Learning Set Functions Under the Optimal Subset Oracle via Equivariant Variational Inference

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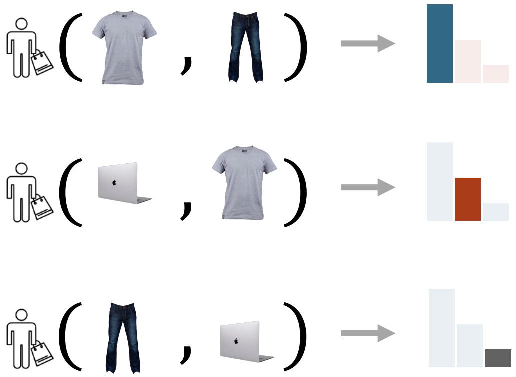
Set Function Learning Applications

Database

Ground set V

Customer



Utility function $F_{\theta^*}(\cdot; V)$

Shopping cart

Optimal subset S^*

Set Function Learning Applications

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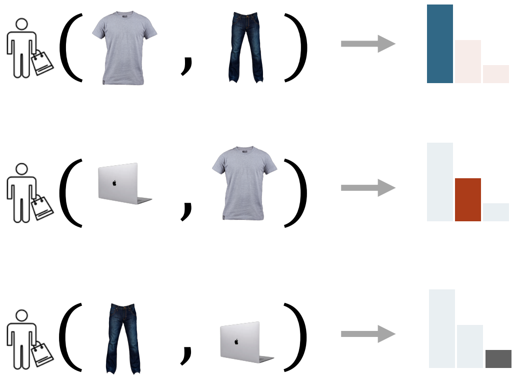


Utility function $F_{\theta^*}(\cdot; V)$

Shopping cart

Optimal subset S^*

Data Generation Process:

$$S^* = \operatorname*{argmax}_{S \in 2^V} F_{\theta^*}(S; V)$$

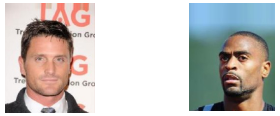
$$\sim \mathbb{p}(S, V) =: \delta_{S=S^*|V}$$

Set Function Learning Applications

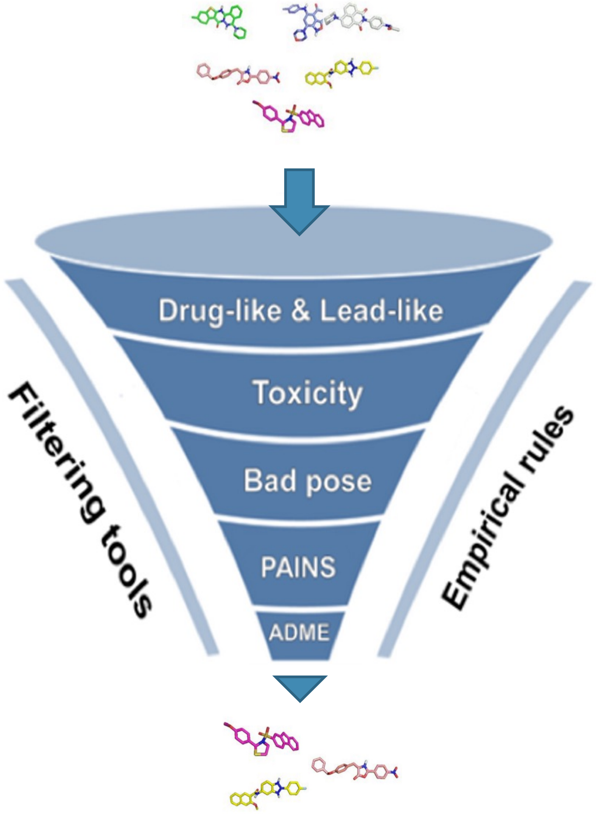
$$S^* = \underset{S \in 2^V}{\operatorname{argmax}} F_{\theta^*}(S;V)$$

Set anomaly detection

$$F_{\theta^*}(S;V) = \sum_{s_i \in S} \mathbb{I}(s_i\ is\ male) - \mathbb{I}(s_i\ is\ femail)$$



Compound selection



Set Function Learning Function Value (FV) Oracle

$$S^* = \underset{S \in 2^V}{\operatorname{argmax}} F_{\theta^*}(S; V)$$

Goal: Learn a surrogate F_θ to approximate the oracle utility function F_{θ^*}.

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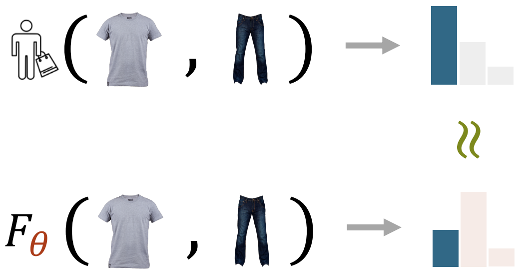
Setting 1, FV oracle:



Matching via empirical risk minimization

$$\theta^* = \min_\theta \sum_i L(F_\theta(S_i; V); F_{\theta^*}(S_i; V))$$

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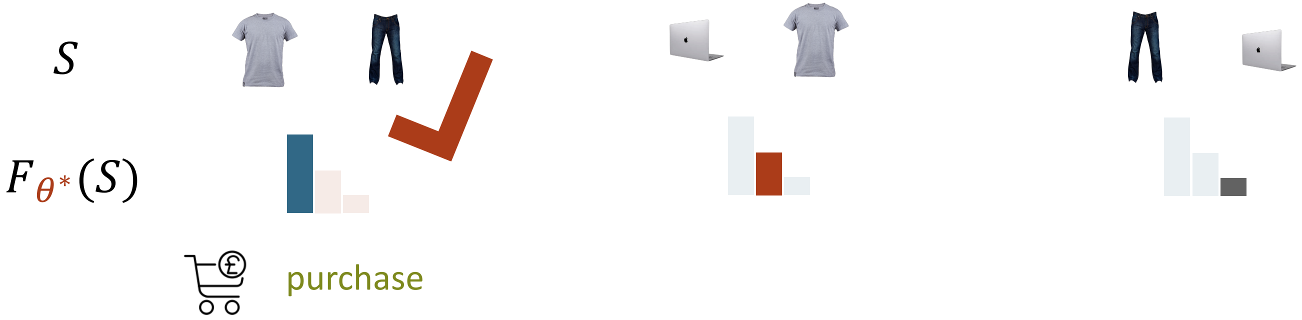

Set Function Learning Function Value (FV) Oracle

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Goal: Learn a surrogate F_θ to approximate the oracle utility function F_{θ^*}.

