# Shape Constraints for Set Functions

Andrew Cotter, Maya R. Gupta, Heinrich Jiang, Erez Louidor, James Muller, Taman Narayan, Serena Wang, <u>Tao Zhu</u>

Google Research

• **Problem**: Learn a **set function** to predict a label given a *variable-size* set of feature vectors.

$$f: \{x_m \in \mathbb{R}^D\} \to y \in \mathbb{R}$$

• **Problem**: Learn a **set function** to predict a label given a *variable-size* set of feature vectors.

$$f: \{x_m \in \mathbb{R}^D\} \to y \in \mathbb{R}$$

• **Use Case:** Classify if a recipe is French given its set of ingredients.

• **Problem**: Learn a **set function** to predict a label given a *variable-size* set of feature vectors.

$$f: \{x_m \in \mathbb{R}^D\} \to y \in \mathbb{R}$$

- Use Case: Classify if a recipe is French given its set of ingredients.
- Use Case: Estimate label given compound sparse categorical features.
  - Predict if a KickStarter campaign will succeed given its **name** "Superhero Teddy Bear".

How likely a campaign succeeds given its **name** "Superhero Teddy Bear"?

**E**(Y | "Superhero Teddy Bear")

How likely a campaign succeeds given its **name** "Superhero Teddy Bear"?

```
E(Y | "Superhero") = 0.3
```

```
E(Y | "Superhero Teddy Bear") -
```

```
└ E(Y | "Teddy Bear") = 0.9
```

Mean  $(\{0.3, 0.9\}) = 0.6$ Min  $(\{0.3, 0.9\}) = 0.3$ Max  $(\{0.3, 0.9\}) = 0.9$ Median  $(\{0.3, 0.9\}) = 0.6$ 

How likely a campaign succeeds given its **name** "Superhero Teddy Bear"?

```
E(Y | "Superhero Teddy Bear") = C(Y | "Superhero") = 0.3
Count("Superhero") = 100
Count("Superhero") = 100
Count("Teddy Bear") = 0.9
Count("Teddy Bear") = 50
```

How likely a campaign succeeds given its **name** "Superhero Teddy Bear"?

E(Y | "Superhero Teddy Bear")

E(Y | "Superhero") = 0.3 Count("Superhero") = 100 Size("Superhero") = 1 E(Y | "Teddy Bear") = 0.9 Count("Teddy Bear") = 50 Size("Teddy Bear") = 2

**0.3**\*100\*1 + **0.9**\*50\*2 100\*1 + 50\*2

How likely a campaign succeeds given its name "Superhero Teddy Bear"?

E(Y | "Superhero Teddy Bear")

E(Y | "Superhero") = 0.3
Count("Superhero") = 100
Size("Superhero") = 1

```
0.3*100*1 + 0.9*50*2
100*1 + 50*2
```

```
E(Y | "Teddy Bear") = 0.9
Count("Teddy Bear") = 50
Size("Teddy Bear") = 2
```



How likely a campaign succeeds given its name "Superhero Teddy Bear"?

E(Y | "Superhero Teddy Bear")

E(Y | "Superhero") = 0.3
Count("Superhero") = 100
Size("Superhero") = 1
E(Y | "Teddy Bear") = 0.9
Count("Teddy Bear") = 50
Size("Teddy Bear") = 2

Learned Set Function ({ [0.3, 100, 1], [0.9, 50, 2]})

$$f(x) = \rho\left(\frac{1}{M(x)}\sum_{m=1}^{M(x)}\phi(x_m)\right)$$

[Deep Sets, Zaheer et al. 2017]

How likely a campaign succeeds given its name "Superhero Teddy Bear"?

E(Y | "Superhero Teddy Bear")

E(Y | "Superhero") = 0.3
Count("Superhero") = 100
Size("Superhero") = 1

E(Y | "Teddy Bear") = 0.9 Count("Teddy Bear") = 50 Size("Teddy Bear") = 2 Learned Set Function ({ [0.3, 100, 1], [0.9, 50, 2]})

> Too flexible "over-fit"



How likely a campaign succeeds given its name "Superhero Teddy Bear"?

