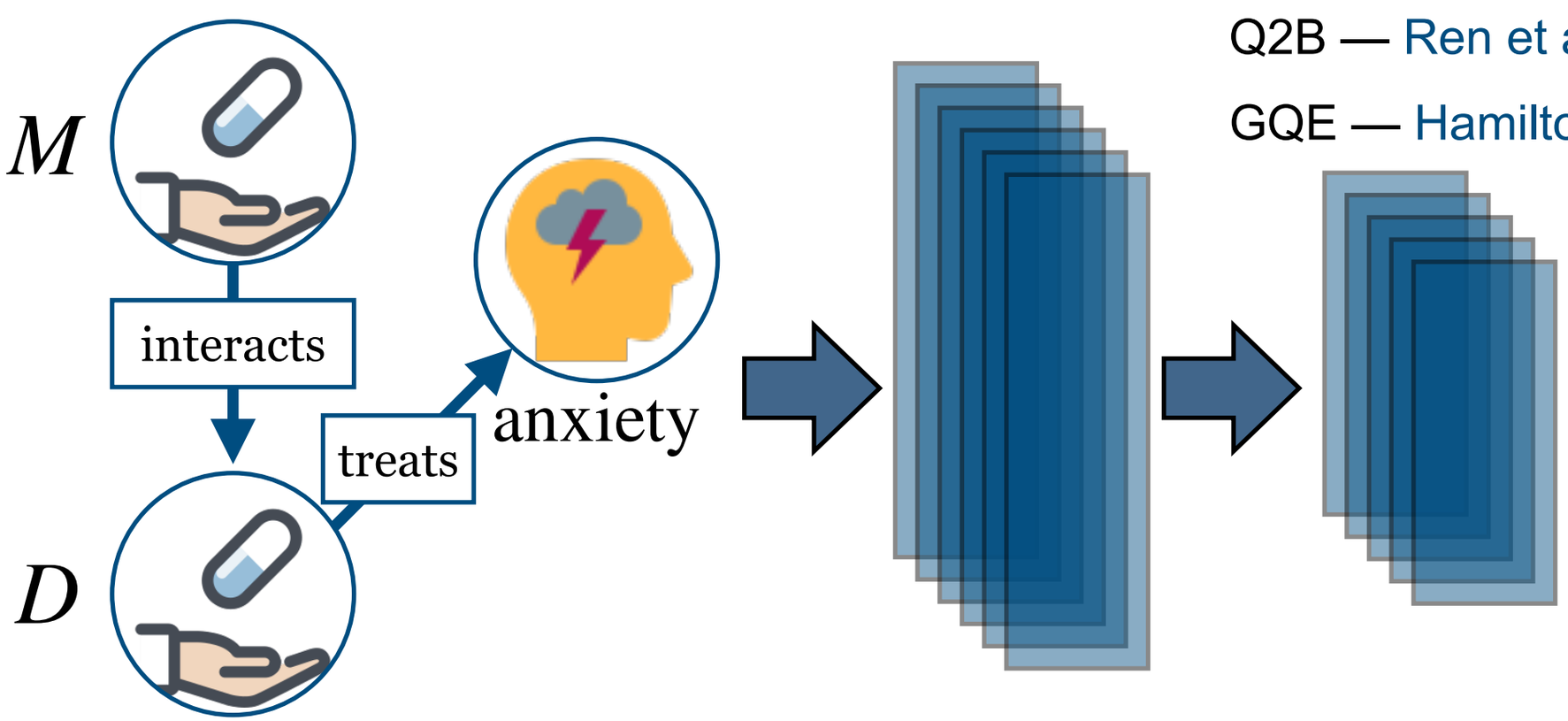
Query: Which medications have side-effects when taken with drugs for treating Anxiety?

$$?M : \exists D \,.\, \text{interacts}\,(M, D) \wedge \text{treats}\,\big(D, \text{anxiety}\big)$$

BetaE — Ren et al. [ICLR 2020]

Q2B — Ren et al. [NeurIPS 2020]

GQE — Hamilton et al. [NeurIPS 2018]



Complex Queries on Incomplete Graphs

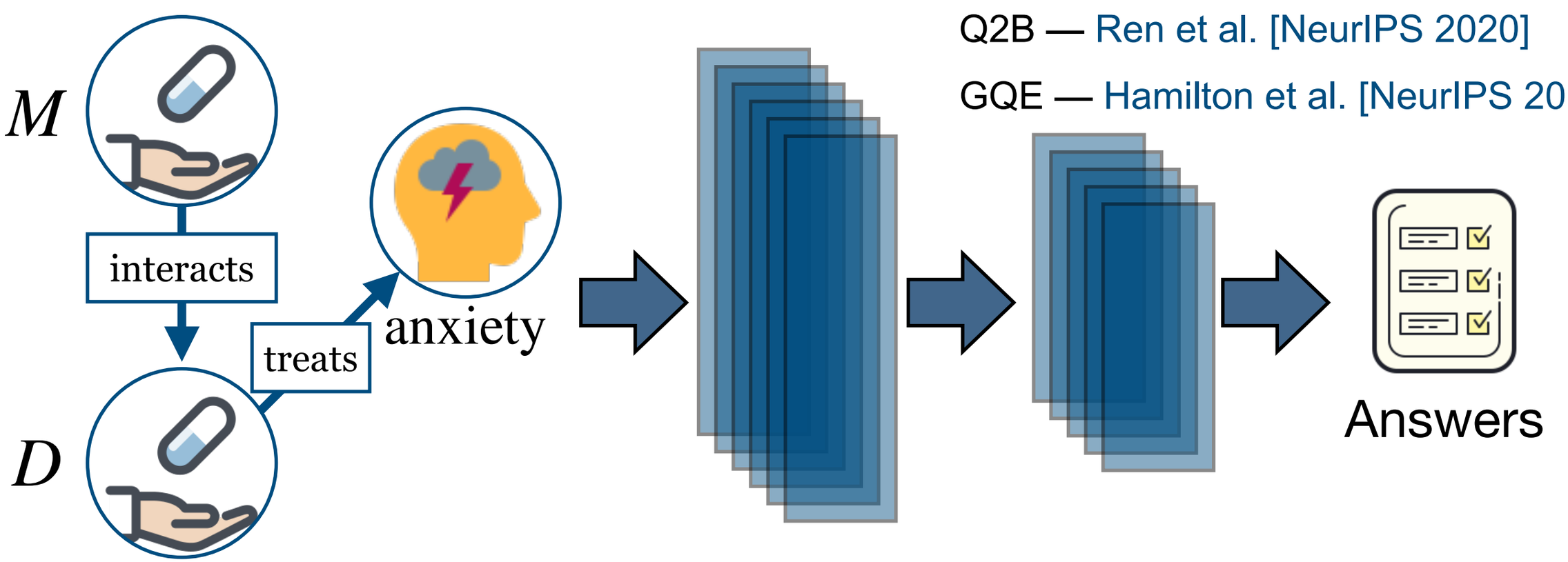
Query: Which medications have side-effects when taken with drugs for treating Anxiety?