Setting 1, FV oracle:

$$\theta^* = \min_{\theta} \sum_i L(F_\theta(S_i;V); F_{\theta^*}(S_i;V))$$

Curse of amounts of supervision signals 😅

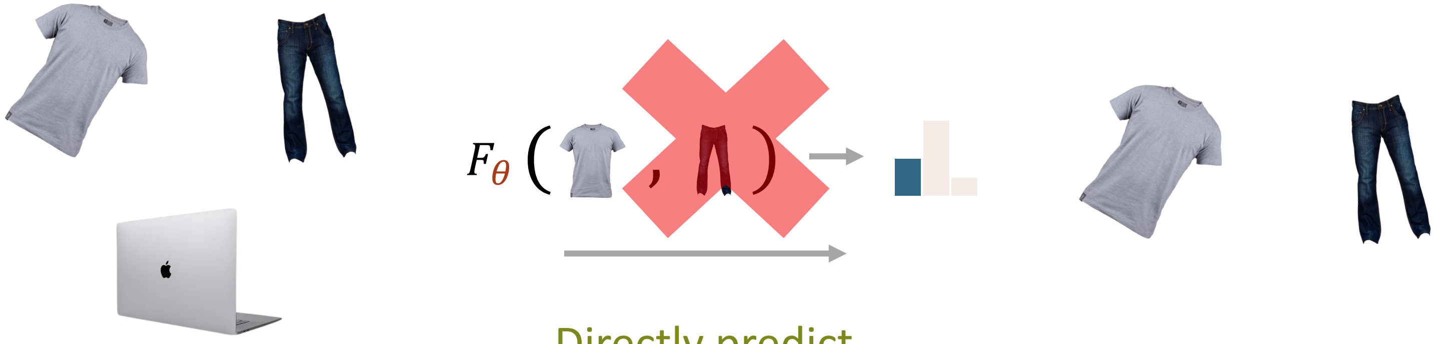
⇒ Training data in form of $\{(S_i, F_{\theta^*}(S_i;V))\}$ for each V

Set Function Learning Optimal Subset (OS) Oracle

$$S^* = \underset{S \in 2^V}{\operatorname{argmax}} F_{\theta^*}(S; V)$$

Goal: Learn a surrogate F_θ to approximate the oracle utility function F_{θ^*}.

Setting 2, OS oracle:



Ground set V

Directly predict

Optimal subset S^*

$\Rightarrow$ Training data in form of $\{(S^*, V)\}$

Learning Set Function Under the OS Oracle

Empirical distribution

↓

$$\underset{\theta}{\operatorname{argmax}}\, \mathbb{E}_{\mathbb{P}(S^*,V)}[\log p_\theta(S^*|V)]$$

$$s.t.\, p_\theta(S|V) \propto F_\theta(S;V), \forall S \in 2^V$$

↑

Monotonically grows with the utility function

Learning Set Function Under the OS Oracle

Empirical distribution

↓

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$$s.t.\, p_\theta(S|V) \propto F_\theta(S;V), \forall S \in 2^V$$

↑

Monotonically grows with the utility function

How to construct a proper set mass function $p_\theta(S|V)$?

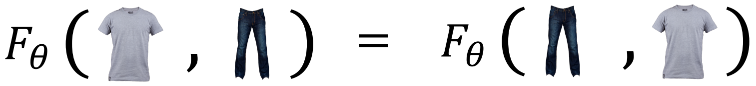
Learning Set Function Under the OS Oracle

$$\underset{\theta}{\operatorname{argmax}}\, \mathbb{E}_{\mathbb{P}(S^*,V)}[\log p_\theta(S^*|V)]$$

$$s.t.\, p_\theta(S|V) \propto F_\theta(S;V), \forall S \in 2^V$$

Desiderata:

Permutation invariance



Learning Set Function Under the OS Oracle

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Desiderata:

Permutation invariance

Varying ground set

Learning Set Function Under the OS Oracle

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Desiderata:

Permutation invariance

Varying ground set

Differentiability; Minimum prior & Scalability

Learning Set Function Under the OS Oracle

$$\underset{\theta}{\operatorname{argmax}}\, \mathbb{E}_{\mathbb{P}(S^*,V)}[\log p_\theta(S^*|V)]$$

$$s.t. p_\theta(S|V) \propto F_\theta(S;V), \forall S \in 2^V$$

Probabilistic greedy model (PGM):

Permutation $\pi = \{s_1, s_2, \dots, s_{|S|}\}$

$$p_\theta(\mathrm{S}|V) = \sum_{\pi\in\Pi^S} p_\theta(\pi|V)$$

The first j chosen elements: $\mathrm{S}_j = \{s_1, s_2, \dots, s_j\}$

$$p_\theta(\pi|V) = \prod_{\mathrm{j}=0}^{|S|-1} \frac{\exp(F_\theta(s_{j+1} \cup S_j)/\gamma)}{\sum_{s\in V\setminus \mathrm{S}_j} \exp(F_\theta(s \cup S_j)/\gamma)}$$

Learning Set Function Under the OS Oracle

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Training:

$$\theta^* = \underset{\theta}{\operatorname{argmax}} \sum\nolimits_{(V,S^*)} \log \sum\nolimits_{\pi\in\Pi^{S^*}} p_\theta(\pi|V)$$

Log-likelihood: approximate with sampling

Learning Set Function Under the OS Oracle

DSF:

Concave function $\rho_i: \mathbb{R}_+ \rightarrow \mathbb{R}_+$

$$F_\theta(S;V) = \sum_i \rho_i\left(\sum_{s\in S} \kappa_i(s)\right)$$

Transform $\kappa_i: V \rightarrow \mathbb{R}_+$

PGM:

$$p_\theta(S|V) = \sum_{\pi\in\Pi^S} p_\theta(\pi|V)$$

$$p_\theta(\pi|V) = \prod_{j=0}^{|S|-1} \frac{\exp(F_\theta(s_{j+1}\cup S_j)/\gamma)}{\sum_{s\in V\setminus S_j} \exp(F_\theta(s\cup S_j)/\gamma)}$$

	Permutation Invariance	Varying Ground Set	Differentiability	Minimum Prior	Scalability	FV/OS Oracle
DSF	✓	✗	✓	-	-	FV
PGM	✓	✗	✓	✗	✗	OS
EquiVSet (Ours)	✓	✓	✓	✓	✓	OS

Bilmes et al. DSF: Deep submodular functions. NIPS 2016
Tschiatschek et al. PGM: Differentiable submodular maximization. IJCAI 2017.

