# Performance-Aligned Learning Algorithms with Statistical Guarantees

**RIZAL FATHONY** 





### Outline









Bipartite Matching in Graphs



Multiclass Classification



Motivation

### **Empirical Risk Minimization (ERM)**

- Assume a family of parametric hypothesis function *f* (e.g. linear discriminator)
- Find the hypothesis  $f^*$  that minimize the empirical risk:

$$\min_{f} \frac{1}{n} \sum_{i=1}^{n} \operatorname{loss}(f(\mathbf{x}_{i}), y_{i}) = \min_{f} \mathbb{E}_{\mathbf{X}, Y \sim \tilde{P}} \left[ \operatorname{loss}(f(\mathbf{X}), Y) \right]$$

Intractable optimization, non-convex, non-continuous Convex surrogate loss need to be employed!

A desirable property of convex surrogates:

### **Fisher Consistency**

Under ideal condition: optimize surrogate  $\rightarrow$  minimizes the loss metric (given the true distribution and fully expressive model)



### **Two Main Approaches**



### Probabilistic Approach

- Construct prediction probability model
- Employ the logistic loss surrogate

### Logistic Regression, Conditional Random Fields (CRF)



### Maximum Margin Approach

- Maximize the margin that separates correct prediction from the incorrect one
- Employ the hinge loss surrogate

Support Vector Machine (SVM), Structured SVM





### Multiclass Classification | Logistic Regression vs SVM



**Multiclass Logistic Regression** 





Statistical guarantee of Fisher consistency (minimizes the zero-one loss metric in the limit)







- Lack Fisher consistency property, or
- Doesn't perform well in practice

Structured Prediction | CRF vs Structured SVM



Conditional Random Fields (CRF)





Statistical guarantee of Fisher consistency







Computation of the normalization term may be intractable





Relatively more efficient in computation

### New Learning Algorithms?



Align better with the loss/performance metric (by incorporating the metric into its learning objective)



Provide Fisher consistency guarantee





#### How?

#### Robust adversarial learning approach

"What predictor best maximizes the performance metric (or minimizes the loss metric) in the worst case given the statistical summaries of the empirical distributions?"

### **Robust Adversarial Formulation**

### Robust Adversarial Formulation (Asif et.al, 2015; Grunwald & Dawid, 2004; Topsoe, 1979)

**Original Loss Metric** Approximate the loss Non-convex, non-continuous with convex surrogates  $\min_{f} \mathbb{E}_{\mathbf{X}, Y \sim \tilde{P}} \left[ \operatorname{loss}(f(\mathbf{X}), Y) \right]$ Probabilistic prediction  $\min_{\hat{P}(\hat{Y}|\mathbf{X})} \mathbb{E}_{\mathbf{X}, Y \sim \tilde{P}; \hat{Y}|\mathbf{X} \sim \hat{P}} \left[ loss(\hat{Y}, Y) \right]$ Evaluate against an adversary, instead of using empirical data Adversary's probabilistic prediction  $\check{P}(\check{Y}|\mathbf{X})$  $\min_{\hat{P}(\hat{Y}|\mathbf{X})} \max_{\check{P}(\check{Y}|\mathbf{X})} \mathbb{E}_{\mathbf{X},Y\sim\tilde{P};\hat{Y}|\mathbf{X}\sim\hat{P};\check{Y}|\mathbf{X}\sim\check{P}} \left[ loss(\hat{Y},\check{Y}) \right]$ 

 $\stackrel{\bullet}{\longrightarrow} \frac{\text{Empirical Risk Minimization}}{\min_{f} \mathbb{E}_{\mathbf{X}, Y \sim \tilde{P}} [\text{surrogate}(f(\mathbf{X}), Y)]} \\ \hat{y} = \operatorname*{argmax}_{j} f_{j}(\mathbf{x})$ 

#### **Robust Adversarial Formulation**

 $\min_{\hat{P}(\hat{Y}|\mathbf{X})} \max_{\check{P}(\check{Y}|\mathbf{X})} \mathbb{E}_{\mathbf{X},Y\sim\tilde{P};\hat{Y}|\mathbf{X}\sim\hat{P};\check{Y}|\mathbf{X}\sim\check{P}} \left[ loss(\hat{Y},\check{Y}) \right]$ s.t.  $\mathbb{E}_{\mathbf{X}\sim\tilde{P};\check{Y}|\mathbf{X}\sim\check{P}} [\phi(\mathbf{X},\check{Y})] = \mathbb{E}_{\mathbf{X},Y\sim\tilde{P}} [\phi(\mathbf{X},Y)]$ 

**Constraint** the **statistics** of the **adversary**'s distribution to match the **empirical** statistics

### **Robust Adversarial Dual Formulation**

### Multiclass Zero-One Classification

Based on:

**Rizal Fathony**, Anqi Liu, Kaiser Asif, Brian D. Ziebart. *"Adversarial Multiclass Classification: A Risk Minimization Perspective"*. Advances in Neural Information Processing Systems 29 (NIPS), 2016.

