Learning Neural Set Functions Under the Optimal Subset Oracle

Zijing Ou[1,2], Tingyang Xu[1],Qinliang Su[3],Yingzhen Li[2],Peilin Zhao[1],Yatao Bian[1]
[1]Tencent AI Lab
[2]Imperial College London
[3]Sun Yat—sen University

Background of Set Function Learning

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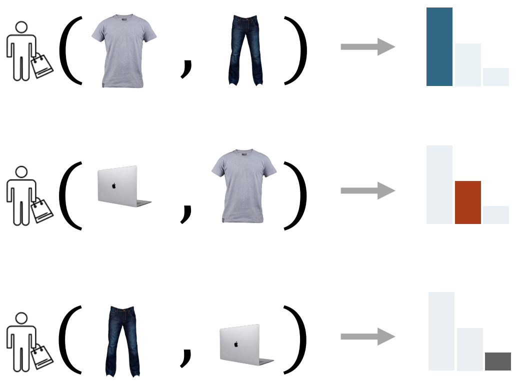
Database

Ground set V

Customer



Utility function

$F_{\theta^*}(\cdot; V): 2^V \to \mathbb{R}$

Shopping cart

Optimal subset S^*

Data Generation Process:

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

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

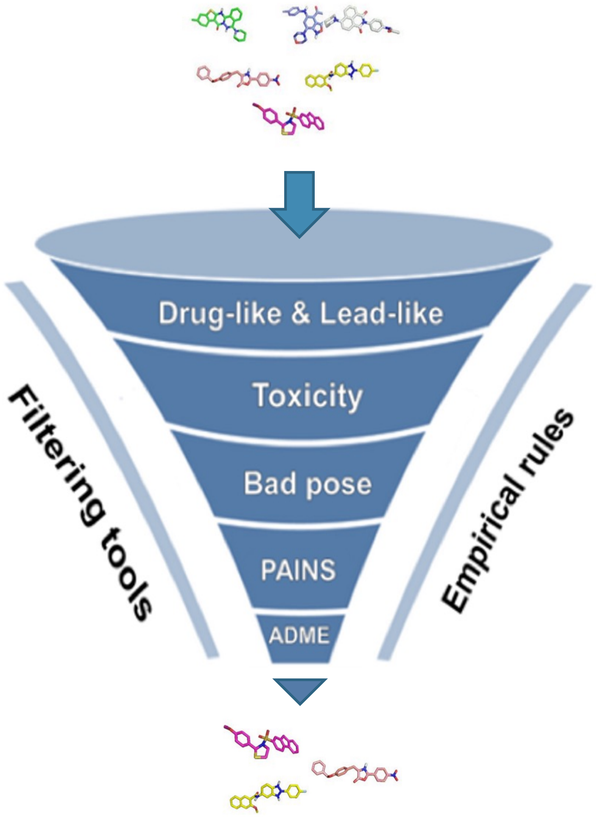
Background of Set Function Learning

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

Set anomaly detection

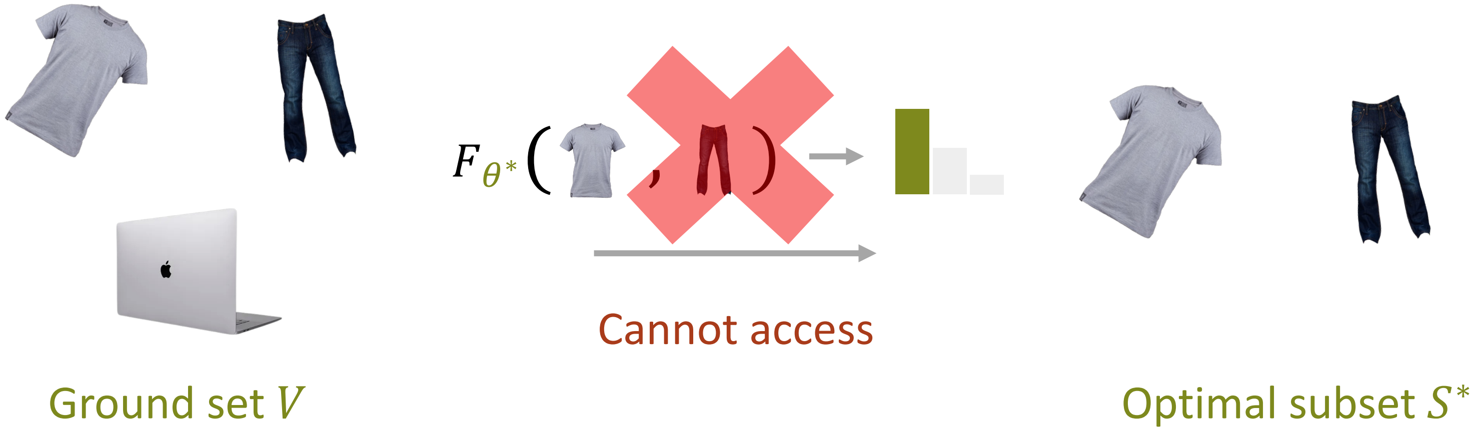
$F_{\theta^*}(S; V) = \sum_{s_i \in S} \mathbb{I}(s_i \text{ is male}) - \mathbb{I}(s_i \text{ is female})$