Energy-based Modeling

$$\mathrm{p}_{\theta}(\mathrm{S}|\mathrm{V}) = \frac{\exp(\mathrm{F}_{\theta}(\mathrm{S};\mathrm{V}))}{Z}$$

← Partition function $Z := \sum_{S \subseteq V} \exp(F_{\theta}(S;V))$

Energy-based Modeling

$$\mathrm{p}_\theta(\mathrm{S}|\mathrm{V}) = \frac{\exp(\mathrm{F}_\theta(\mathrm{S};\mathrm{V}))}{Z}$$

← Partition function $Z \coloneqq \sum_{S \subseteq V} \exp(F_\theta(S;V))$

EBMs for Minimum Prior:

Energy-based modeling has **maximum entropy**

Energy-based Modeling

$$\mathrm{p}_\theta(\mathrm{S}|\mathrm{V}) = \frac{\exp(\mathrm{F}_\theta(\mathrm{S};\mathrm{V}))}{Z}$$

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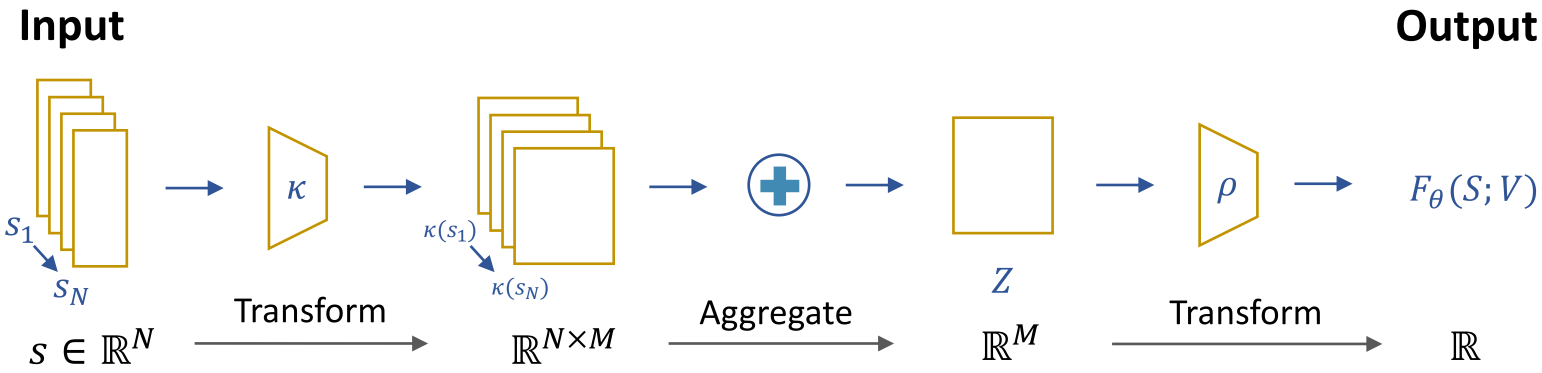
DeepSet for Permutation Invariance:



Zaheer Kottur, Ravanbakhsh, Poczos, Salakhutdinov and Smola. Deep sets. NIPS 2017.

Approximate MLE

$$p_\theta(S|V) = \frac{\exp(F_\theta(S;V))}{Z}$$

← Partition function $Z := \sum_{S\subseteq V} \exp(F_\theta(S;V))$

Training Discrete EBMs:

Contrastive Divergence ⇒ Hard to converge

Score Matching ⇒ NonDifferentiable

Ratio Matching ⇒ Unstable

Separate training and inference procedure 😤

Approximate MLE

$$\mathrm{p}_\theta(\mathrm{S}|\mathrm{V}) = \frac{\exp(\mathrm{F}_\theta(\mathrm{S};\mathrm{V}))}{Z}$$

← Partition function $Z \coloneqq \sum_{S\subseteq V} \exp(F_\theta(S;V))$

Marginal-based Loss:

$\psi \in [0,1]^{|V|}$: odds that $s \in V$ shall be selected in the OS S^*

$$\psi^* = \underset{\psi}{\operatorname{argmax}}\, \mathrm{D}(q(S;\psi)||p_\theta(S))$$

$$L(\theta;\psi^*) = \sum_{i=1}^{N}[-\sum_{j\in S_i^*}\log\psi_j^* - \sum_{j\in V_i\backslash \mathrm{S}_i^*}\log(1-\psi_j^*)]$$

Cohesive training and inference procedure 😀

Domke J. Learning graphical model parameters with approximate marginal inference. PAMI 2013.

Approximate MLE

$$\mathrm{p}_\theta(\mathrm{S}|\mathrm{V}) = \frac{\exp(\mathrm{F}_\theta(\mathrm{S};\mathrm{V}))}{Z}$$

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$$L(\theta;\psi^*) = \sum_{i=1}^{N}[-\sum_{j \in S_i^*} \log \psi_j^* - \sum_{j \in V_i \backslash S_i^*} \log(1-\psi_j^*)]$$

↑

Require ψ^* is differentiable w.r.t. θ 🤔

Differentiable MFVI

Variational distribution $q(S;\psi) = \prod_{i\in S}\psi_i \prod_{j\notin S}(1-\psi_j)\,, \psi \in [0,1]^{|V|}$

$$\min_{\psi} \mathbb{KL}(q(S;\psi) \| p_\theta(S))$$

$$\Leftrightarrow \max_{\psi} f_{mt}^{F_\theta}(\psi) + \mathbb{H}\big(q(S;\psi)\big) =: \text{ELBO}$$

multilinear extension $f_{mt}^{F_\theta}(\psi) \coloneqq \sum_{S\subseteq V} F_\theta(S) \prod_{i\in S}\psi_i \prod_{j\notin S}(1-\psi_j)$

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↑

multilinear extension $f_{mt}^{F_\theta}(\psi) := \sum_{S \subseteq V} F_\theta(S) \prod_{i \in S} \psi_i \prod_{j \notin S}(1-\psi_j)$

RNN-like fixed-point iteration:

$$\left.\begin{aligned} \psi^{(0)} &\leftarrow \text{Initialize in } [0,1]^{|V|} \\ \psi_\theta^{(k)} &\leftarrow \left(1 + \exp\left(-\nabla_{\psi^{(k-1)}} f_{mt}^{F_\theta}\left(\psi^{(k-1)}\right)\right)\right)^{-1} \\ \psi_\theta^{*} &\leftarrow \psi_\theta^{(K)} \end{aligned}\right\} \mathrm{MFVI}\left(\psi^{(0)}, V, K\right)$$