Set function properties for more regularization and better interpretability

- **Monotonicity**: output does not decrease as E(Y | "Superhero") or E(Y | "Teddy Bear") increases.
- **Conditioning**: *conditioning* feature (count/size) tells how much to trust *primary* feature.

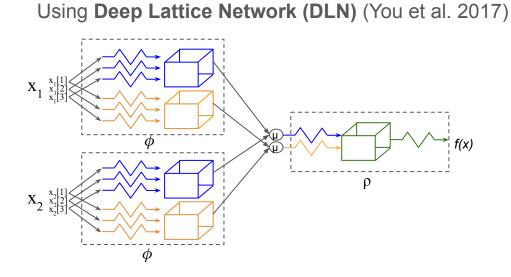
How likely a campaign succeeds given its name "Superhero Teddy Bear"?

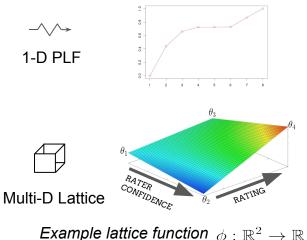
Set function properties for more regularization and better interpretability

- **Monotonicity**: output does not decrease as E(Y | "Superhero") or E(Y | "Teddy Bear") increases.
- **Conditioning**: *conditioning* feature (count/size) tells how much to trust *primary* feature.

#### Can we learn flexible set functions while satisfying such properties?

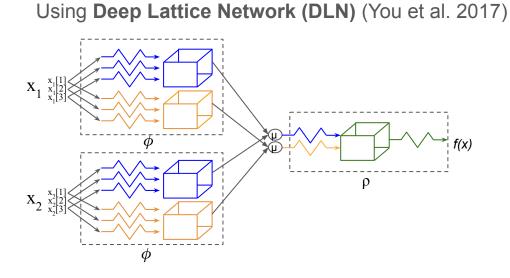
#### Our approach: DLN with Shape Constraints



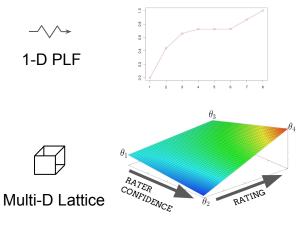


- Monotonicity  $\phi(\theta_3) \ge \phi(\theta_1), \phi(\theta_4) \ge \phi(\theta_2)$
- Conditioning (Edgeworth)  $\phi(\theta_4) - \phi(\theta_2) \ge \phi(\theta_3) - \phi(\theta_1)$
- Conditioning (Trapezoid)  $\phi(\theta_1) \ge \phi(\theta_2), \phi(\theta_4) \ge \phi(\theta_3)$

#### Our approach: DLN with Shape Constraints



- Constrained empirical risk minimization based on SGD
- Shapes constraints work for normal functions (set size = 1) using DLN as well



Example lattice function  $\phi : \mathbb{R}^2 \to \mathbb{R}$ 

- Monotonicity  $\phi(\theta_3) \ge \phi(\theta_1), \phi(\theta_4) \ge \phi(\theta_2)$
- Conditioning (Edgeworth)  $\phi(\theta_4) - \phi(\theta_2) \ge \phi(\theta_3) - \phi(\theta_1)$
- Conditioning (Trapezoid)  $\phi(\theta_1) \ge \phi(\theta_2), \phi(\theta_4) \ge \phi(\theta_3)$

### Semantic Feature Engine

• Estimate E(Y | "Superhero Teddy Bear")



- Shape constraints
  - **Monotonicity**: Output monotonically increasing wrt. each ngram estimate.
  - **Conditioning**: Trust more frequent ngrams more...
- Similar accuracy as Deep Sets (Zaheer et al. 2017) and DNN, but with guarantees on model behavior producing better generalization and more debuggability.

## Poster Tonight 06:30 -- 09:00 PM @ Pacific Ballroom #127