Compound selection



Background of Set Function Learning

Setting: Training data is given in form of $\{(V_i, S_i^*)\}_{i=1}^{N}$



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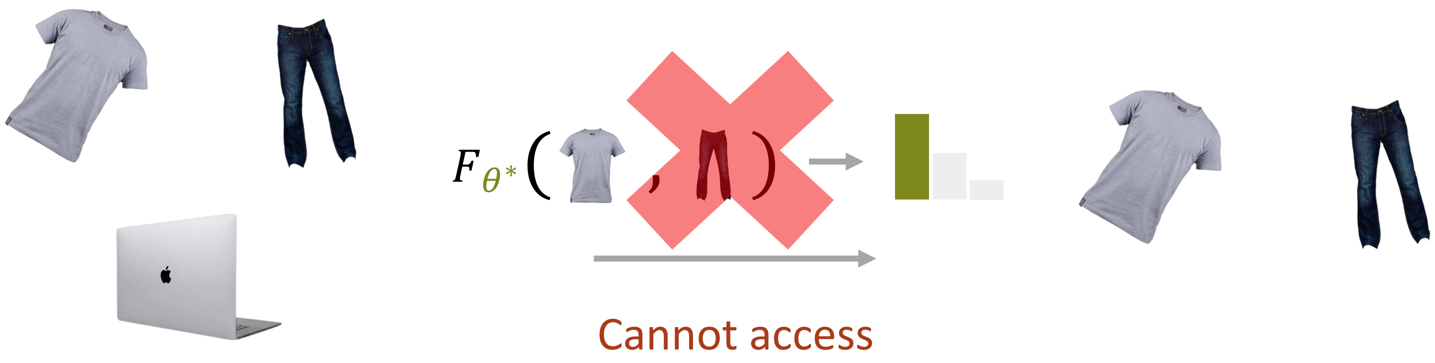

Ground set V Optimal subset S^*

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

$$S^* = \underset{S \in 2^V}{\operatorname{argmax}} F_\theta(S; V), \forall (V, S^*) \in \{(\mathrm{V}_i, \mathrm{S}_\mathrm{i}^*)\}_{\mathrm{i}=1}^{\mathrm{N}}$$

Learning Set Function Under the OS Oracle

Maximum Likelihood:

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 MLE

Maximum Likelihood:

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Monotonically grows with the utility function

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

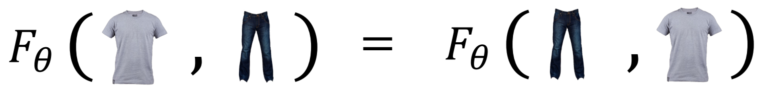
Maximum Likelihood:

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

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

Desiderata:

Permutation invariance



Varying ground set

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Energy-based Modeling for Set

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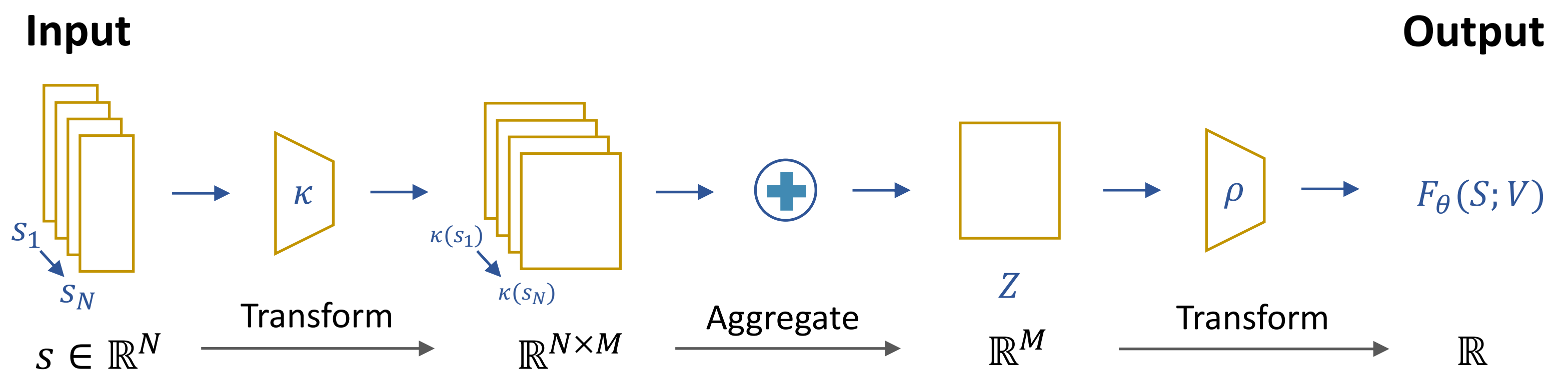
$$p_\theta(S|V) = \frac{\exp(F_\theta(S;V))}{Z}$$