### Multiclass Classification | Zero-One Loss

#### Example: Digit Recognition

#### Loss Metric: Zero-One Loss



Loss Metric:  $loss(\hat{y}, y) = I(\hat{y} \neq y)$ 

$$\mathbf{L} = \begin{bmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{bmatrix}$$

### Multiclass Classification | Related Works

#### Multiclass Support Vector Machine (SVM)

Fisher Consistent? (Tewari and Bartlett, 2007) (Liu, 2007) Perform well in low dimensional feature? (Dogan et.al., 2016)



**Relative Margin Model** 

3. The LLW Model (Lee et.al., 2004)

$$loss_{LLW}(\mathbf{x}_i, y_i) = \sum_{j \neq y_i} [1 + f_j(\mathbf{x}_i)]_+$$
  
with:  $\sum_j f_j(\mathbf{x}_i) = 0$   
Absolute Margin Model



### Adversarial Surrogate Loss for Zero-One Loss (AL<sup>0-1</sup>)

#### Adversarial Surrogate Loss

$$AL(\mathbf{f}, y) = \max_{\mathbf{q} \in \Delta} \min_{\mathbf{p} \in \Delta} \mathbf{p}^{\mathsf{T}} \mathbf{L} \mathbf{q} + \mathbf{f}^{\mathsf{T}} \mathbf{q} - f_y$$

#### Convert to Linear Program

$$\begin{aligned} AL(\mathbf{f}, y) &= \max_{\mathbf{q}, v} v + \mathbf{f}^{\mathsf{T}} \mathbf{q} - f_y \\ \text{s.t.: } \mathbf{L}_{(i,:)} \mathbf{q} \geq v \quad \forall i \in [k] \\ q_i \geq 0 \qquad \forall i \in [k] \\ \mathbf{q}^{\mathsf{T}} \mathbf{1} = 1 \end{aligned}$$

#### Convex Polytope formed by the constraints

$$C = \left\{ \begin{bmatrix} \mathbf{q} \\ v \end{bmatrix} \middle| \mathbf{A} \begin{bmatrix} \mathbf{q} \\ v \end{bmatrix} \ge \mathbf{b}, \text{ where } \mathbf{A} = \begin{bmatrix} \mathbf{L} & -\mathbf{1} \\ \mathbf{I} & \mathbf{0} \\ \mathbf{1}^{\mathsf{T}} & \mathbf{0} \\ -\mathbf{1}^{\mathsf{T}} & \mathbf{0} \end{bmatrix}, \mathbf{b} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{1} \\ -\mathbf{1} \end{bmatrix} \right\}$$

#### Example for a four class classification



#### Extreme points of the (bounded) polytope

There is always an optimal solution that is an extreme point of the domain.

Computing AL = finding the best extreme point

### AL<sup>0-1</sup> | Convex Polytope

#### Convex Polytope of the AL<sup>0-1</sup>

$$\mathbb{C} = \left\{ \begin{bmatrix} \mathbf{q} \\ v \end{bmatrix} \middle| \mathbf{A} \begin{bmatrix} \mathbf{q} \\ v \end{bmatrix} \ge \mathbf{b}, \text{ where } \mathbf{A} = \begin{bmatrix} \mathbf{L} & -\mathbf{1} \\ \mathbf{I} & \mathbf{0} \\ \mathbf{1}^{\mathsf{T}} & \mathbf{0} \\ -\mathbf{1}^{\mathsf{T}} & \mathbf{0} \end{bmatrix}, \mathbf{b} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{1} \\ -\mathbf{1} \end{bmatrix} \right\}$$
$$\mathbf{L} = \begin{bmatrix} \mathbf{0} & \mathbf{1} & \mathbf{1} & \mathbf{1} \\ \mathbf{1} & \mathbf{0} & \mathbf{1} & \mathbf{1} \\ \mathbf{1} & \mathbf{1} & \mathbf{0} & \mathbf{1} \\ \mathbf{1} & \mathbf{1} & \mathbf{0} \end{bmatrix}$$

#### Extreme points of the polytope

$$D = \left\{ \begin{bmatrix} \mathbf{q} \\ v \end{bmatrix} = \frac{1}{|S|} \begin{bmatrix} \sum_{i \in S} \mathbf{e}_i \\ |S| - 1 \end{bmatrix} \ \middle| \ \emptyset \neq S \subseteq [k] \right\}$$

 $e_i$  is a vector with a single 1 at the *i*-th index, and 0 elsewhere.