$$?M : \exists D \,.\, \text{interacts}\,(M, D) \wedge \text{treats}\,\big(D, \text{anxiety}\big)$$

BetaE — Ren et al. [ICLR 2020]

Q2B — Ren et al. [NeurIPS 2020]

GQE — Hamilton et al. [NeurIPS 2018]



Complex Queries on Incomplete Graphs

Query: Which medications have side-effects when taken with drugs for treating Anxiety?

$$?M : \exists D \,.\, \text{interacts}\,(M, D) \wedge \text{treats}\,\big(D, \text{anxiety}\big)$$

BetaE — Ren et al. [ICLR 2020]

Problems

Complex Queries on Incomplete Graphs

Query: Which medications have side-effects when taken with drugs for treating Anxiety?

$$?M : \exists D \,.\, \text{interacts}\,(M, D) \wedge \text{treats}\,\big(D, \text{anxiety}\big)$$

BetaE — Ren et al. [ICLR 2020]

Problems

- Need to train the model on *millions* of generated queries — not clear what happens when evaluating on queries outside of training distribution

Complex Queries on Incomplete Graphs

Query: Which medications have side-effects when taken with drugs for treating Anxiety?

$$?M : \exists D \,.\, \text{interacts}\,(M, D) \wedge \text{treats}\,\big(D, \text{anxiety}\big)$$

BetaE — Ren et al. [ICLR 2020]

Problems

- Need to train the model on *millions* of generated queries — not clear what happens when evaluating on queries outside of training distribution
- No explanation on the reasons *why* a given answer was produced by the model

Query Answering as Optimisation

Proposed solution: train a neural model ϕ for answering atomic (simple) queries (e.g. “which drugs treat Anxiety?”), and cast the query answering task as an *optimisation problem*

$$?M : \exists D \,.\, \text{interacts}\,(M, D) \wedge \text{treats}\,\left(D, \text{anxiety}\right)$$

Query Answering as Optimisation

Proposed solution: train a neural model ϕ for answering atomic (simple) queries (e.g. “which drugs treat Anxiety?”), and cast the query answering task as an *optimisation problem*

$$?M : \exists D \,.\, \text{interacts}(M, D) \wedge \text{treats}\left(D, \text{anxiety}\right)$$

Optimisation problem

$$\arg\max_{M,D \in \mathscr{E}}$$

Query Answering as Optimisation

Proposed solution: train a neural model ϕ for answering atomic (simple) queries (e.g. “which drugs treat Anxiety?”), and cast the query answering task as an *optimisation problem*

$$?M : \exists D \,.\, \text{interacts}\,(M, D) \wedge \text{treats}\,\left(D, \text{anxiety}\right)$$

Optimisation problem

$$\arg\max_{M,D \in \mathcal{E}} \left[\phi_{\text{interacts}}\left(\mathbf{e}_M, \mathbf{e}_D\right) \quad \phi_{\text{treats}}\left(\mathbf{e}_D, \mathbf{e}_{\text{anxiety}}\right) \right]$$

Likelihood that M interacts with D

Likelihood that D treats anxiety

Query Answering as Optimisation

Proposed solution: train a neural model ϕ for answering atomic (simple) queries (e.g. “which drugs treat Anxiety?”), and cast the query answering task as an *optimisation problem*

$$?M : \exists D \,.\, \text{interacts}(M, D) \wedge \text{treats}\left(D, \text{anxiety}\right)$$

Optimisation problem

Continuous relaxation of the logical AND (**t-norm**)

$$\arg\max_{M,D \in \mathcal{E}} \left[\phi_{\text{interacts}}\left(\mathbf{e}_M, \mathbf{e}_D\right) \top \phi_{\text{treats}}\left(\mathbf{e}_D, \mathbf{e}_{\text{anxiety}}\right) \right]$$

Likelihood that M interacts with D

Likelihood that D treats anxiety

Query Answering as Optimisation

$$\arg \max_{M,D \in \mathcal{E}} \left[\phi_{\text{interacts}} \left(\mathbf{e}_M, \mathbf{e}_D \right) \top \phi_{\text{treats}} \left(\mathbf{e}_D, \mathbf{e}_{\text{anxiety}} \right) \right]$$

Query Answering as Optimisation

$$\arg \max_{M,D \in \mathcal{E}} \left[\phi_{\text{interacts}} \left(\mathbf{e}_M, \mathbf{e}_D \right) \top \phi_{\text{treats}} \left(\mathbf{e}_D, \mathbf{e}_{\text{anxiety}} \right) \right]$$

Greedy Search

Query Answering as Optimisation

$$\arg \max_{M,D \in \mathscr{E}} \left[\phi_{\text{interacts}}\left(\mathbf{e}_M, \mathbf{e}_D\right) \top \phi_{\text{treats}}\left(\mathbf{e}_D, \mathbf{e}_{\text{anxiety}}\right) \right]$$

Greedy Search

- Identify the k most likely values for D

Query Answering as Optimisation

$$\arg \max_{M,D \in \mathscr{E}} \left[\phi_{\text{interacts}}\left(\mathbf{e}_M, \mathbf{e}_D\right) \top \phi_{\text{treats}}\left(\mathbf{e}_D, \mathbf{e}_{\text{anxiety}}\right) \right]$$

Greedy Search

- Identify the k most likely values for D
- For each value of D:

