

Domain Adaptation for Flavour Tagging at LHCb

Mirko Bunse and Quentin Führung

Lamarr Physics Monthly – April 7th, 2025

Partner institutions:



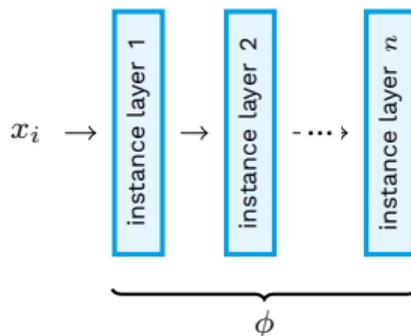
Institutionally funded by:



Ministerium für
Kultur und Wissenschaft
des Landes Nordrhein-Westfalen



Recap: Deep Sets

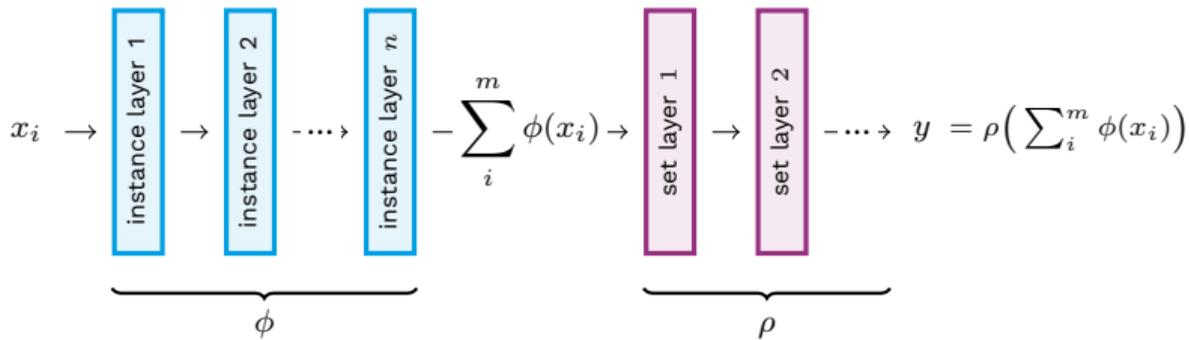


- Each event is a **set of tracks** $\{x_i \in \mathcal{X} : 1 \leq i \leq m\}$ of variable size m

¹ Zaheer et al., “Deep sets”, 2017

² Lee et al., “Set Transformer: A Framework for Attention-based Permutation-Invariant Neural Networks”, 2019

Recap: Deep Sets

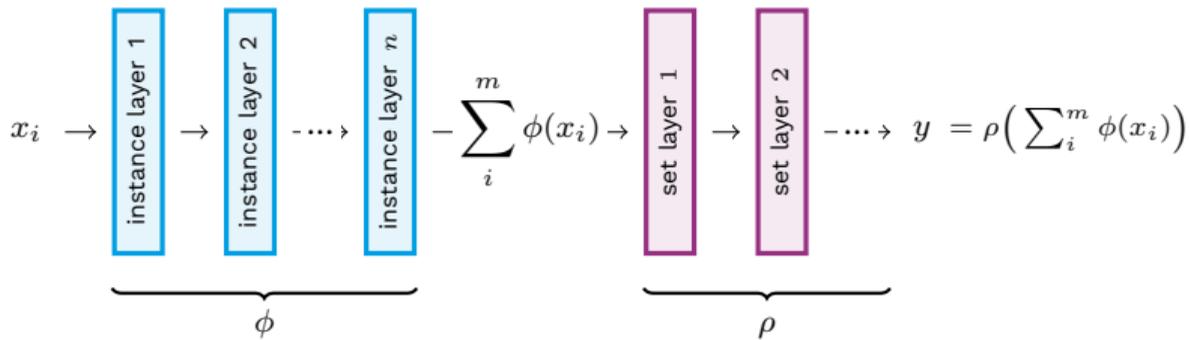


- Each event is a **set of tracks** $\{x_i \in \mathcal{X} : 1 \leq i \leq m\}$ of variable size m
- Track representations $\phi(x_i)$ are aggregated by (un-weighted) **sum pooling**

¹ Zaheer et al., “Deep sets”, 2017

² Lee et al., “Set Transformer: A Framework for Attention-based Permutation-Invariant Neural Networks”, 2019