 $[k] \triangleq \{1, \dots, k\}$ 

The Adversarial Surrogate Loss for Zero-One Loss Metrics (AL<sup>0-1</sup>)

$$AL^{0-1}(\mathbf{f}, y) = \max_{S \subseteq [k], S \neq \emptyset} \frac{\sum_{i \in S} f_i + |S| - 1}{|S|} - f_y$$

#### Computation of $AL^{0-1}$

- Sort  $f_i$  in non-increasing order
- Incrementally add potentials to the set *S*, until adding more potential decrease the loss value

 $O(k \log k)$ , where k is the number of classes

### AL<sup>0-1</sup> | Loss Surface

#### **Binary Classification**



- Plots over the space of potential differences  $\psi_i = f_i - f_y$ - The true label is y = 1



**Three Class Classification** 



### **Fisher Consistency**

#### Fisher Consistency Requirement in Classification

$$f^* \in \mathcal{F}^* \triangleq \underset{f}{\operatorname{argmin}} \mathbb{E}_{Y|\mathbf{x} \sim P} \left[ \operatorname{surrogate}_f(\mathbf{x}, Y) \right] \implies \underset{y}{\operatorname{argmax}} f^*(\mathbf{x}, y) \subseteq \mathcal{Y}^\diamond \triangleq \underset{y'}{\operatorname{argmin}} \mathbb{E}_{Y|\mathbf{x} \sim P} \left[ \operatorname{loss}(y', Y) \right]$$

- P(Y|x) is the true conditional distribution

- f is optimized over all measurable functions

Bayes risk minimizer

#### The property of the minimizer for AL

Loss reflective property of AL, for any loss metrics  $f^*(\mathbf{x}, y) + loss(y^\diamond, y) = constant$ , i.e., is invariant to y  $y^\diamond$  is the Bayes risk minimizer.

$$\operatorname{argmax}_y f^*(\mathbf{x}, y) = \operatorname{argmin}_y \mathbf{L}_{(y^\diamond, y)}$$
  
Fisher consistent

### AL<sup>0-1</sup> | Optimization

#### Primal

Stochastic sub-gradient descent

$$\partial_{\theta} AL^{0-1}(\mathbf{x}, y, \theta) \ni \frac{1}{|S^*|} \sum_{j \in S^*} \phi(\mathbf{x}, j) - \phi(\mathbf{x}, y)$$

 $S^*$  is the set that maximize  $AL^{0-1}$ 

#### Kernel trick



#### **Dual Optimization**

Exp. number of constraints (primal)  $\rightarrow$  Exp. number of variables (dual) Constraint Generation Algorithm

#### Dual

#### **Constrained Primal QP**

$$\begin{split} \min_{\theta} \frac{1}{2} \|\theta\|^2 + C \sum_{i=1}^n \xi_i \\ \text{subject to:} \quad \xi_i \ge \Delta_{i,k} \quad \forall i \in \{1, \dots, n\} k \in \{1, \dots, 2^{|\mathcal{Y}|} - 1\} \end{split}$$

 $\Delta$  enumerate all  $2^{|\mathcal{Y}|} - 1$  possible values of AL<sup>0-1</sup> for each sample

#### **Dual QP Formulation**

$$\begin{split} \max_{\alpha} \sum_{i=1}^{n} \sum_{k=1}^{2^{|\mathcal{Y}|-1}} \nu_{i,k} \, \alpha_{i,k} - \frac{1}{2} \sum_{i,j=1}^{m} \sum_{k,l=1}^{2^{|\mathcal{Y}|-1}} \alpha_{i,k} \alpha_{j,l} \left[\Lambda_{i,k} \cdot \Lambda_{j,l}\right] \\ \text{subject to} \quad \alpha_{i,k} \ge 0, \ \sum_{k=1}^{2^{|\mathcal{Y}|-1}} \alpha_{i,k} = C, \ i \in \{1, \dots, n\}, \ k \in \{1, \dots, 2^{|\mathcal{Y}|} - 1\} \\ \text{where:} \\ \Lambda_{i,k} = \frac{d\Delta_{i,k}}{d\theta} \text{ , and } \nu_{i,k} \text{ is the constant part of } \Delta_{i,k} \\ \Lambda_{i,k} \cdot \Lambda_{j,l} = c_{(i,k),(j,l)} K(\mathbf{x}_i, \mathbf{x}_j) \end{split}$$

for some constants  $c_{(i,k)}$  and  $c_{(j,l)}$ 

### AL<sup>0-1</sup> | Experiments

#### Dataset properties and AL<sup>0-1</sup> constraints

	Dataset		Prop	erties		SVM	$AL^{0-1}$ of	constrai	nts added ar	nd active
		#class	#train	# test	#feat.	constraints	Linear	kernel	Gauss	. kernel
(1)	iris	3	105	45	4	210	213	13	223	38
(2)	$\operatorname{glass}$	6	149	65	9	745	578	125	490	252
(3)	redwine	10	1119	480	11	10071	5995	1681	3811	1783
(4)	ecoli	8	235	101	7	1645	614	117	821	130
(5)	vehicle	4	592	254	18	1776	1310	311	1201	248
(6)	segment	7	1617	693	19	9702	4410	244	4312	469
(7)	sat	7	4435	2000	36	26610	11721	1524	11860	6269
(8)	opt digits	10	3823	1797	64	34407	7932	597	10072	2315
(9)	pageblocks	<b>5</b>	3831	1642	10	15324	9459	427	9155	551
(10)	libras	15	252	108	90	3528	1592	389	1165	353
(11)	vertebral	3	217	93	6	434	344	78	342	86
(12)	breasttissue	6	74	32	9	370	258	65	271	145