Query Answering as Optimisation

$$\arg \max_{M,D \in \mathcal{E}} \left[\phi_{\text{interacts}}\left(\mathbf{e}_M, \mathbf{e}_D\right) \top \phi_{\text{treats}}\left(\mathbf{e}_D, \mathbf{e}_{\text{anxiety}}\right) \right]$$

Greedy Search

- Identify the k most likely values for D
- For each value of D:
  - Identify the k most likely values for M

Query Answering as Optimisation

$$\arg\max_{M,D \in \mathcal{E}} \left[\phi_{\text{interacts}}\left(\mathbf{e}_M, \mathbf{e}_D\right) \top \phi_{\text{treats}}\left(\mathbf{e}_D, \mathbf{e}_{\text{anxiety}}\right) \right]$$

Greedy Search

- Identify the k most likely values for D
- For each value of D:
  - Identify the k most likely values for M
- Compute the query score for all (M, D) combinations

Query Answering as Optimisation

$$\arg\max_{M,D \in \mathcal{E}} \left[\phi_{\text{interacts}}\left(\mathbf{e}_M, \mathbf{e}_D\right) \top \phi_{\text{treats}}\left(\mathbf{e}_D, \mathbf{e}_{\text{anxiety}}\right) \right]$$

Greedy Search

- Identify the k most likely values for D
- For each value of D:
  - Identify the k most likely values for M
- Compute the query score for all (M, D) combinations
- Return the most likely value for (M, D)

Query Answering as Optimisation

$$\arg \max_{\mathbf{e}_M, \mathbf{e}_D \in \mathbb{R}^k} \left[\phi_{\text{interacts}}\left(\mathbf{e}_M, \mathbf{e}_D\right) \top \phi_{\text{treats}}\left(\mathbf{e}_D, \mathbf{e}_{\text{anxiety}}\right) \right]$$

Query Answering as Optimisation

$$\arg \max_{\mathbf{e}_M, \mathbf{e}_D \in \mathbb{R}^k} \left[\phi_{\text{interacts}}(\mathbf{e}_M, \mathbf{e}_D) \top \phi_{\text{treats}}(\mathbf{e}_D, \mathbf{e}_{\text{anxiety}}) \right]$$

Gradient-Based Search

Query Answering as Optimisation

$$\arg \max_{\mathbf{e}_M, \mathbf{e}_D \in \mathbb{R}^k} \left[\phi_{\text{interacts}}(\mathbf{e}_M, \mathbf{e}_D) \top \phi_{\text{treats}}(\mathbf{e}_D, \mathbf{e}_{\text{anxiety}}) \right]$$

Gradient-Based Search

- Initialise $\mathbf{e}_M$ and $\mathbf{e}_D$ randomly

Query Answering as Optimisation

$$\arg \max_{\mathbf{e}_M, \mathbf{e}_D \in \mathbb{R}^k} \left[\phi_{\text{interacts}}\left(\mathbf{e}_M, \mathbf{e}_D\right) \top \phi_{\text{treats}}\left(\mathbf{e}_D, \mathbf{e}_{\text{anxiety}}\right) \right]$$

Gradient-Based Search

- Initialise $\mathbf{e}_M$ and $\mathbf{e}_D$ randomly
- Optimise $\mathbf{e}_M$ and $\mathbf{e}_D$ via Gradient Ascent to maximise the score of the query