Recap: Deep Sets



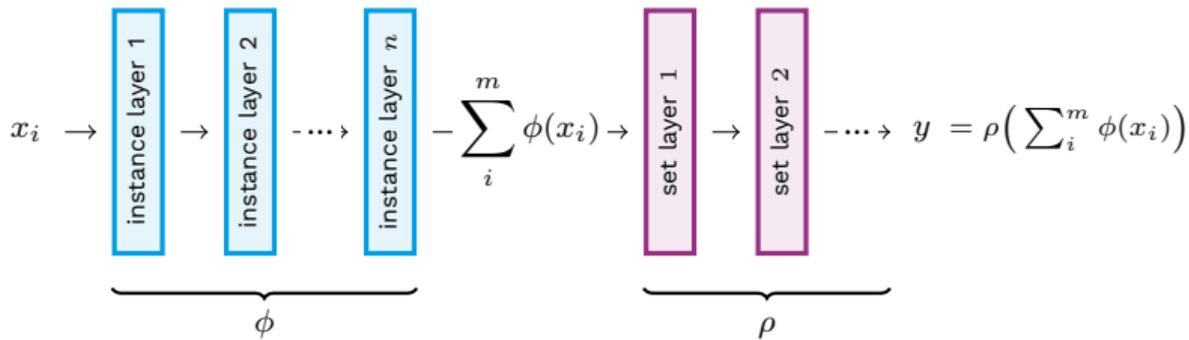
- Each event is a **set of tracks** $\{x_i \in \mathcal{X} : 1 \leq i \leq m\}$ of variable size m
- Track representations $\phi(x_i)$ are aggregated by (un-weighted) **sum pooling**

Deep Sets are **universal approximators** of permutation-invariant functions¹ (✓), but they ...

¹ Zaheer et al., “Deep sets”, 2017

² Lee et al., “Set Transformer: A Framework for Attention-based Permutation-Invariant Neural Networks”, 2019

Recap: Deep Sets



- Each event is a **set of tracks** $\{x_i \in \mathcal{X} : 1 \leq i \leq m\}$ of variable size m
- Track representations $\phi(x_i)$ are aggregated by (un-weighted) **sum pooling**

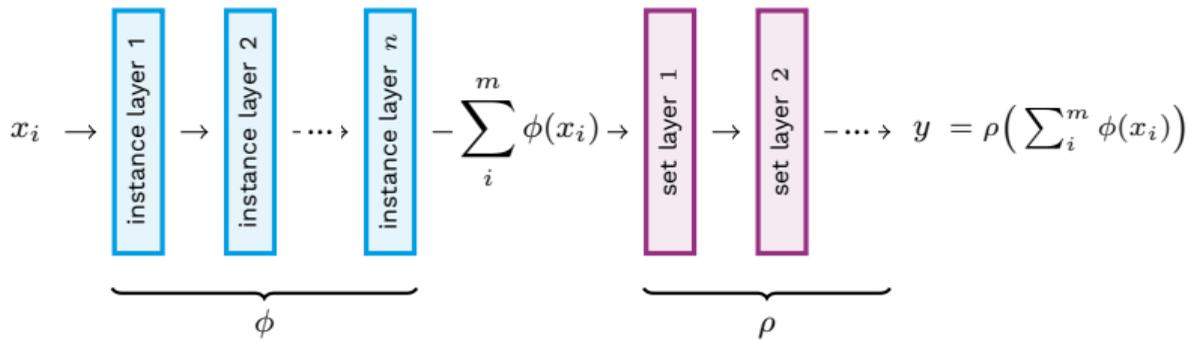
Deep Sets are **universal approximators** of permutation-invariant functions¹ (✓), but they ...

- might be inefficient in representing interactions between tracks² ✗

¹ Zaheer et al., “Deep sets”, 2017

² Lee et al., “Set Transformer: A Framework for Attention-based Permutation-Invariant Neural Networks”, 2019

Recap: Deep Sets



- Each event is a **set of tracks** $\{x_i \in \mathcal{X} : 1 \leq i \leq m\}$ of variable size m
- Track representations $\phi(x_i)$ are aggregated by (un-weighted) **sum pooling**

Deep Sets are **universal approximators** of permutation-invariant functions¹ (✓), but they ...

- might be inefficient in representing interactions between tracks² ✗
- might over-fit to simulated training data ✗

¹ Zaheer et al., “Deep sets”, 2017

² Lee et al., “Set Transformer: A Framework for Attention-based Permutation-Invariant Neural Networks”, 2019

Set Transformers



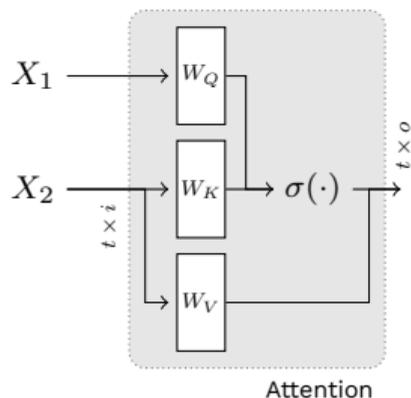
Idea: Model track interactions through Self-Attention²