$\psi_\theta^{*} = \mathrm{MFVI}\left(\psi^{(0)}, V, K\right)$ is **differentiable** w.r.t. θ 😌

Differentiable MFVI

$$L(\theta;\psi^*) = \sum_{i=1}^{N}[-\sum_{j\in S_i^*}\log\psi_j^* - \sum_{j\in V_i\backslash S_i^*}\log(1-\psi_j^*)]$$

Algorithm $\mathrm{DiffMF}(V, S^*)$:

```
Initialize variational parameter $\psi$
    $\psi^{(0)} \leftarrow 0.5 * \mathbf{1}$
Compute the variational marginals
    $\psi^* \leftarrow \mathrm{MFVI}(\psi^{(0)}, V, K)$
Update parameter $\theta$
    $\theta \leftarrow \theta - \eta\nabla_\theta L(\theta;\psi^*)$
```

Differentiable MFVI

$$L(\theta;\psi^*) = \sum_{i=1}^{N}[-\sum_{j\in S_i^*}\log\psi_j^* - \sum_{j\in V_i\backslash S_i^*}\log(1-\psi_j^*)]$$

Training:

```
Initialize variational parameter $\psi$
    $\psi^{(0)} \leftarrow 0.5 * \mathbf{1}$
Compute the variational marginals
    $\psi^* \leftarrow \mathrm{MFVI}(\psi^{(0)}, V, K)$
Update parameter $\theta$
    $\theta \leftarrow \theta - \eta\nabla_\theta L(\theta;\psi^*)$
```

Inference:

$$S = \mathrm{topN}(\psi^*)$$

$$\psi^* = \mathrm{MFVI}(\psi^{(0)}, V, K)$$

Amortizing MFVI Open problems of DiffMF

- Expensive computation complexity

$$\psi_{\theta}^{(k)} \leftarrow \left(1+\exp\left(-\nabla_{\psi^{(k-1)}} f_{mt}^{F_\theta}\left(\underset{\substack{\uparrow \\ \text{expensive sampling loop per data point}}}{\psi^{(k-1)}}\right)\right)\right)^{-1}$$

- Discard interaction pattern

$$q(S;\underset{\substack{\uparrow \\ \text{Independent assumption}}}{\psi}) = \prod_{i\in S}\psi_i \prod_{j\notin S}(1-\psi_j)\,,\psi \in [0,1]^{|V|}$$

Amortizing MFVI

Reduce computational complexity

$$\psi_\theta^{(k)} \leftarrow \left(1 + \exp\left(-\nabla_{\psi^{(k-1)}} f_{mt}^{F_\theta}\left(\psi^{(k-1)}\right)\right)\right)^{-1}$$

$$\uparrow$$

expensive sampling loop per data point

Approximate with neural networks:

neural network $q_\phi : \mathbb{R}^{|V|} \rightarrow \mathbb{R}^{|V|}$

$$\downarrow$$

$$L = \mathbb{KL}(q_\phi(S;\psi) \| p_\theta(S))$$

$$= f_{mt}^{F_\theta}(\psi) + \mathbb{H}\left(q_\phi(S;\psi)\right) + const$$

$q_\phi(S;\psi)$ should satisfy **equivariant**

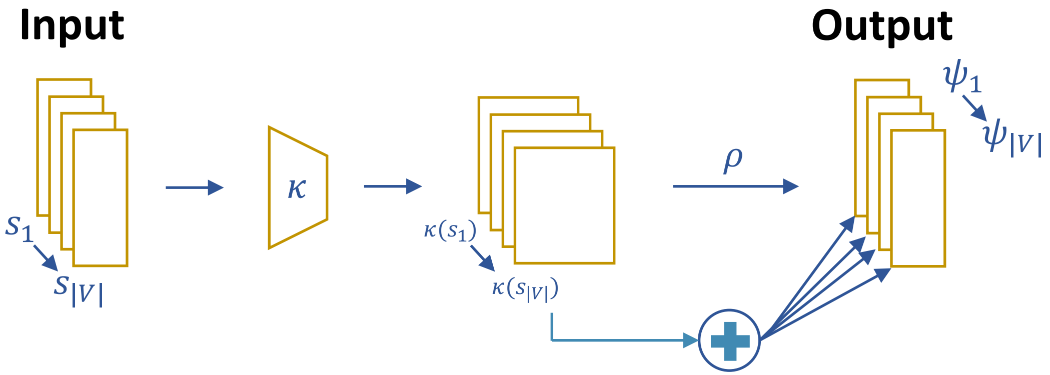
Amortizing MFVI

Reduce computational complexity

$$\psi_\theta^{(k)} \leftarrow \left(1 + \exp\left(-\nabla_{\psi^{(k-1)}} f_{mt}^{F_\theta}\left(\psi^{(k-1)}\right)\right)\right)^{-1}$$

expensive sampling loop per data point

$\mathrm{EquiNet}(V;\phi)$ with permutation equivariance



Zaheer Kottur, Ravanbakhsh, Poczos, Salakhutdinov and Smola. Deep sets. NIPS 2017.

Amortizing MFVI Induce interaction pattern

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$$q(S;\psi) = \prod_{i\in S}\psi_i \prod_{j\notin S}(1-\psi_j)\,, \psi \in [0,1]^{|V|}$$

Independent assumption

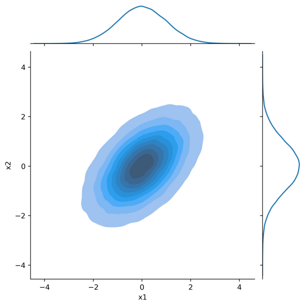
Correlation-aware inference:

Copula density

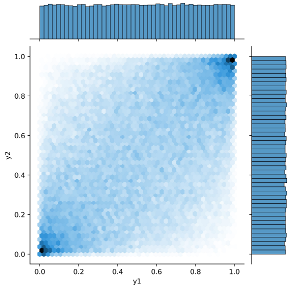
Marginal distribution

$$q\left(s_1, s_2, \ldots, s_{|V|}\right) = \mathrm{c}\left(Q_1(s_1), Q_2(s_2), \ldots, Q_{|V|}\left(s_{|V|}\right)\right)\prod_{i=1}^{|V|} q_i(s_i)$$