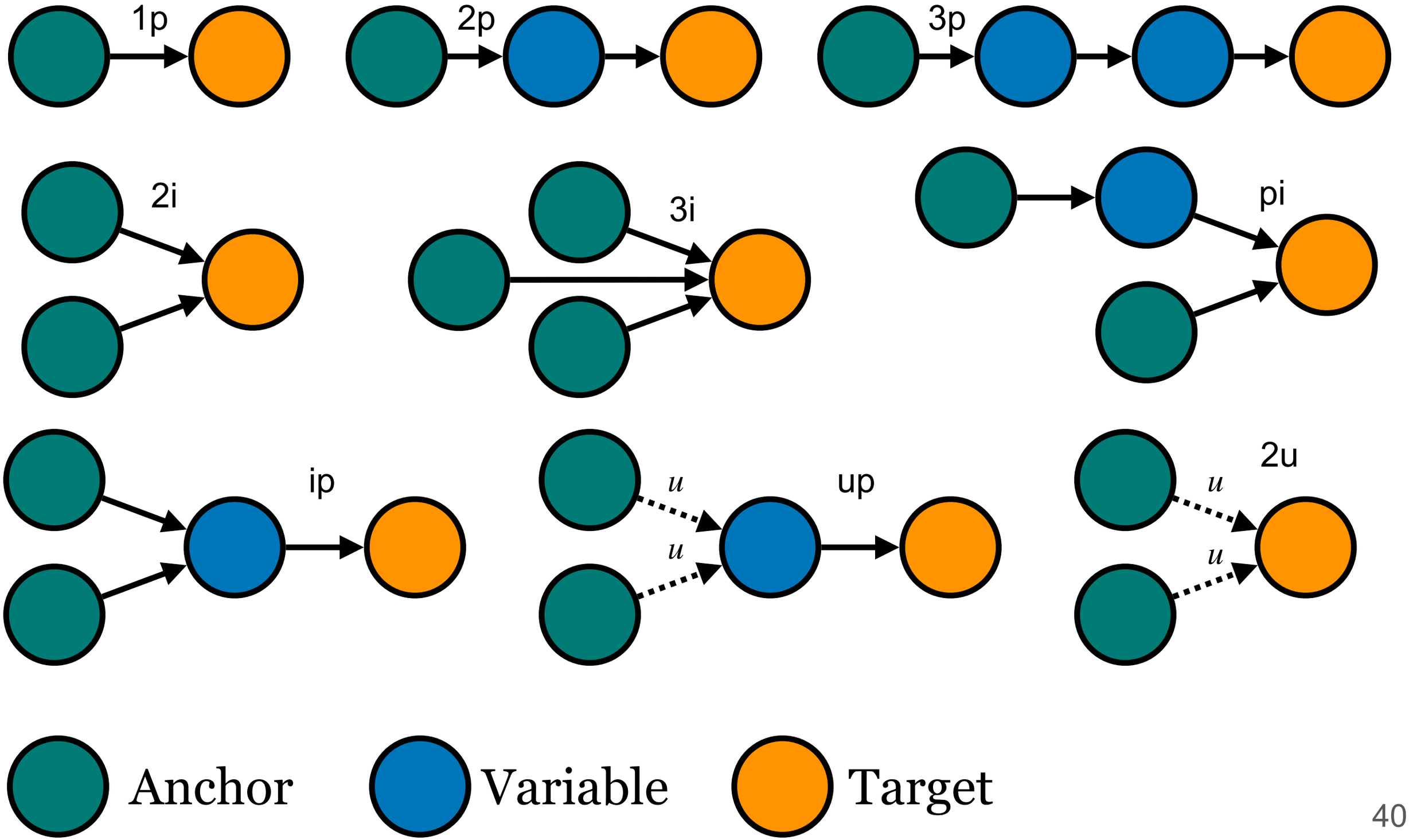
Query Answering as Optimisation

$$\arg \max_{\mathbf{e}_M, \mathbf{e}_D \in \mathbb{R}^k} \left[\phi_{\text{interacts}}\left(\mathbf{e}_M, \mathbf{e}_D\right) \top \phi_{\text{treats}}\left(\mathbf{e}_D, \mathbf{e}_{\text{anxiety}}\right) \right]$$

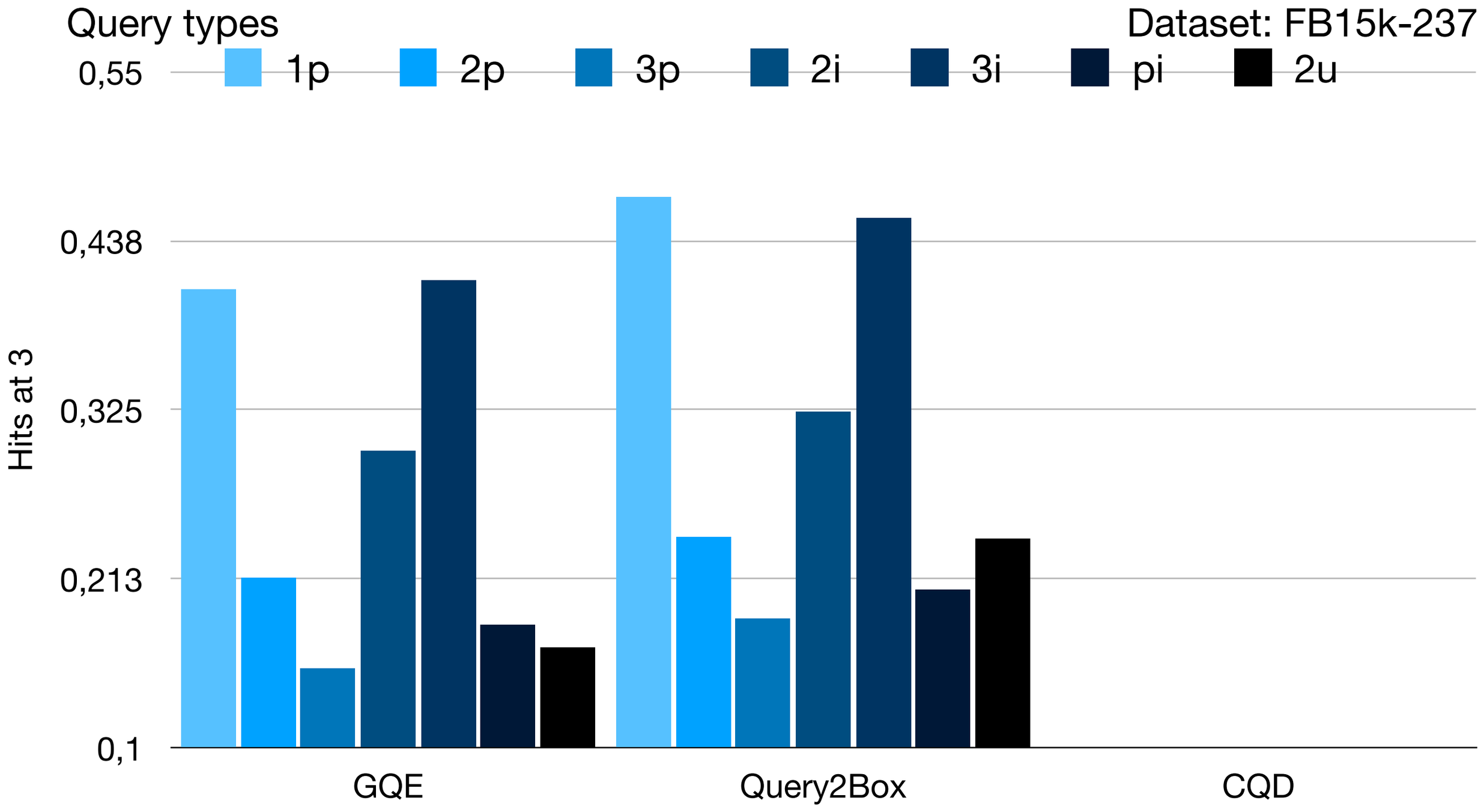
Gradient-Based Search

- Initialise $\mathbf{e}_M$ and $\mathbf{e}_D$ randomly
- Optimise $\mathbf{e}_M$ and $\mathbf{e}_D$ via Gradient Ascent to maximise the score of the query
- Replace $\mathbf{e}_M$ with the representations of all entities, and rank them based on the resulting query score