Set Transformers



Idea: Model track interactions through Self-Attention²

$$\text{Attention}(X_1, X_2) = \sigma\left((X_1 W_Q)(X_2 W_K)^\top\right) X_2 W_V$$

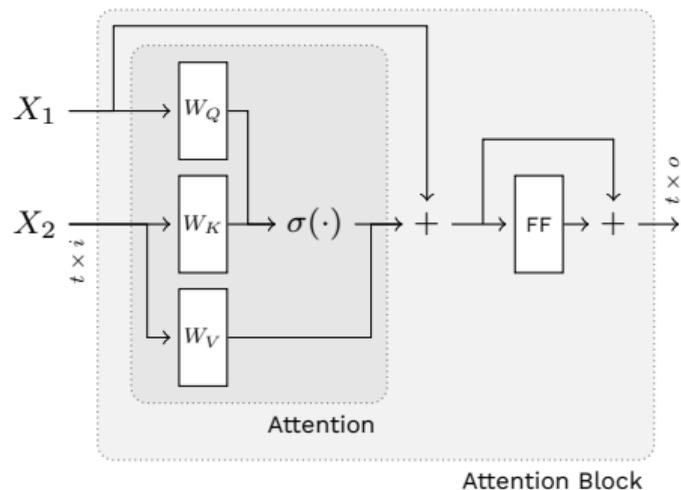


Set Transformers



Idea: Model track interactions through Self-Attention²

$$\text{Attention}(X_1, X_2) = \sigma\left((X_1 W_Q)(X_2 W_K)^\top\right) X_2 W_V$$

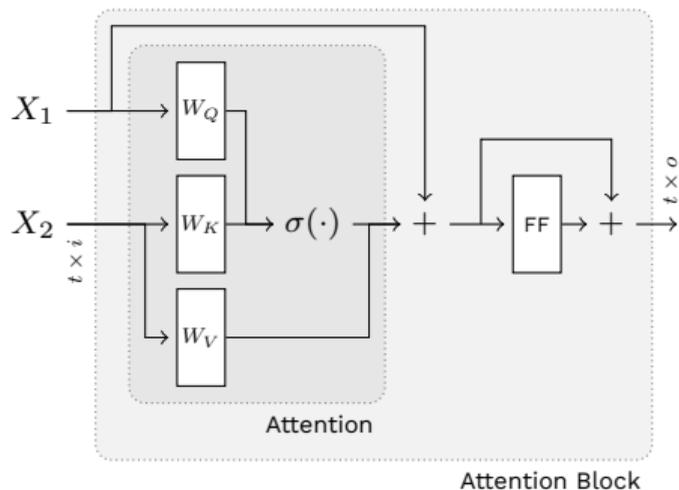


Set Transformers

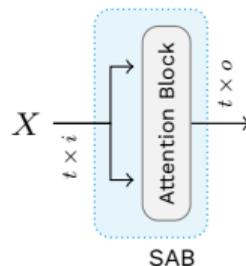


Idea: Model track interactions through Self-Attention²

$$\text{Attention}(X_1, X_2) = \sigma\left((X_1 W_Q)(X_2 W_K)^T\right) X_2 W_V$$



Self-Attention Block:

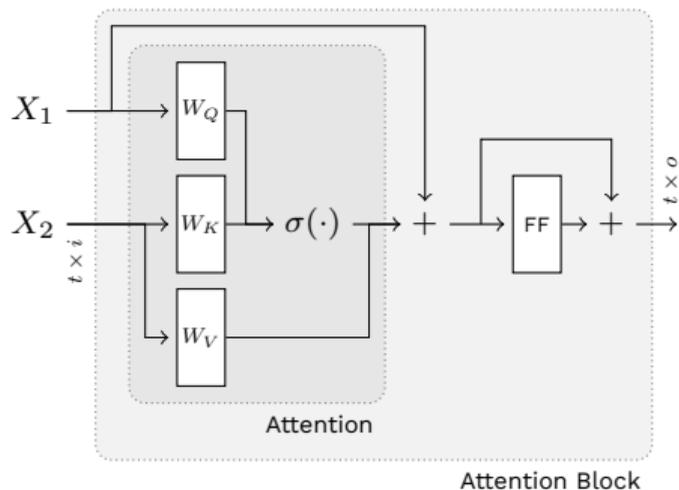


Set Transformers

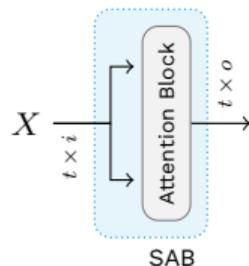


Idea: Model track interactions through Self-Attention²

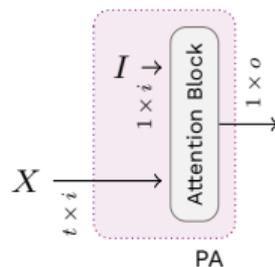
$$\text{Attention}(X_1, X_2) = \sigma\left((X_1 W_Q)(X_2 W_K)^T\right) X_2 W_V$$