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

DeepSet for Permutation Invariance & Varying Ground Set:



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

Training Discrete EBMs

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Marginal-based Loss:

ψ^* is differentiable w.r.t. θ

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

$$\psi^{*|\theta} = \underset{\psi}{\operatorname{argmin}}\, \mathbb{KL}(q_\phi(S;\psi)\|p_\theta(S))$$

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

Training θ by differentiating through ψ^* using cross entropy loss

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

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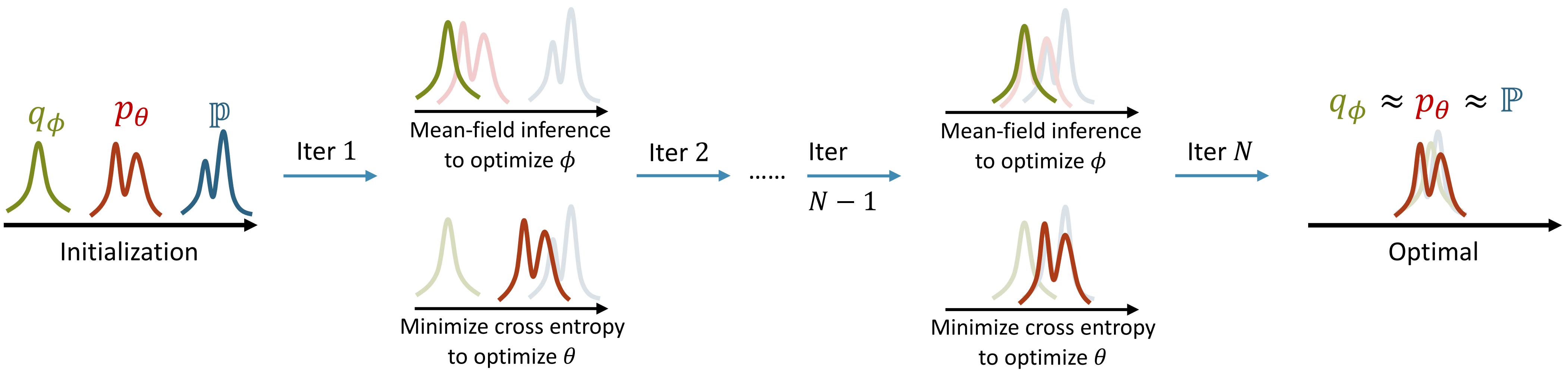
Training θ by differentiating through ψ^* using cross entropy loss



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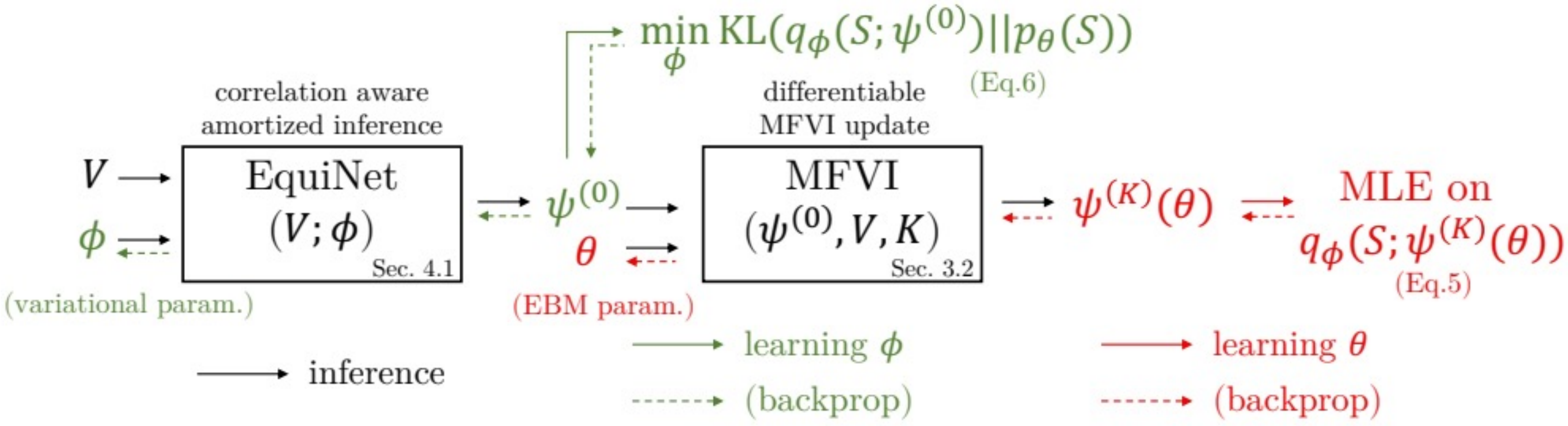
EquiVSet Overview