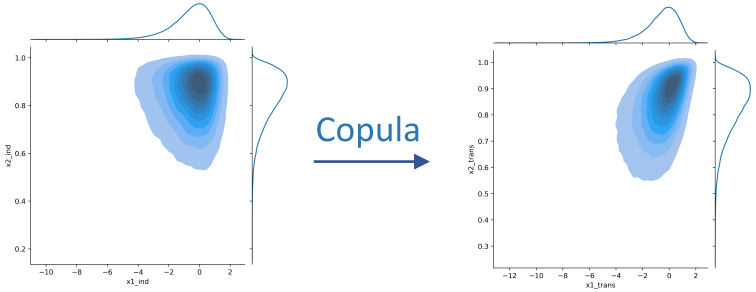
Cumulative distribution function



$$\begin{bmatrix}x_1\\x_2\end{bmatrix} \sim N\left(\begin{bmatrix}0\\0\end{bmatrix}, \begin{bmatrix}1 & 0.5\\0.5 & 1\end{bmatrix}\right)$$



$$\begin{bmatrix}y_1\\y_2\end{bmatrix} \sim c(Q_1(x_1), Q_2(x_2))$$



$$x_{1_{trans}} \sim Gumbel$$
$$x_{2_{trans}} \sim Beta$$

Amortizing MFVI Induce interaction pattern

$$q(s_1, s_2, \dots, s_{|V|}) = \underset{\uparrow}{\mathrm{c}}\left(Q_1(s_1), Q_2(s_2), \dots, Q_{|V|}(s_{|V|})\right) \prod_{i=1}^{|V|} q_i(s_i)$$

Apply Gaussian copula here

Induce Gaussian copula:

Sample an auxiliary noise

$$g \sim N(0, \Sigma)$$ → Covariance matrix , parameterized by neural network

Apply element-wise Gaussian CDF

$$u = \Phi_{diag(\Sigma)}(g)$$

Obtain binary sample

$$s = \mathbb{I}(\psi \leq u)$$ → Original logits of Bernoulli

Amortizing MFVI

$$\phi^* = \underset{\phi}{\operatorname{argmax}}\, f_{mt}^{F_\theta}(\psi) + \mathbb{H}\left(q_\phi(S;\psi)\right) \coloneqq \text{ELBO}$$

$$\theta^* = \underset{\theta}{\operatorname{argmin}} \textstyle\sum_{i=1}^{N}[-\sum_{j\in S_i^*} \log \underset{\substack{\uparrow \\ \psi^* = \text{MFVI}(\psi^{(0)}, V, K)}}{\psi_j^*} - \sum_{j\in V_i \backslash S_i^*} \log(1-\psi_j^*)]$$

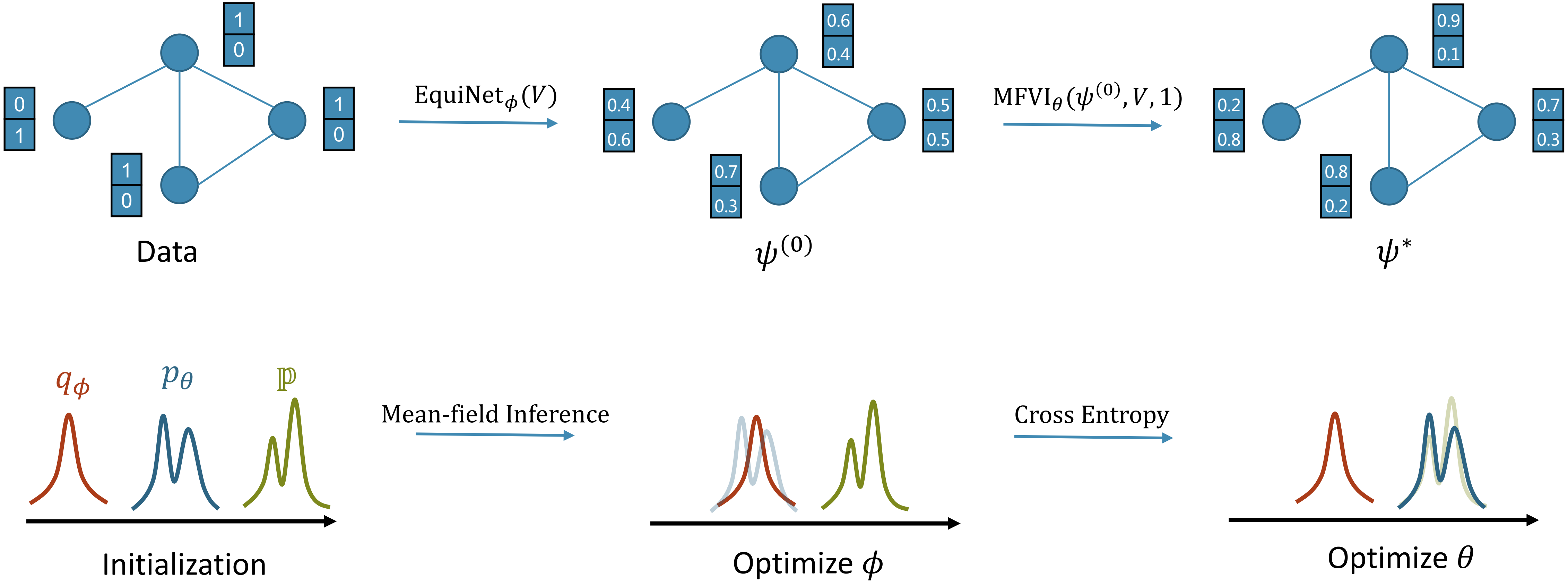
Algorithm $\text{EquiVSet}(V, S^*)$:

```
Update parameter $\phi$
    $\phi \leftarrow \phi + \eta\nabla_\phi \text{ELBO}(\phi)$                → Optimize $\phi$
Initialize variational parameter
    $\psi^{(0)} \leftarrow \text{EquiNet}(V;\phi)$                   ⎫
One step fixed point iteration                         ⎬ Mean-field Iteration
    $\psi^* \leftarrow \text{MFVI}(\psi^{(0)}, V, K = 1)$             ⎭
Update parameter $\theta$
    $\theta \leftarrow \theta - \eta\nabla_\theta L(\theta;\psi^*)$                   → Optimize $\theta$
```

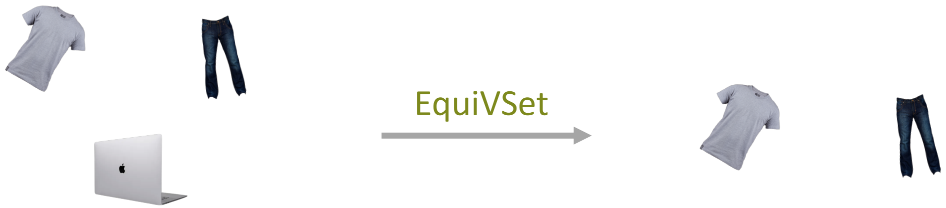
Cooperative training

EquiVSet is a cooperative training framework

$$\theta^* = \underset{\theta}{\operatorname{argmin}} \sum_{i=1}^{N} [-\sum_{j \in S_i^*} \log \psi_j^* - \sum_{j \in V_i \setminus S_i^*} \log(1 - \psi_j^*)]$$