Self-Attention Block:



Pooling by Attention:

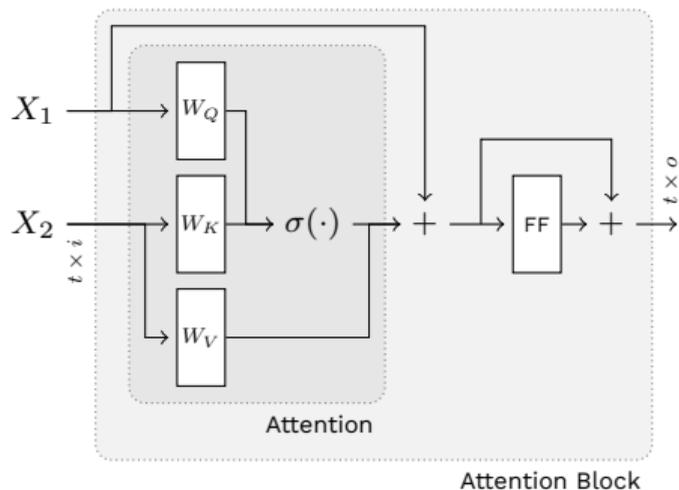


Set Transformers

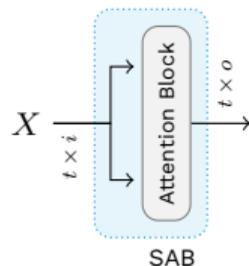


Idea: Model track interactions through Self-Attention²

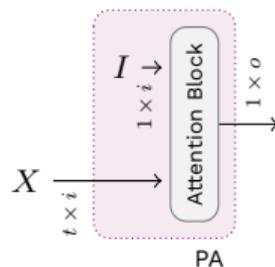
$$\text{Attention}(X_1, X_2) = \sigma\left((X_1 W_Q)(X_2 W_K)^T\right) X_2 W_V$$



Self-Attention Block:



Pooling by Attention:



Set Encoder:

SAB \circ ... \circ SAB \circ PA



Set Transformers

Universal Approximation ✓

Track interactions ✓

Over-fitting to simulations ✗

Unsupervised Domain Adaptation



Problem: Simulations and real data do not match perfectly, i.e. $\mathbb{P}_{\mathcal{S}}(X, Y) \neq \mathbb{P}_{\mathcal{T}}(X, Y)$

³ Ganin et al., “Domain-Adversarial Training of Neural Networks”, 2016

Unsupervised Domain Adaptation



Problem: Simulations and real data do not match perfectly, i.e. $\mathbb{P}_{\mathcal{S}}(X, Y) \neq \mathbb{P}_{\mathcal{T}}(X, Y)$

- Assume Concept Shift: $\mathbb{P}_{\mathcal{S}}(X | Y) \neq \mathbb{P}_{\mathcal{T}}(X | Y)$ and $\mathbb{P}_{\mathcal{S}}(Y) = \mathbb{P}_{\mathcal{T}}(Y)$
- Employ Unlabeled Data: $D_{\mathcal{T}} = \{x \sim \mathbb{P}_{\mathcal{T}}(X)\}$

³ Ganin et al., “Domain-Adversarial Training of Neural Networks”, 2016

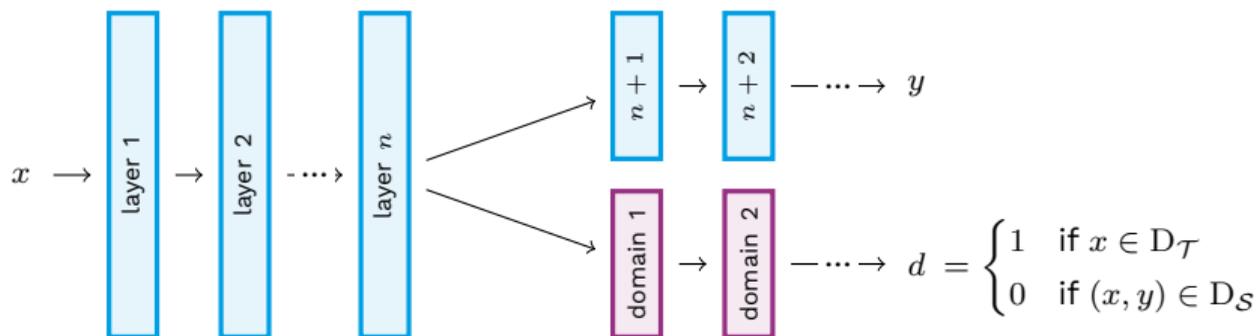
Unsupervised Domain Adaptation



Problem: Simulations and real data do not match perfectly, i.e. $\mathbb{P}_{\mathcal{S}}(X, Y) \neq \mathbb{P}_{\mathcal{T}}(X, Y)$