### AL<sup>0-1</sup> | Experiments | Results

#### **Results for Linear Kernel and Gaussian Kernel**

The mean (standard deviation) of the accuracy. Bold numbers: best or not significantly worse than the best

D		Linear	Kernel		Gaussian Kernel			
	$AL^{0-1}$	WW	$\mathbf{CS}$	LLW	$AL^{0-1}$	WW	$\mathbf{CS}$	LLW
(1)	<b>96.3</b> (3.1)	<b>96.0</b> (2.6)	<b>96.3</b> (2.4)	79.7(5.5)	<b>96.7</b> (2.4)	<b>96.4</b> (2.4)	<b>96.2</b> (2.3)	95.4(2.1)
(2)	<b>62.5</b> (6.0)	<b>62.2</b> (3.6)	<b>62.5</b> (3.9)	52.8(4.6)	<b>69.5</b> (4.2)	66.8(4.3)	<b>69.4</b> (4.8)	<b>69.2</b> (4.4)
(3)	<b>58.8</b> (2.0)	<b>59.1</b> (1.9)	56.6(2.0)	57.7(1.7)	63.3(1.8)	64.2(2.0)	64.2(1.9)	<b>64.7</b> (2.1)
(4)	<b>86.2</b> (2.2)	85.7(2.5)	<b>85.8</b> (2.3)	74.1(3.3)	<b>86.0</b> (2.7)	84.9(2.4)	<b>85.6</b> (2.4)	<b>86.0</b> (2.5)
(5)	<b>78.8</b> (2.2)	<b>78.8</b> (1.7)	<b>78.4</b> $(2.3)$	69.8(3.7)	<b>84.3</b> (2.5)	<b>84.4</b> (2.6)	83.8(2.3)	<b>84.4</b> (2.6)
(6)	94.9(0.7)	94.9(0.8)	<b>95.2</b> (0.8)	75.8(1.5)	<b>96.5</b> (0.6)	<b>96.6</b> (0.5)	96.3(0.6)	96.4(0.5)
(7)	84.9(0.7)	<b>85.4</b> (0.7)	84.7(0.7)	74.9(0.9)	<b>91.9</b> (0.5)	<b>92.0</b> (0.6)	<b>91.9</b> (0.5)	<b>91.9</b> (0.4)
(8)	<b>96.6</b> (0.6)	96.5(0.7)	96.3(0.6)	76.2(2.2)	98.7(0.4)	98.8(0.4)	98.8(0.3)	<b>98.9</b> (0.3)
(9)	96.0(0.5)	96.1 (0.5)	<b>96.3</b> (0.5)	92.5(0.8)	<b>96.8</b> (0.5)	96.6(0.4)	96.7(0.4)	96.6(0.4)
(10)	<b>74.1</b> (3.3)	72.0(3.8)	71.3(4.3)	34.0(6.4)	83.6(3.8)	83.8(3.4)	<b>85.0</b> (3.9)	83.2 (4.2)
(11)	<b>85.5</b> (2.9)	<b>85.9</b> (2.7)	<b>85.4</b> (3.3)	79.8(5.6)	<b>86.0</b> (3.1)	<b>85.3</b> (2.9)	85.5(3.3)	84.4 (2.7)
(12)	<b>64.4</b> (7.1)	59.7(7.8)	<b>66.3</b> (6.9)	58.3(8.1)	<b>68.4</b> (8.6)	<b>68.1</b> (6.5)	<b>66.6</b> (8.9)	<b>68.0</b> (7.2)
avg	81.59	81.02	81.25	68.80	85.14	84.82	85.00	84.93
#b	9	6	8	0	9	6	6	7

### **Multiclass Zero-One Classification**



### Other results

General Multiclass Classification

#### **General Multiclass Classification**

Zero-One Loss Metric (NIPS 2016) 1 Ordinal Classification with the Absolute 2. (NIPS 2017) Loss Metric Ordinal Classification with the Squared 3. Loss Metric (JMLR submission 4. Weighted Multiclass Loss Metrics in preparation) Classification with Abstention / Reject 5. Option

### Conditional Graphical Models

Based on:

**Rizal Fathony**, Ashkan Rezaei, Mohammad Bashiri, Xinhua Zhang, Brian D. Ziebart. "*Distributionally Robust Graphical Models*". Advances in Neural Information Processing Systems 31 (NIPS), 2018

### **Conditional Graphical Models**

Some Popular Graphical Structure in Structured Prediction

**Chain Structure** 



Activity Prediction, Sequence Tagging, NLP tasks: e.g. Named Entity Recognition

#### **Tree Structure**



Parse Tree-Based NLP tasks: Semantic Role Labeling and Sentiment Analysis

#### Lattice Structure



Computer Vision Tasks: e.g. Image Segmentation

### Previous Approaches for Conditional Graphical Models



Conditional Random Fields (CRF)

(Lafferty et. al., 2001)



Fisher Consistent Produce Bayes optimal prediction in ideal case.