$$\psi^{*|\theta} = \underset{\psi}{\operatorname{argmin}}\, \mathbb{KL}(q(S;\psi) \| p_\theta(S))$$

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

Equivariant **V**ariational inference for **Set** function learning (**EquiVSet**)

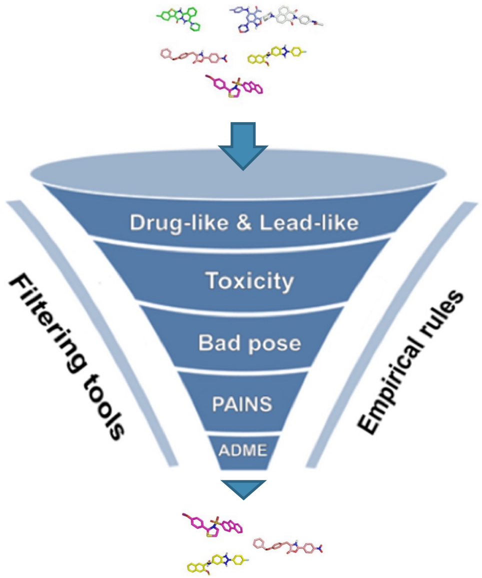


Applications

EquiVSet achieves **SOTA** results on 3 different tasks!!!

Product Recommendation

Set Anomaly Detection



Compound Selection

Applications: product recommendation

Table 2: Product recommendation results on the Amazon dataset with different categories.

Categories	Random	PGM	DeepSet (NoSetFn)	DiffMF (ours)	$\texttt{EquiVSet}_{\text{ind}}$ (ours)	$\texttt{EquiVSet}_{\text{copula}}$ (ours)
Toys	0.083	0.441 ± 0.004	0.429 ± 0.005	0.610 ± 0.010	0.650 ± 0.015	**0.680 ± 0.020**
Furniture	0.065	0.175 ± 0.007	**0.176 ± 0.007**	0.170 ± 0.010	0.170 ± 0.011	0.172 ± 0.009
Gear	0.077	0.471 ± 0.004	0.381 ± 0.002	0.560 ± 0.020	0.610 ± 0.020	**0.700 ± 0.020**
Carseats	0.066	**0.230 ± 0.010**	0.210 ± 0.010	0.220 ± 0.010	0.214 ± 0.007	0.210 ± 0.010
Bath	0.076	0.564 ± 0.008	0.424 ± 0.006	0.690 ± 0.006	0.650 ± 0.020	**0.757 ± 0.009**
Health	0.076	0.449 ± 0.002	0.448 ± 0.004	0.565 ± 0.009	0.630 ± 0.020	**0.700 ± 0.020**
Diaper	0.084	0.580 ± 0.009	0.457 ± 0.005	0.700 ± 0.010	0.730 ± 0.020	**0.830 ± 0.010**
Bedding	0.079	0.480 ± 0.006	0.482 ± 0.008	0.641 ± 0.009	0.630 ± 0.020	**0.770 ± 0.010**
Safety	0.065	0.250 ± 0.006	0.221 ± 0.004	0.200 ± 0.050	0.230 ± 0.030	**0.250 ± 0.030**
Feeding	0.093	0.560 ± 0.008	0.430 ± 0.002	0.750 ± 0.010	0.696 ± 0.006	**0.810 ± 0.007**
Apparel	0.090	0.533 ± 0.005	0.507 ± 0.004	0.670 ± 0.020	0.650 ± 0.020	**0.750 ± 0.010**
Media	0.094	0.441 ± 0.009	0.420 ± 0.010	0.510 ± 0.010	0.551 ± 0.007	**0.570 ± 0.010**

EquiVSet achieves improvements up to 33% on average

Thank you!

Code is available at: https://github.com/SubsetSelection/EquiVSet

✓ Welcome to try it out in Colab: Open in Colab