- Assume Concept Shift: $\mathbb{P}_{\mathcal{S}}(X | Y) \neq \mathbb{P}_{\mathcal{T}}(X | Y)$ and $\mathbb{P}_{\mathcal{S}}(Y) = \mathbb{P}_{\mathcal{T}}(Y)$
- Employ Unlabeled Data: $D_{\mathcal{T}} = \{x \sim \mathbb{P}_{\mathcal{T}}(X)\}$

Domain-Adversarial UDA:³



³ Ganin et al., "Domain-Adversarial Training of Neural Networks", 2016

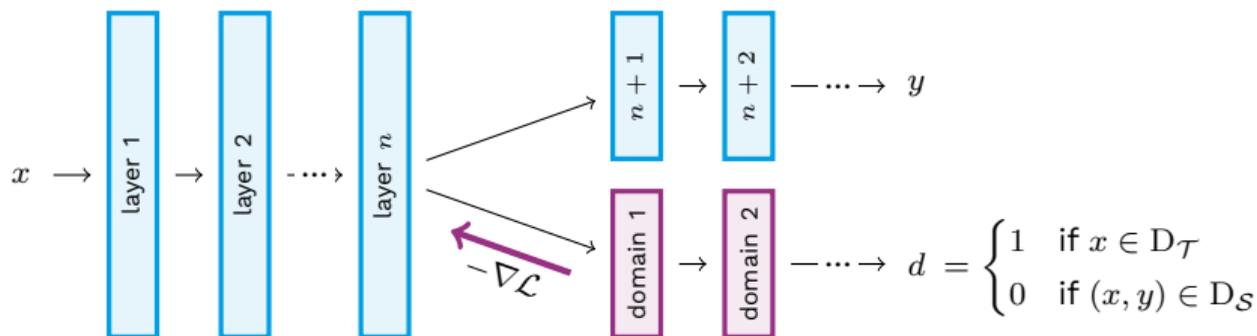
Unsupervised Domain Adaptation



Problem: Simulations and real data do not match perfectly, i.e. $\mathbb{P}_{\mathcal{S}}(X, Y) \neq \mathbb{P}_{\mathcal{T}}(X, Y)$

- Assume Concept Shift: $\mathbb{P}_{\mathcal{S}}(X | Y) \neq \mathbb{P}_{\mathcal{T}}(X | Y)$ and $\mathbb{P}_{\mathcal{S}}(Y) = \mathbb{P}_{\mathcal{T}}(Y)$
- Employ Unlabeled Data: $D_{\mathcal{T}} = \{x \sim \mathbb{P}_{\mathcal{T}}(X)\}$

Domain-Adversarial UDA:³



³ Ganin et al., "Domain-Adversarial Training of Neural Networks", 2016

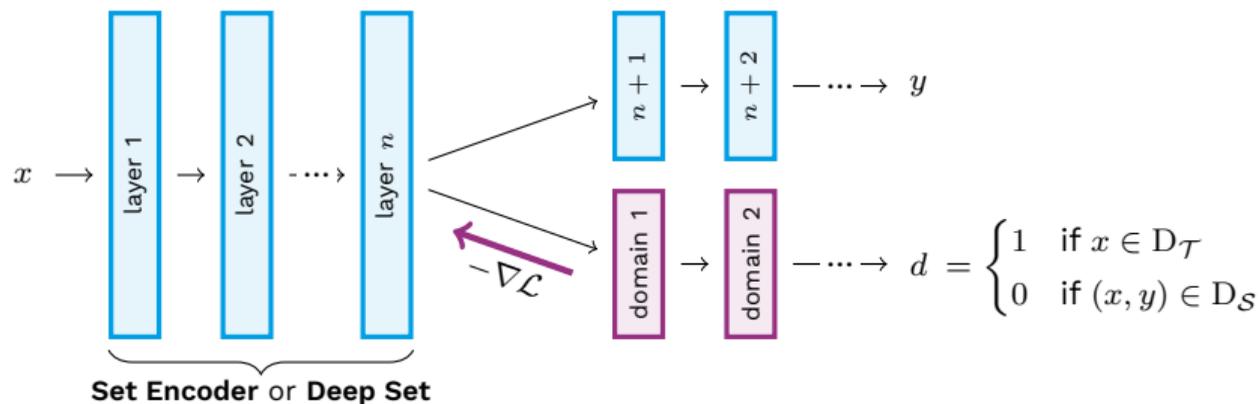
Unsupervised Domain Adaptation



Problem: Simulations and real data do not match perfectly, i.e. $\mathbb{P}_{\mathcal{S}}(X, Y) \neq \mathbb{P}_{\mathcal{T}}(X, Y)$