No Fisher consistency guarantee Based on Multiclass SVM-CS. Not consistent for distribution with no majority label.



No easy mechanism to incorporate customized loss/performance metrics The algorithm optimized the conditional likelihood. Loss/performance metric-based prediction can be performed after learning process. Align with the loss/performance metrics The algorithm accept customized loss/performance metric in its optimization objective.

### Adversarial Graphical Models (AGM)

#### Primal:

 $\min_{\hat{P}(\hat{\mathbf{y}}|\mathbf{x})} \max_{\check{P}(\check{\mathbf{y}}|\mathbf{x})} \mathbb{E}_{\mathbf{X} \sim \tilde{P}; \hat{\mathbf{Y}}|\mathbf{X} \sim \hat{P}; \check{\mathbf{Y}}|\mathbf{X} \sim \check{P}} \left[ loss(\hat{\mathbf{Y}}, \check{\mathbf{Y}}) \right] s.t.: \mathbb{E}_{\mathbf{X} \sim \tilde{P}; \check{\mathbf{Y}}|\mathbf{X} \sim \check{P}} \left[ \Phi(\mathbf{X}, \check{\mathbf{Y}}) \right] = \tilde{\Phi}$ 

- Feature function  $\Phi(\mathbf{X}, \mathbf{Y})$  is additively decomposed over cliques,  $\Phi(\mathbf{x}, \mathbf{y}) = \sum_{c} \phi(\mathbf{x}, \mathbf{y}_{c})$
- The loss metric is additively decomposed over each  $y_i$  variables,  $loss(\hat{y}, \check{y}) = \sum_{i=1}^{n} loss(\hat{y_i}, \check{y_i})$
- Focus on pairwise graphical models: interactions between label = edges in graphs

#### Dual:

$$\min_{\theta_{e},\theta_{v}} \mathbb{E}_{\mathbf{X},\mathbf{Y}\sim\tilde{P}} \max_{\check{P}(\check{\mathbf{y}}|\mathbf{x})} \min_{\hat{P}(\hat{\mathbf{y}}|\mathbf{x})} \sum_{\hat{\mathbf{y}},\check{\mathbf{y}}} \hat{P}(\hat{\mathbf{y}}|\mathbf{x}) \check{P}(\check{\mathbf{y}}|\mathbf{x}) \Big[ \sum_{i}^{n} \operatorname{loss}(\hat{y}_{i},\check{y}_{i}) \\
+ \theta_{e} \cdot \sum_{(i,j)\in E} \left[ \phi(\mathbf{x},\check{y}_{i},\check{y}_{j}) - \phi(\mathbf{x},y_{i},y_{j}) \right] + \theta_{v} \cdot \sum_{i}^{n} \left[ \phi(\mathbf{x},\check{y}_{i}) - \phi(\mathbf{x},y_{i}) \right] \Big]$$

 $\theta_e$ : Lagrange multipliers for constraints with edge features  $\theta_v$ : Lagrange multipliers for constraints with node features

### AGM | Marginal Formulation

Dual:

$$\min_{\theta_{e},\theta_{v}} \mathbb{E}_{\mathbf{X},\mathbf{Y}\sim\tilde{P}} \max_{\check{P}(\check{\mathbf{y}}|\mathbf{x})} \min_{\hat{P}(\hat{\mathbf{y}}|\mathbf{x})} \sum_{\hat{\mathbf{y}},\check{\mathbf{y}}} \hat{P}(\hat{\mathbf{y}}|\mathbf{x}) \check{P}(\check{\mathbf{y}}|\mathbf{x}) \Big[ \sum_{i}^{n} \log(\hat{y}_{i},\check{y}_{i}) \\
+ \theta_{e} \cdot \sum_{(i,j)\in E} \left[ \phi(\mathbf{x},\check{y}_{i},\check{y}_{j}) - \phi(\mathbf{x},y_{i},y_{j}) \right] + \theta_{v} \cdot \sum_{i}^{n} \left[ \phi(\mathbf{x},\check{y}_{i}) - \phi(\mathbf{x},y_{i}) \right] \Big]$$