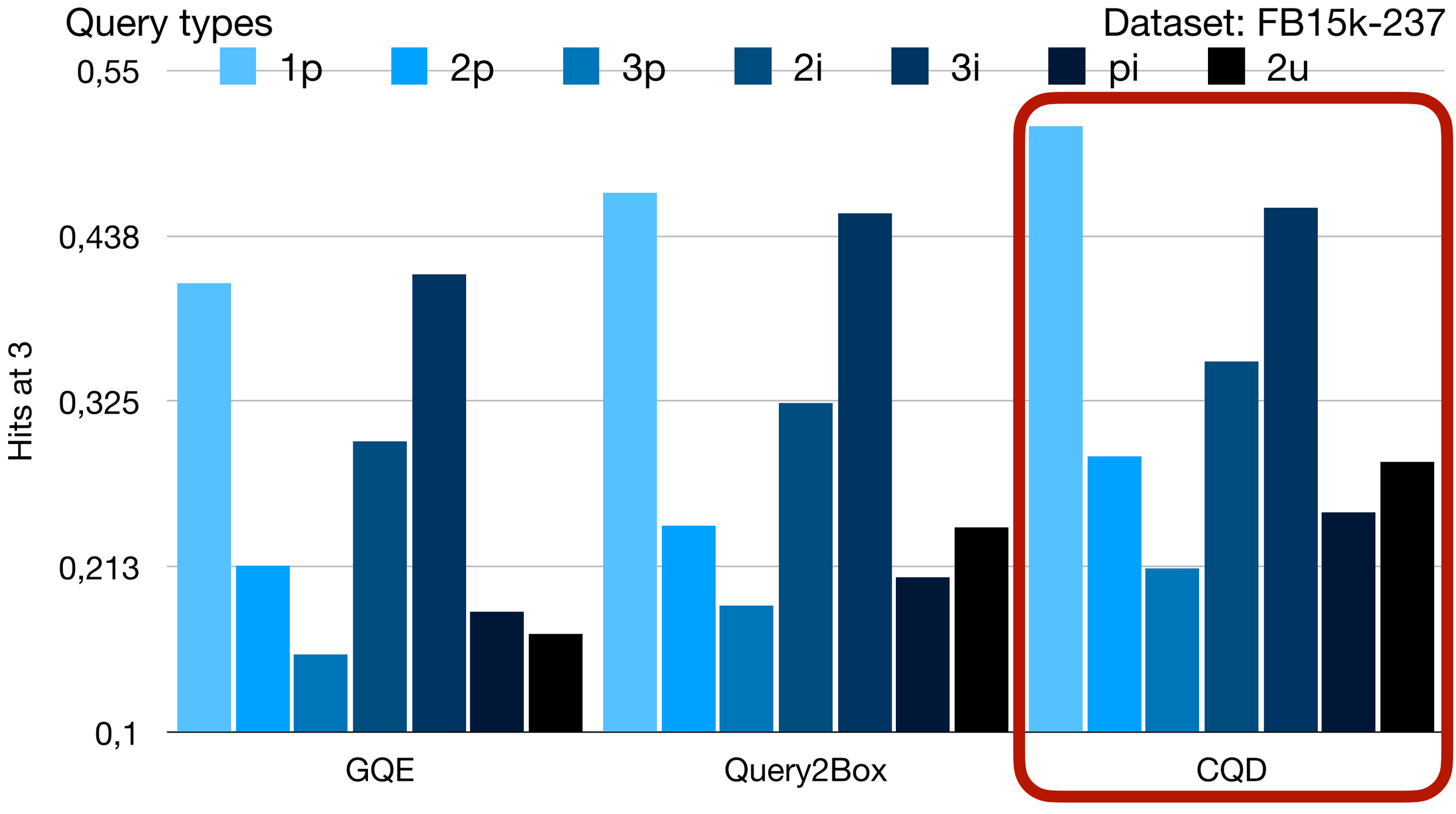
Types of Complex Queries



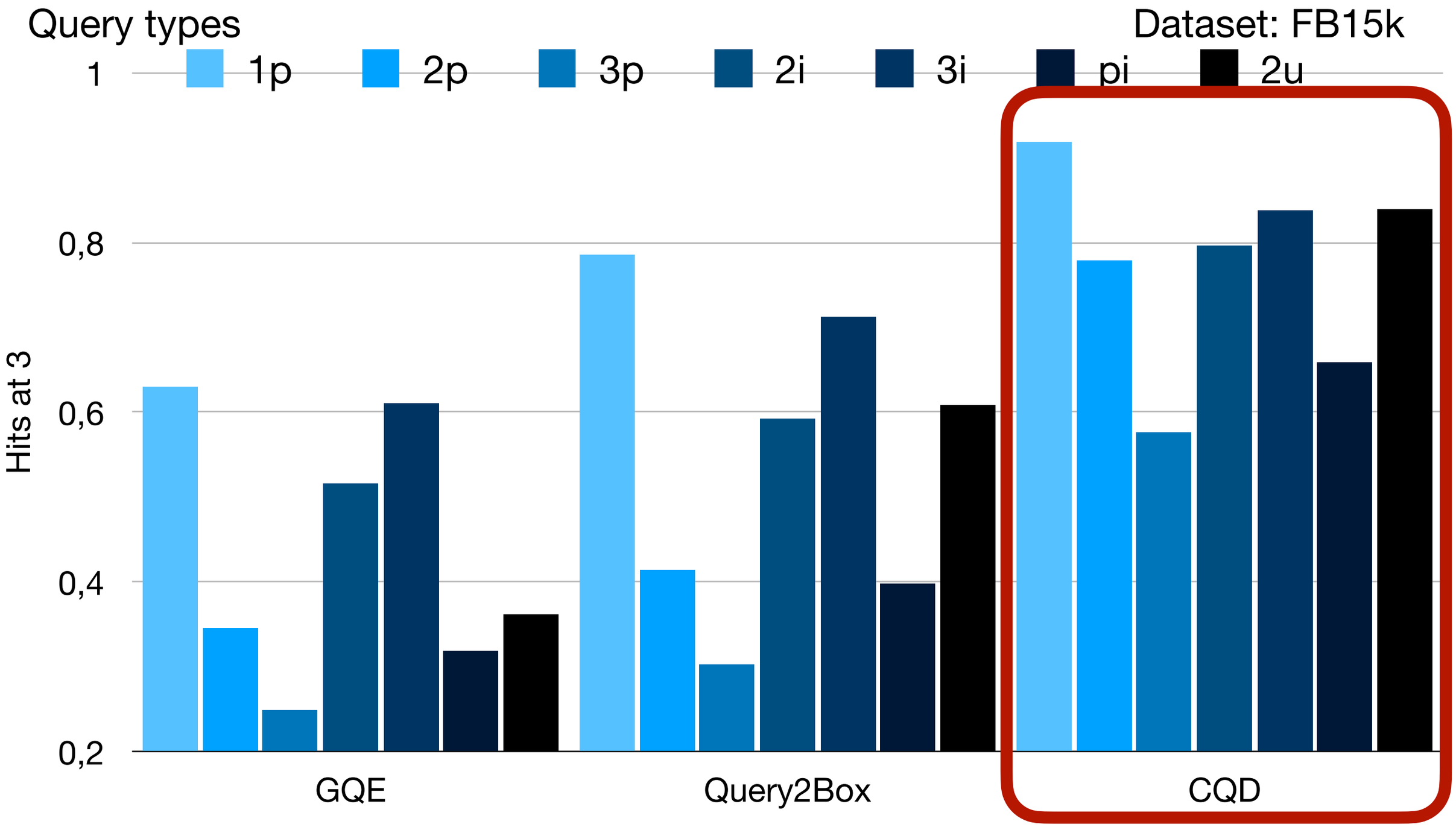
Experiments



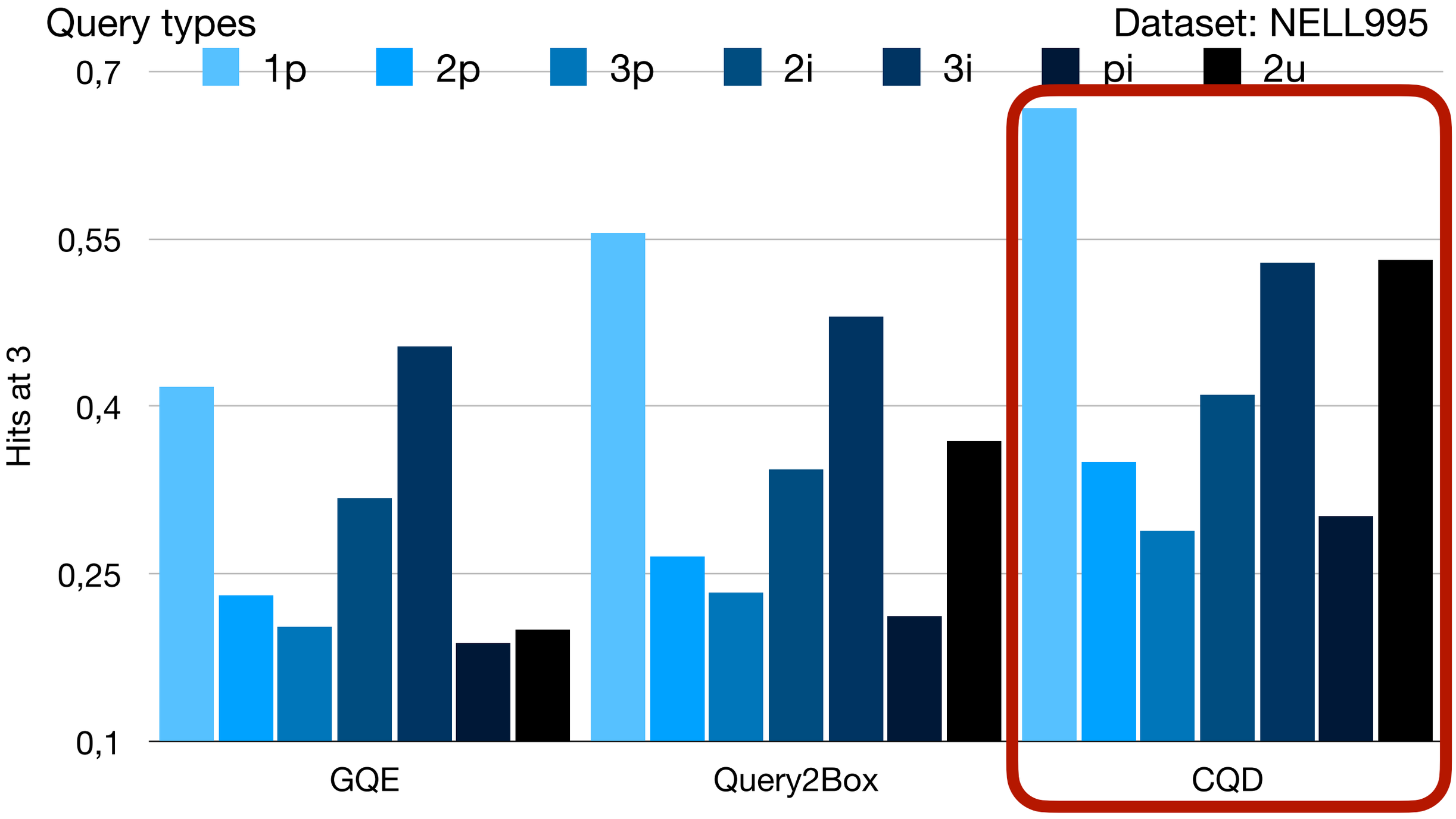
Experiments



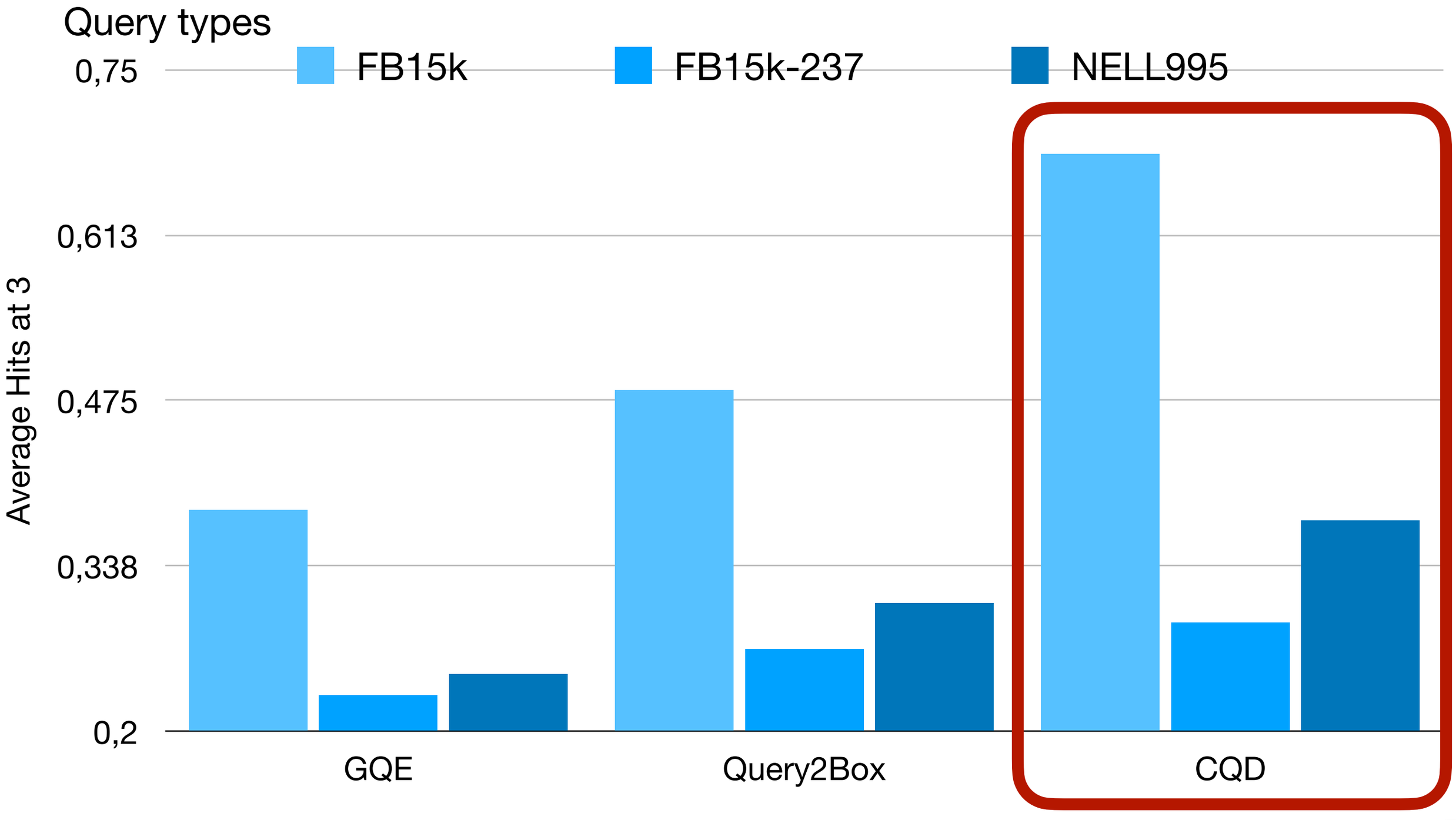
Experiments



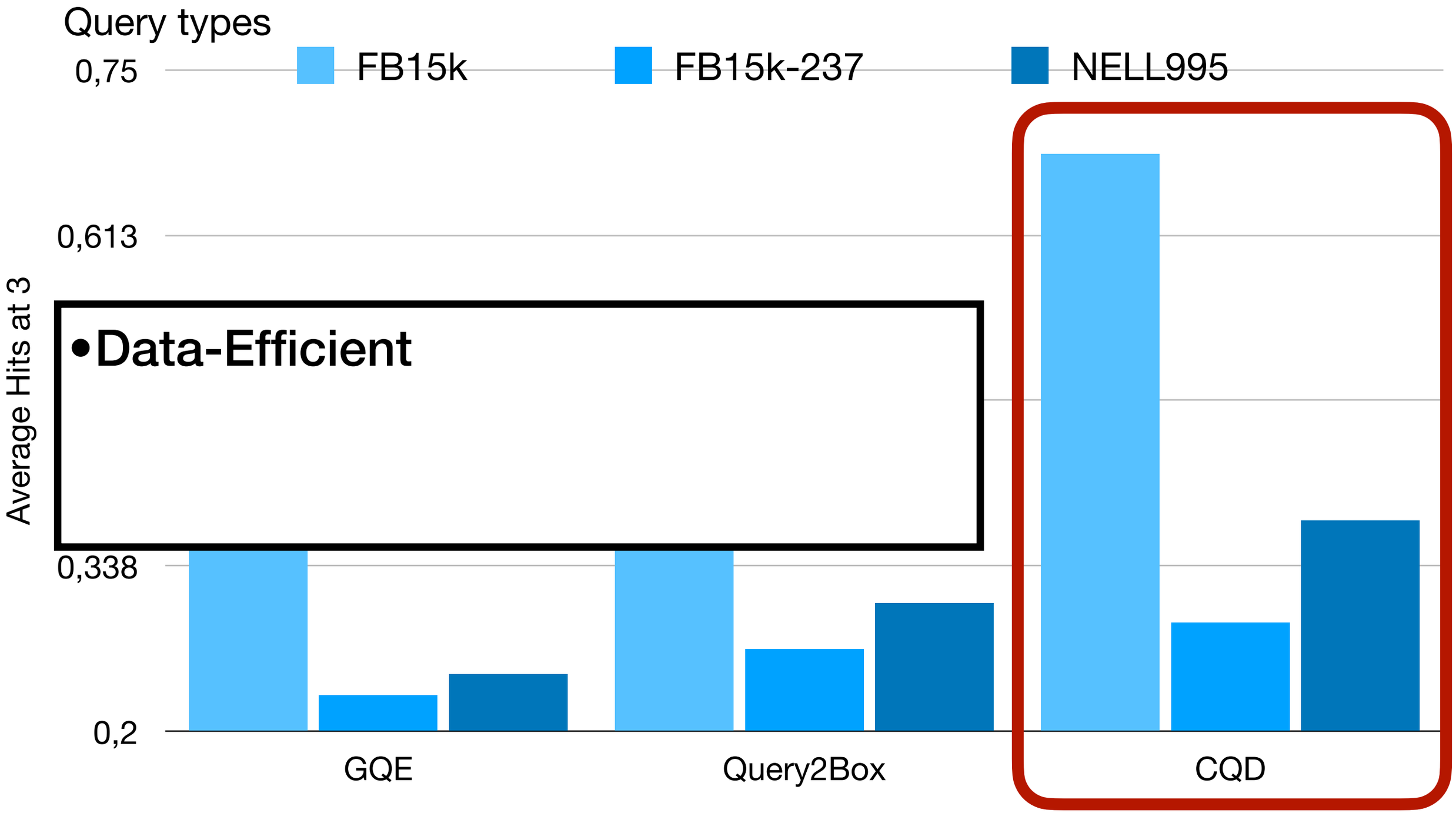
Experiments



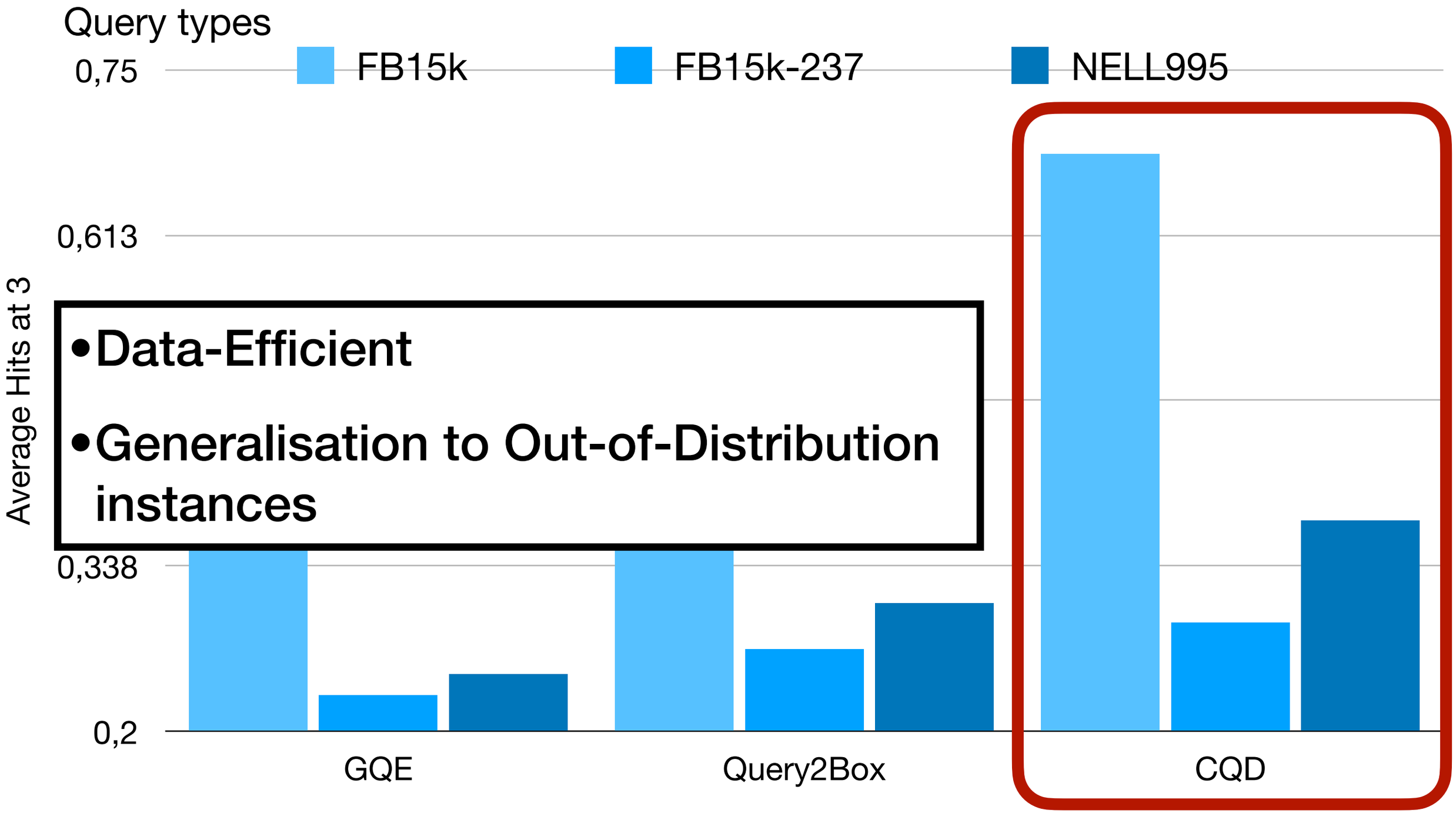
Experiments



Experiments



Experiments



Explainability

Query: Which medications have side-effects when taken with drugs for treating Anxiety?

$$?M : \exists D \,.\, \text{interacts}\,(M, D) \wedge \text{treats}\,\big(D, \text{anxiety}\big)$$

M
Apixaban
Amitriptyline
Phenytoin
Duloxetine