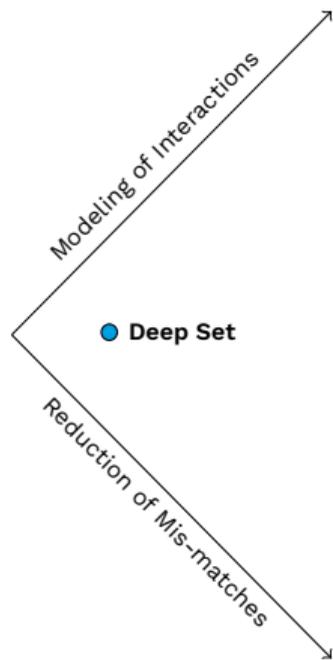
- Assume Concept Shift: $\mathbb{P}_{\mathcal{S}}(X | Y) \neq \mathbb{P}_{\mathcal{T}}(X | Y)$ and $\mathbb{P}_{\mathcal{S}}(Y) = \mathbb{P}_{\mathcal{T}}(Y)$
- Employ Unlabeled Data: $D_{\mathcal{T}} = \{x \sim \mathbb{P}_{\mathcal{T}}(X)\}$

Domain-Adversarial UDA:³

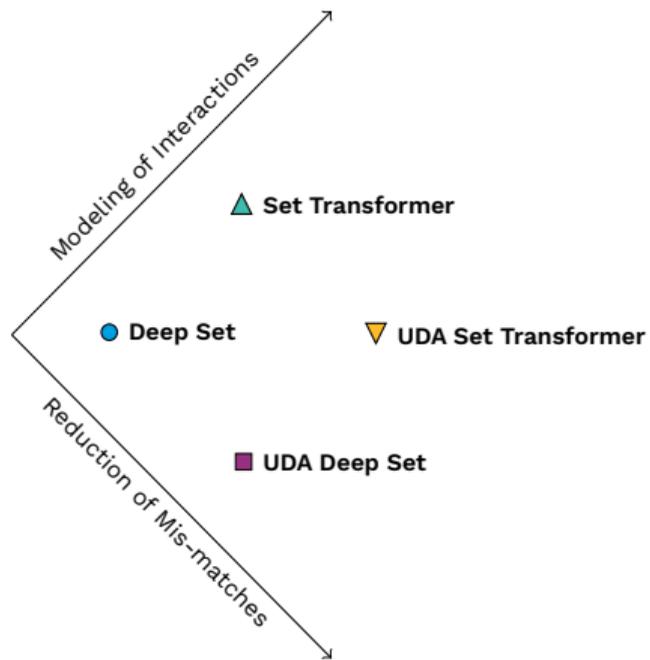


³ Ganin et al., "Domain-Adversarial Training of Neural Networks", 2016

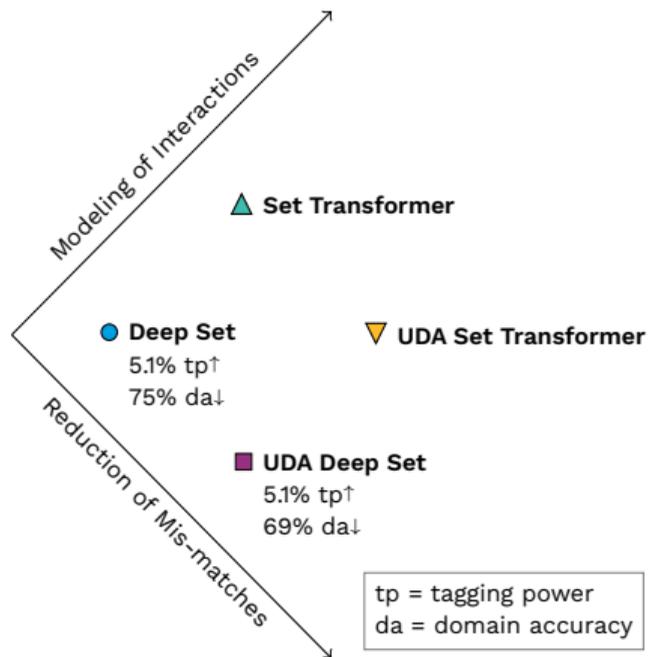
(Preliminary) Performance



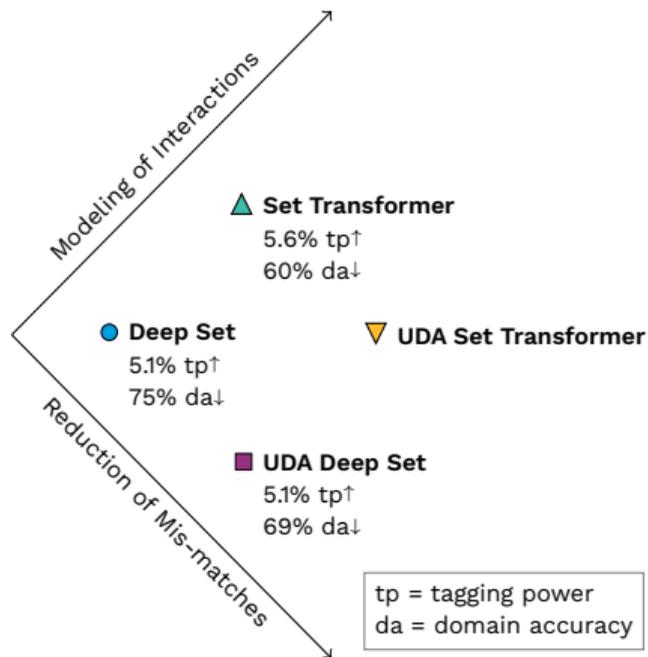
(Preliminary) Performance



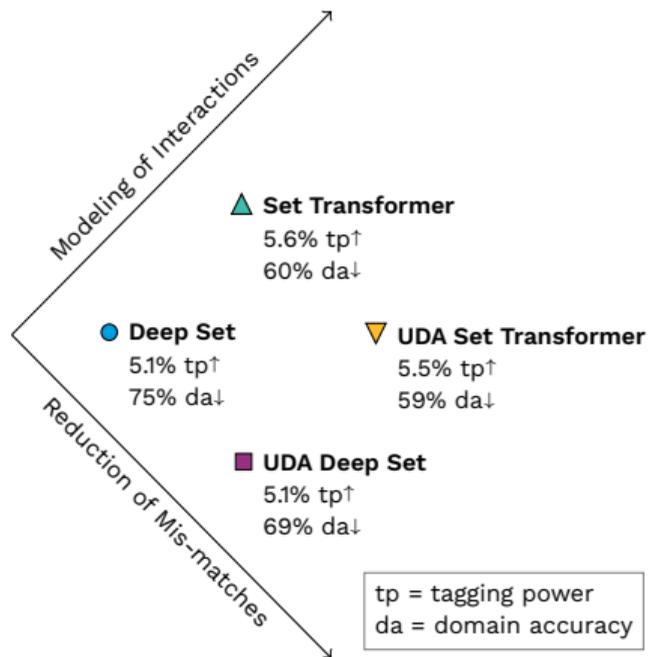
(Preliminary) Performance



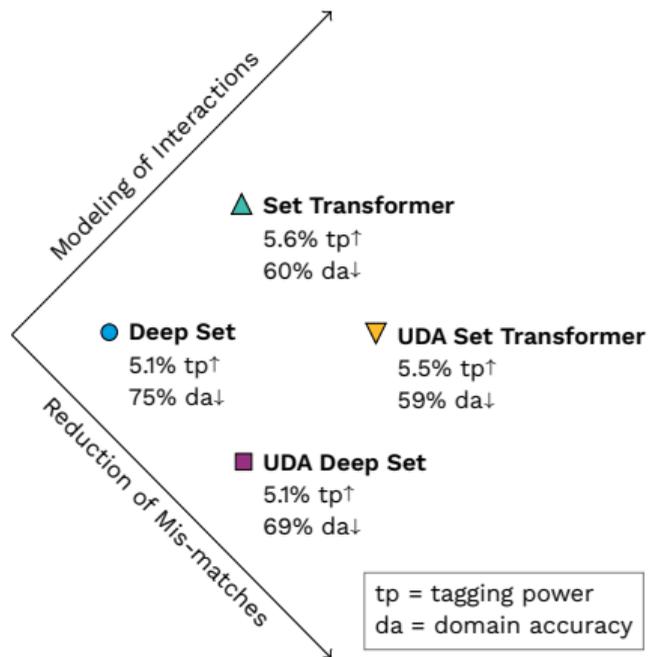