#### Dual | Marginal Formulation:

$$\min_{\theta_{e},\theta_{v}} \mathbb{E}_{\mathbf{X},\mathbf{Y}\sim\tilde{P}} \max_{\check{P}(\check{\mathbf{y}}|\mathbf{x})} \min_{\hat{P}(\hat{\mathbf{y}}|\mathbf{x})} \left[ \sum_{i}^{n} \sum_{\hat{y}_{i},\check{y}_{i}} \hat{P}(\hat{y}_{i}|\mathbf{x})\check{P}(\check{y}_{i}|\mathbf{x}) loss(\hat{y}_{i},\check{y}_{i}) + \sum_{(i,j)\in E} \sum_{\check{y}_{i},\check{y}_{j}} \check{P}(\check{y}_{i},\check{y}_{j}|\mathbf{x}) \left[ \theta_{e} \cdot \phi(\mathbf{x},\check{y}_{i},\check{y}_{j}) \right] - \sum_{(i,j)\in E} \theta_{e} \cdot \phi(\mathbf{x},y_{i},y_{j}) + \sum_{i}^{n} \sum_{\check{y}_{i}} \check{P}(\check{y}_{i}|\mathbf{x}) \left[ \theta_{v} \cdot \phi(\mathbf{x},\check{y}_{i}) \right] - \sum_{i}^{n} \theta_{v} \cdot \phi(\mathbf{x},y_{i}) \right],$$

Similar to CRF and SSVM: General Graphical Models: Intractable Focus: Graphs with low tree-width,

e.g.: chain, tree. Tractable optimization

Predictor's probability  $\hat{P}(\hat{y}|x)$  can be decomposed into node marginal probability  $\hat{P}(\hat{y}_i|x)$ Adversary's probability  $\check{P}(\check{y}|x)$  can be decomposed into node and edge marginal probability  $\check{P}(\check{y}_i|x)$  and  $\check{P}(\check{y}_i,\check{y}_j|x)$ 

### AGM | Optimization

#### Matrix Notation (Tree Structure AGM):

$$\begin{split} \min_{\theta_{e},\theta_{v}} \mathbb{E}_{\mathbf{X},\mathbf{Y}\sim\tilde{P}} \max_{\mathbf{Q}} \min_{\mathbf{p}} \sum_{i}^{n} \left[ \mathbf{p}_{i} \mathbf{L}_{i} (\mathbf{Q}_{pt(i);i}^{\mathrm{T}} \mathbf{1}) + \left\langle \mathbf{Q}_{pt(i);i} - \mathbf{Z}_{pt(i);i}, \sum_{l} \theta_{e}^{(l)} \mathbf{W}_{pt(i);i;l} \right\rangle \\ &+ (\mathbf{Q}_{pt(i);i}^{\mathrm{T}} \mathbf{1} - \mathbf{z}_{i})^{\mathrm{T}} (\sum_{l} \theta_{v}^{(l)} \mathbf{w}_{i;l}) \right] \\ \text{subject to: } \mathbf{Q}_{pt(pt(i));pt(i)}^{\mathrm{T}} \mathbf{1} = \mathbf{Q}_{pt(i);i} \mathbf{1}, \ \forall i \in \{1, \dots, n\}, \end{split}$$

#### **Optimization Techniques:**

- Stochastic (sub)-gradient descent
- (outer optimization for  $\theta_e$  and  $\theta_v$ )
- Dual decomposition (inner  $oldsymbol{Q}$  optimization)
- Discrete optimal transport solver (recovering  $oldsymbol{Q}$ )
- Closed-form solution (inner  $oldsymbol{p}$  optimization)

Runtime (for a single subgradient update):

- Depends on the loss metric used
- For the additive zero-one loss metric (Hamming loss)  $O(nlk \log k + nk^2)$ 
  - k: # classes, n: # nodes,
  - *l*: # iterations in dual decomposition

CRF	SSVM
$O(nk^2)$	$O(nk^2)$

General graphs low tree-width

 $O(nlwk^{(w+1)}\log k + nk^{2(w+1)})$ n: # cliques, w: treewidth of the graph

### AGM | Consistency

#### If the loss function is additive

#### AGM is consistent

when f is optimized over all measurable functions on the input space

#### AGM is also consistent

when f is optimized over a restricted set of functions:

all measurable function that are additive over the edge and node potentials.

### AGM | Experiments (1)

#### Facial Emotion Intensity Prediction (Chain Structure, Labels with Ordinal Category)

- Each node: 3 class classification: neutral = 1< increasing = 2 < apex = 3
- 167 sequences
- Ordinal loss metrics: zero-one loss, absolute loss, and squared loss
- Weighted and unweighted. Weights reflect the focus of prediction (e.g. focus more on latest nodes)
- **Results:** Table 1: The average loss metrics for the emotion intensity prediction. Bold numbers indicate the best or not significantly worse than the best results (paired t-test with  $\alpha = 0.05$ ).