Buprenorphine

Explainability

Query: Which medications have side-effects when taken with drugs for treating Anxiety?

$$?M : \exists D \,.\, \text{interacts}\,(M, D) \wedge \text{treats}\,\big(D, \text{anxiety}\big)$$

- **Explainable**

M	*D*
Apixaban	Paroxetine
Amitriptyline	Paroxetine
Phenytoin	Paroxetine
Duloxetine	Pregabalin
Buprenorphine	Pregabalin

Explainability

Query: What international organisations contain the country of nationality of Thomas Aquinas?

$$?O : \exists C \,.\, \text{nationality}\left(\text{T}\,.\,\text{Aquinas}, C\right) \wedge \text{member}\,(C, O)$$

O	*C*
NATO	United States
OECD	United States
EU	United States
NATO	United Kingdom
OECD	United Kingdom
EU	United Kingdom
OECD	Germany
EU	Germany
WTO	Germany

Summary

Summary

Novel approach to answering Complex Queries on large-scale incomplete Knowledge Graphs:

Summary

Novel approach to answering Complex Queries on large-scale incomplete Knowledge Graphs:

- Train a neural link predictor on atomic queries

Summary

Novel approach to answering Complex Queries on large-scale incomplete Knowledge Graphs:

- Train a neural link predictor on atomic queries
- Answer complex queries by formulating the task as an optimisation problem

Summary

Novel approach to answering Complex Queries on large-scale incomplete Knowledge Graphs:

- Train a neural link predictor on atomic queries
- Answer complex queries by formulating the task as an optimisation problem

Generalises extremely well to complex queries, despite not being trained on them

Summary

Novel approach to answering Complex Queries on large-scale incomplete Knowledge Graphs:

- Train a neural link predictor on atomic queries
- Answer complex queries by formulating the task as an optimisation problem

Generalises extremely well to complex queries, despite not being trained on them

Source code: https://github.com/uclnlp/ctp/