Application: Product Recommender



EquiVSet

Ground set V

Optimal subset S^*

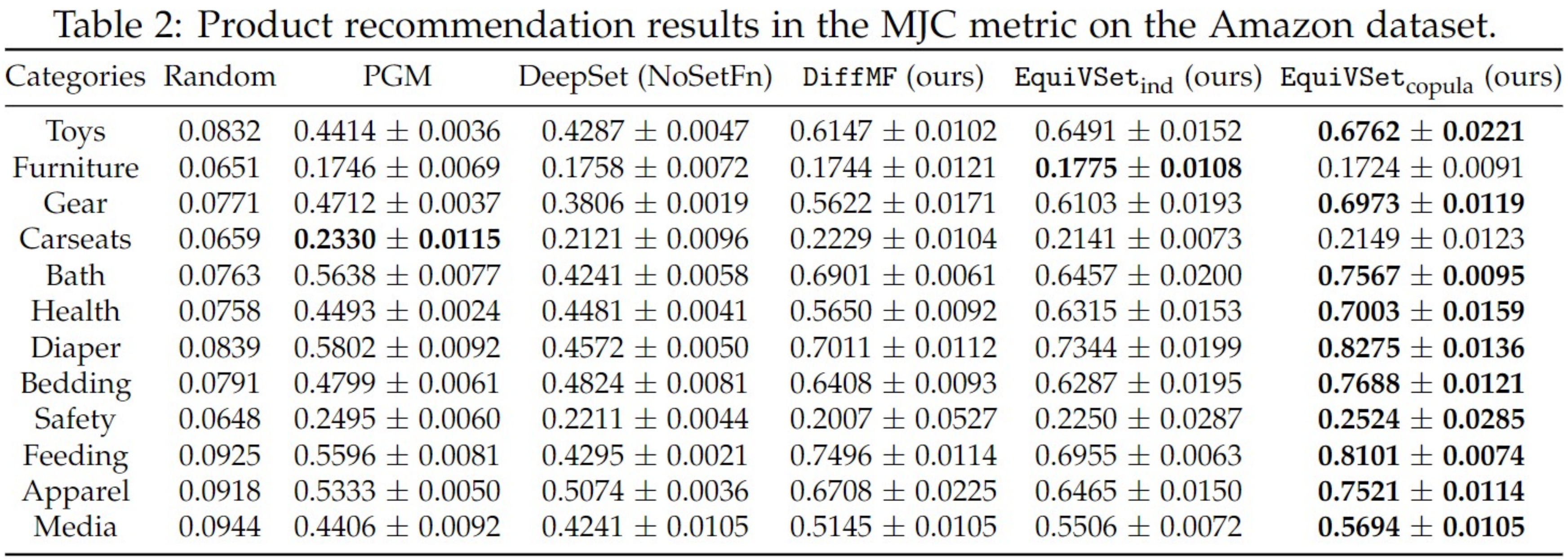
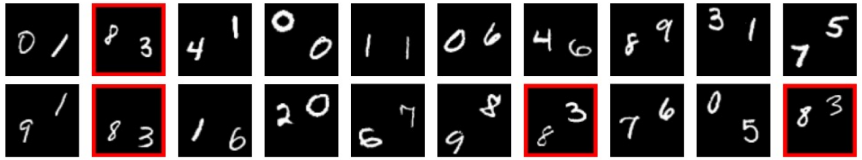


Table 2: Product recommendation results in the MJC metric on the Amazon dataset.

Categories	Random	PGM	DeepSet (NoSetFn)	`DiffMF` (ours)	$\texttt{EquiVSet}_{\text{ind}}$ (ours)	$\texttt{EquiVSet}_{\text{copula}}$ (ours)
Toys	0.0832	0.4414 ± 0.0036	0.4287 ± 0.0047	0.6147 ± 0.0102	0.6491 ± 0.0152	**0.6762 ± 0.0221**
Furniture	0.0651	0.1746 ± 0.0069	0.1758 ± 0.0072	0.1744 ± 0.0121	**0.1775 ± 0.0108**	0.1724 ± 0.0091
Gear	0.0771	0.4712 ± 0.0037	0.3806 ± 0.0019	0.5622 ± 0.0171	0.6103 ± 0.0193	**0.6973 ± 0.0119**
Carseats	0.0659	**0.2330 ± 0.0115**	0.2121 ± 0.0096	0.2229 ± 0.0104	0.2141 ± 0.0073	0.2149 ± 0.0123
Bath	0.0763	0.5638 ± 0.0077	0.4241 ± 0.0058	0.6901 ± 0.0061	0.6457 ± 0.0200	**0.7567 ± 0.0095**
Health	0.0758	0.4493 ± 0.0024	0.4481 ± 0.0041	0.5650 ± 0.0092	0.6315 ± 0.0153	**0.7003 ± 0.0159**
Diaper	0.0839	0.5802 ± 0.0092	0.4572 ± 0.0050	0.7011 ± 0.0112	0.7344 ± 0.0199	**0.8275 ± 0.0136**
Bedding	0.0791	0.4799 ± 0.0061	0.4824 ± 0.0081	0.6408 ± 0.0093	0.6287 ± 0.0195	**0.7688 ± 0.0121**
Safety	0.0648	0.2495 ± 0.0060	0.2211 ± 0.0044	0.2007 ± 0.0527	0.2250 ± 0.0287	**0.2524 ± 0.0285**
Feeding	0.0925	0.5596 ± 0.0081	0.4295 ± 0.0021	0.7496 ± 0.0114	0.6955 ± 0.0063	**0.8101 ± 0.0074**
Apparel	0.0918	0.5333 ± 0.0050	0.5074 ± 0.0036	0.6708 ± 0.0225	0.6465 ± 0.0150	**0.7521 ± 0.0114**
Media	0.0944	0.4406 ± 0.0092	0.4241 ± 0.0105	0.5145 ± 0.0105	0.5506 ± 0.0072	**0.5694 ± 0.0105**

$$\text{Metric: MJC} := \frac{1}{|\mathcal{D}_t|} \sum_{(V,S^*)\in\mathcal{D}_t} \frac{|S^* \cap S|}{|S^* \cup S|}$$