Loss metrics	AGM	CRF	SSVM
zero-one, unweighted	0.34	0.32	0.37
absolute, unweighted	0.33	0.34	0.40
quadratic, unweighted	0.38	0.38	0.40
zero-one, weighted	0.28	0.32	0.29
absolute, weighted	0.29	0.36	0.29
quadratic, weighted	0.36	0.40	0.33
average	0.33	0.35	0.35
# bold	4	2	2

### AGM | Experiments (2)

### Semantic Role Labeling (Tree Structure)

- Predict label of each node given known parse tree.
- Cost-sensitive loss metric is used reflect the importance of each label
- CoNLL 2005 dataset

#### **Results:**

Table 2: The average loss metrics for the semantic role labeling task.

Loss metrics	AGM	CRF	SSVM
cost-sensitive loss	0.14	0.19	0.14

### **Conditional Graphical Models**



### Bipartite Matching in Graphs

Based on:

**Rizal Fathony\***, Sima Behpour\*, Xinhua Zhang, Brian D. Ziebart. "*Efficient and Consistent Adversarial Bipartite Matching*". International Conference on Machine Learning (ICML), 2018.

### **Bipartite Matching Task**



Maximum weighted bipartite matching:

$$\max_{\pi \in \Pi} \psi(\pi) = \max_{\pi \in \Pi} \sum_{i} \psi_i(\pi_i)$$

Machine learning task:

Learn the appropriate weights  $\psi_i(\cdot)$ 

Objective:

Minimize a loss metric, e.g., the Hamming loss

$$loss_{Ham}(\pi, \pi') = \sum_{i=1}^{n} 1(\pi'_i \neq \pi_i)$$

### Learning Bipartite Matching | Applications

#### 1 Word alignment

(Taskar et. al., 2005; Pado & Lapta, 2006; Mac-Cartney et. al., 2008)



#### **2** Correspondence between images

(Belongie et. al., 2002; Dellaert et. al., 2003)



#### **3** Learning to rank documents

(Dwork et. al., 2001; Le & Smola, 2007)



e	bipa	rtite match	ning					٩
	All	Videos	Images	News	Shopping	More	Settings	Tools
	Abou	t 213,000 re	sults (0.37 se	econds)				

Maximum Bipartite Matching - GeeksforGeeks https://www.geeksforgeeks.org/maximum-bipartite-matching/ • In a maximum matching, if any edge is added to it, it is no longer a matching. There can be more than one maximum matchings for a given Bipartite Graph.

[PDF] CMSC 451: Maximum Bipartite Matching

https://www.cs.cmu.edu/~ckings/fbioinfo-lectures/matching.pdf 
CMSC 451: Maximum Bipartite Matching. Sildes By: Carl Kingsford. Department of Computer Science. University of Maryland, College Park, Based on Section ...

Matching (graph theory) - Wikipedia

https://en.wikipedia.org/wiki/Matching\_(graph\_theory) \* Jump to in unweighted bipartite graphs - Matching problems are often concerned with bipartite ... a maximum cardinality bipartite matching) in a bipartite ... Biossom algorithm - Hopcroft-Karp algorithm - Edge cover

A non-bipartite matching task can be converted to a bipartite matching problem

### **Previous Approaches for Bipartite Matching**



CRF (Petterson et. al., 2009; Volkovs & Zemel, 2012)

$$P_{\psi}(\pi) = \frac{1}{Z_{\psi}} \exp\left(\sum_{i=1}^{n} \psi_i(\pi_i)\right)$$
$$Z_{\psi} = \sum_{\pi} \prod_{i=1}^{n} \exp\left(\psi_i(\pi_i)\right) = \operatorname{perm}(\mathbf{M})$$
$$\operatorname{where} M_{i,j} = \exp\left(\psi_i(j)\right)$$

Fisher Consistent Produce Bayes optimal prediction in ideal case

Computationally intractable
 Normalization term requires matrix permanent computation (a #P-hard problem).
 An approximation is needed.



solved using constraint generation

$$\min_{\psi} \mathbb{E}_{\pi \sim \tilde{P}} \left[ \max_{\pi'} \left\{ loss(\pi, \pi') + \psi(\pi') \right\} - \psi(\pi) \right]$$

 $\tilde{P}$  is the empirical distribution

Computationally Efficient Hungarian algorithm for computing the maximum violated constraints