(Preliminary) Performance



(Preliminary) Performance



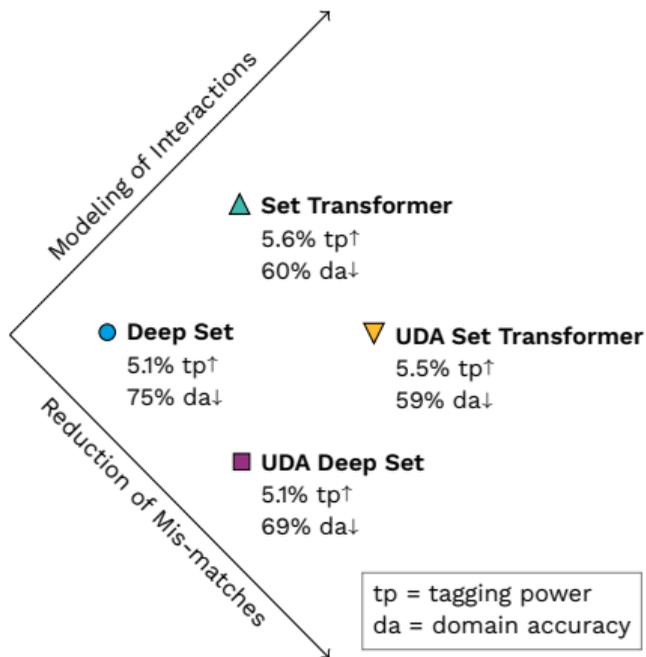
(Preliminary) Performance



(Preliminary) conclusions:

- Set Transformers increase tagging power and reduce mis-matches
- UDA does not improve tagging power (for now)

(Preliminary) Performance



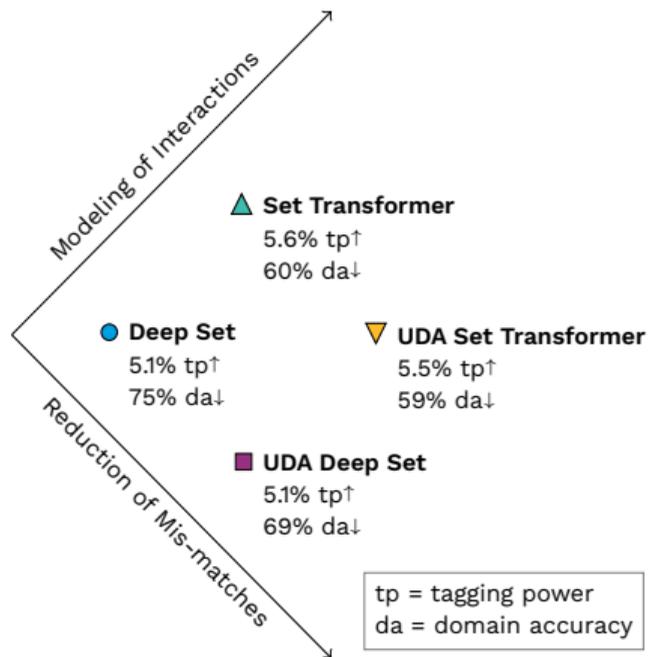
(Preliminary) conclusions:

- Set Transformers increase tagging power and reduce mis-matches
- UDA does not improve tagging power (for now)

Grains of salt:

- Difficulties in balancing the influence of UDA (currently: via multiple training phases)

(Preliminary) Performance



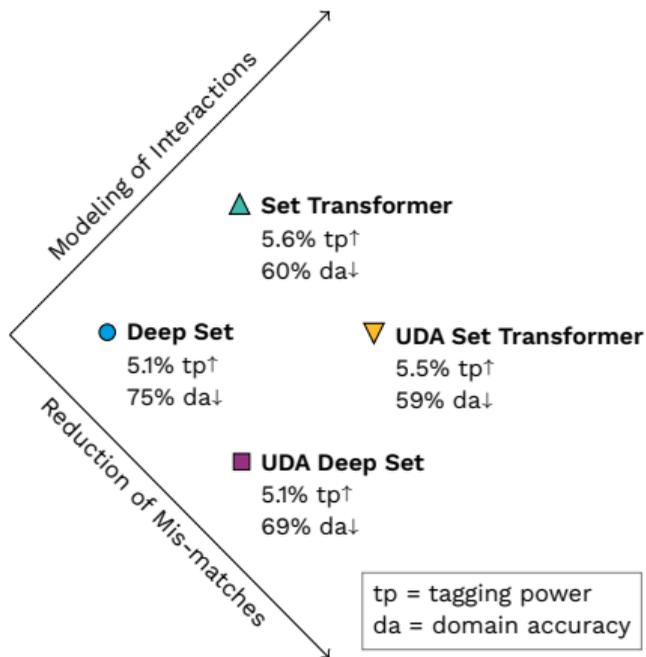
(Preliminary) conclusions:

- Set Transformers increase tagging power and reduce mis-matches
- UDA does not improve tagging power (for now)

Grains of salt:

- Difficulties in balancing the influence of UDA (currently: via multiple training phases)
- Unclear influence of factors besides mis-matches, like background and sweights

(Preliminary) Performance



(Preliminary) conclusions:

- Set Transformers increase tagging power and reduce mis-matches
- UDA does not improve tagging power (for now)

Grains of salt:

- Difficulties in balancing the influence of UDA (currently: via multiple training phases)
- Unclear influence of factors besides mis-matches, like background and sweights

Let's discuss!