Application: Anomaly Detection



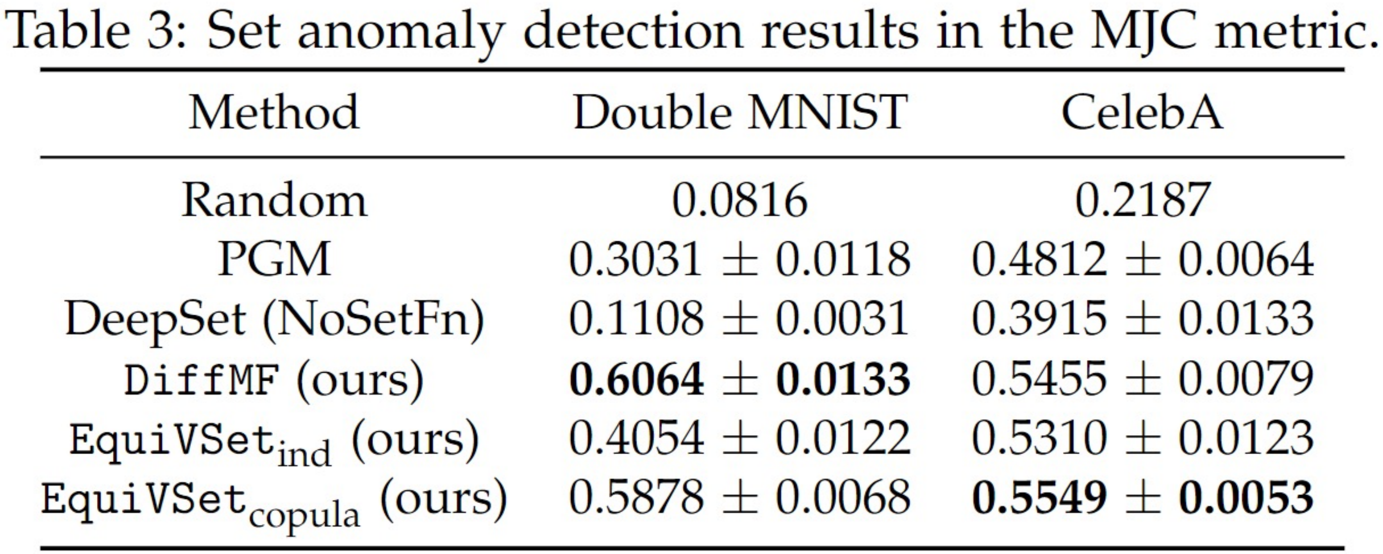
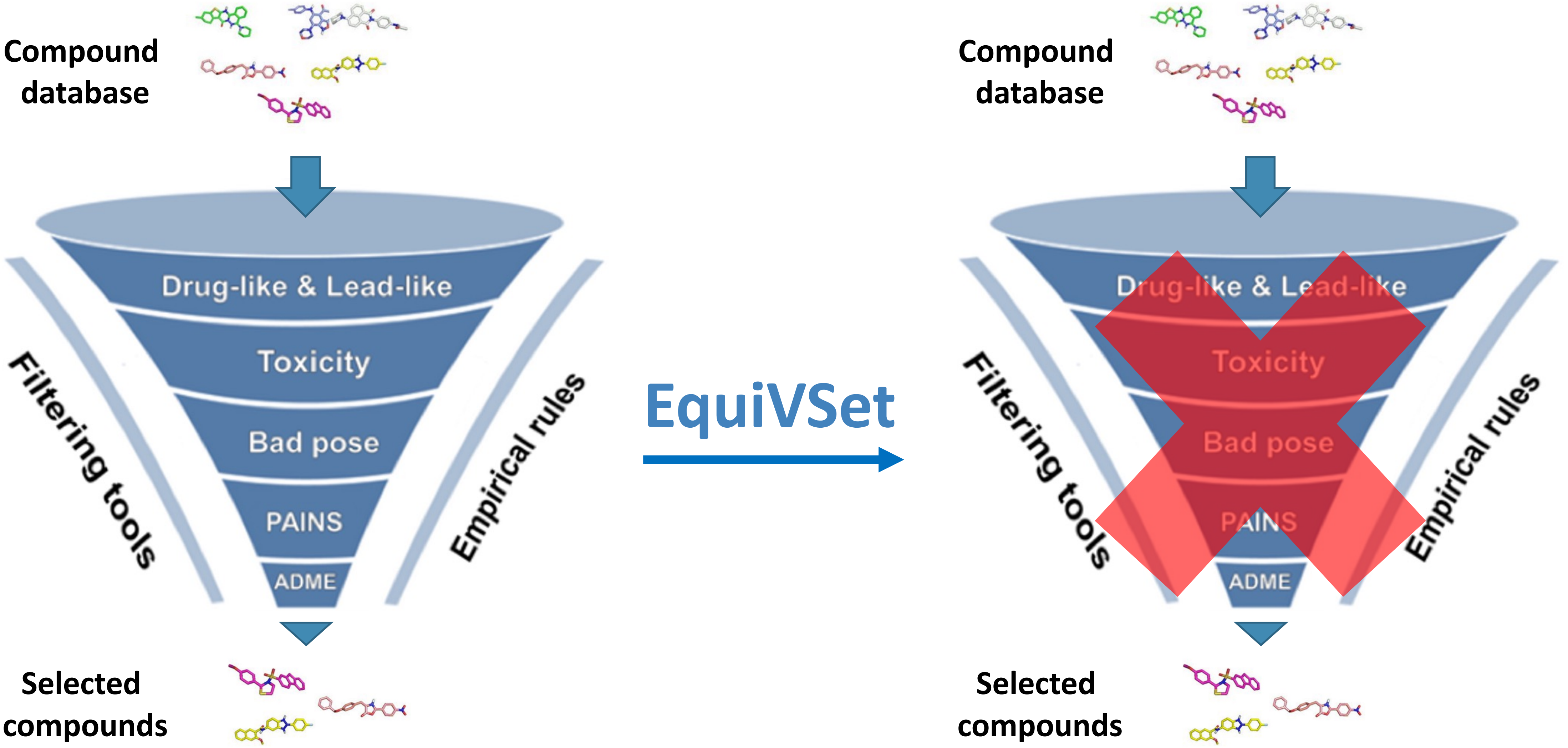


Table 3: Set anomaly detection results in the MJC metric.

Method	Double MNIST	CelebA
Random	0.0816	0.2187
PGM	0.3031 ± 0.0118	0.4812 ± 0.0064
DeepSet (NoSetFn)	0.1108 ± 0.0031	0.3915 ± 0.0133
`DiffMF` (ours)	**0.6064** ± **0.0133**	0.5455 ± 0.0079
$\texttt{EquiVSet}_{\text{ind}}$ (ours)	0.4054 ± 0.0122	0.5310 ± 0.0123
$\texttt{EquiVSet}_{\text{copula}}$ (ours)	0.5878 ± 0.0068	**0.5549** ± **0.0053**

Application: Compound Selection



Compound database

Drug-like & Lead-like

Toxicity

Bad pose

PAINS

ADME

Filtering tools

Empirical rules

Selected compounds

EquiVSet

Compound database

Drug-like & Lead-like

Toxicity

Bad pose

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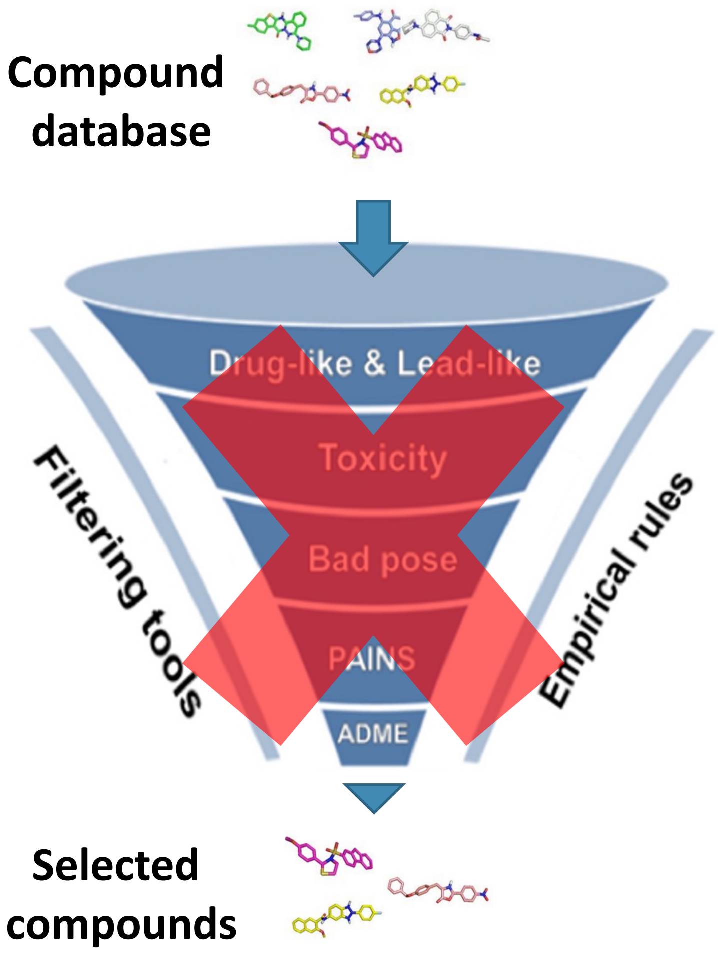
Filtering tools

Empirical rules

Selected compounds

Lionta et al. Structure-based virtual screening for drug discovery: principles, applications and recent advances. Current Topics in Medicinal Chemistry, 2014.

Application: Compound Selection



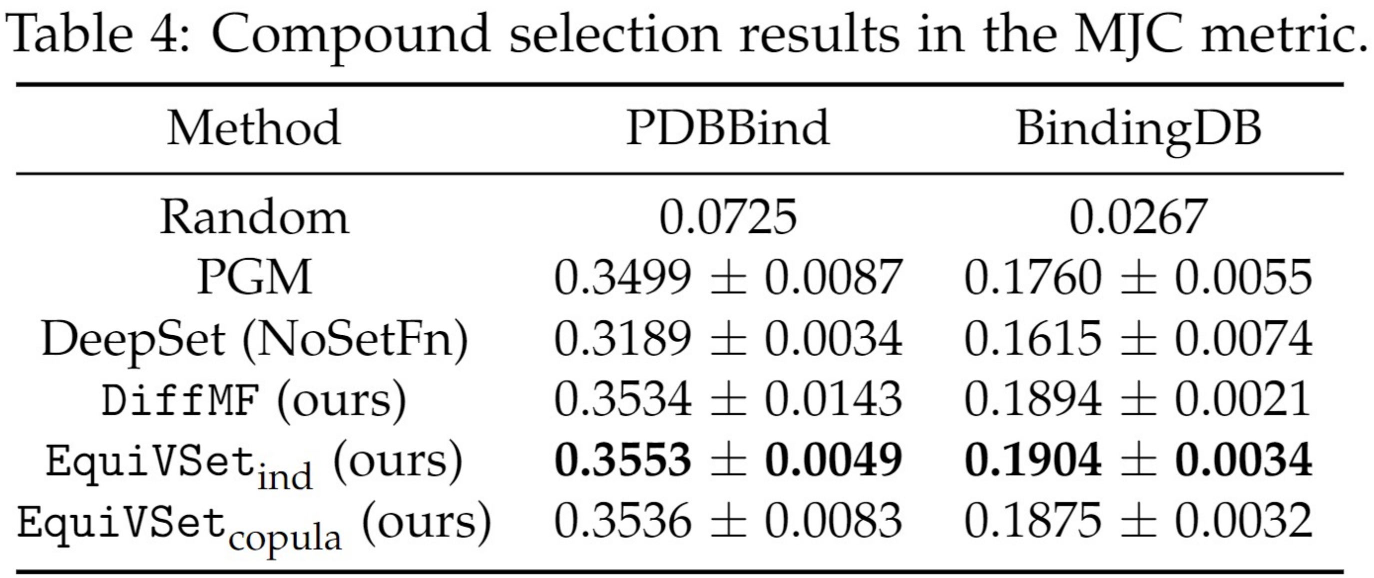


Table 4: Compound selection results in the MJC metric.

Method	PDBBind	BindingDB
Random	0.0725	0.0267
PGM	0.3499 ± 0.0087	0.1760 ± 0.0055
DeepSet (NoSetFn)	0.3189 ± 0.0034	0.1615 ± 0.0074
`DiffMF` (ours)	0.3534 ± 0.0143	0.1894 ± 0.0021
$\texttt{EquiVSet}_{\text{ind}}$ (ours)	$\mathbf{0.3553 \pm 0.0049}$	$\mathbf{0.1904 \pm 0.0034}$
$\texttt{EquiVSet}_{\text{copula}}$ (ours)	0.3536 ± 0.0083	0.1875 ± 0.0032

Tencent
AI Lab

Thank you!