No Fisher consistency guarantee Based on Multiclass SVM-CS

Not consistent for distribution with no majority label

### Adversarial Bipartite Matching (our approach)

#### Primal:



#### Augmented Hamming loss matrix for n = 3 permutations

	$\check{\pi} = 123$	$\check{\pi} = 132$	$\check{\pi} = 213$	$\check{\pi} = 231$	$\check{\pi} = 312$	$\check{\pi} = 321$
$\hat{\pi} = 123$	$0 + \delta_{123}$	$2 + \delta_{132}$	$2 + \delta_{213}$	$3 + \delta_{231}$	$3 + \delta_{312}$	$2 + \delta_{321}$
$\hat{\pi} = 132$	$2 + \delta_{123}$	$0 + \delta_{132}$	$3 + \delta_{213}$	$2 + \delta_{231}$	$2 + \delta_{312}$	$3 + \delta_{321}$
$\hat{\pi} = 213$	$2 + \delta_{123}$	$3 + \delta_{132}$	$0 + \delta_{213}$	$2 + \delta_{231}$	$2 + \delta_{312}$	$3 + \delta_{321}$
$\hat{\pi} = 231$	$3 + \delta_{123}$	$2 + \delta_{132}$	$2 + \delta_{213}$	$0 + \delta_{231}$	$3 + \delta_{312}$	$2 + \delta_{321}$
$\hat{\pi} = 312$	$3 + \delta_{123}$	$2 + \delta_{132}$	$2 + \delta_{213}$	$3 + \delta_{231}$	$0 + \delta_{312}$	$2 + \delta_{321}$
$\hat{\pi} = 321$	$2 + \delta_{123}$	$3 + \delta_{132}$	$3 + \delta_{213}$	$2 + \delta_{231}$	$2 + \delta_{312}$	$0 + \delta_{321}$

size:Intractable $n! \times n!$ for modestly-sized n

Dual:

$$\min_{\theta} \mathbb{E}_{x,\pi\sim\tilde{P}} \min_{\hat{P}(\hat{\pi}|x)} \max_{\check{P}(\check{\pi}|x)} \mathbb{E}_{\substack{\hat{\pi}|x\sim\tilde{P}\\\check{\pi}|x\sim\tilde{P}}} \left[ loss(\hat{\pi},\check{\pi}) + \theta \cdot \sum_{i=1}^{n} \left(\phi_i(x,\check{\pi}_i) - \phi_i(x,\pi_i)\right) \right]$$

$$\text{Hamming loss} \qquad \text{Lagrangian term } \delta$$

### Polytope of the Permutation Mixtures

Dual:  

$$\min_{\theta} \mathbb{E}_{(x,\pi)\sim\tilde{P}} \min_{\hat{P}(\hat{\pi}|x)} \max_{\check{P}(\check{\pi}|x)} \mathbb{E}_{\hat{\pi}|x\sim\tilde{P};\check{\pi}|x\sim\tilde{P}} \left[ \sum_{i=1}^{n} I(\pi'_{i}\neq\pi_{i}) + \theta \cdot \sum_{i=1}^{n} (\phi_{i}(x,\check{\pi}_{i}) - \phi_{i}(x,\pi_{i})) \right]$$

Marginal Distribution Matrices:

Birkhoff – Von Neumann theorem:

Predictor





		1	2	3	
0	$\check{\pi}_1$	$q_{1,1}$	$q_{1,2}$	$q_{1,3}$	
<b>Q</b> =	$\check{\pi}_2$	$q_{2,1}$	$q_{2,2}$	$q_{2,3}$	
	$\check{\pi}_3$	$q_{3,1}$	$q_{3,2}$	$q_{3,3}$	
$q_{i,j} = \breve{P} \; (\breve{\pi}_i = j)$					



 convex polytope whose points are doubly stochastic matrix

$$\mathbf{P}\mathbf{1} = \mathbf{P}^\top \mathbf{1} = \mathbf{Q}\mathbf{1} = \mathbf{Q}^\top \mathbf{1} = \mathbf{1}$$

reduce the space of optimization: from O(n!) to  $O(n^2)$ 

### **Marginal Distribution Formulation**

Dual:

$$\min_{\theta} \mathbb{E}_{(x,\pi)\sim\tilde{P}} \min_{\hat{P}(\hat{\pi}|x)} \max_{\check{P}(\check{\pi}|x)} \mathbb{E}_{\hat{\pi}|x\sim\hat{P};\check{\pi}|x\sim\check{P}} \left[ \sum_{i=1}^{n} I(\pi'_{i}\neq\pi_{i}) + \theta \cdot \sum_{i=1}^{n} (\phi_{i}(x,\check{\pi}_{i}) - \phi_{i}(x,\pi_{i})) \right]$$

#### Marginal Formulation:

Rearrange the optimization order and add regularization and smoothing penalties

$$\max_{\mathbf{Q} \ge \mathbf{0}} \min_{\theta} \frac{1}{m} \sum_{i=1}^{m} \min_{\mathbf{P}_i \ge \mathbf{0}} \left[ \langle \mathbf{Q}_i - \mathbf{Y}_i, \sum_k \theta_k \mathbf{X}_{i,k} \rangle - \langle \mathbf{P}_i, \mathbf{Q}_i \rangle + \frac{\mu}{2} \|\mathbf{P}_i\|_F^2 - \frac{\mu}{2} \|\mathbf{Q}_i\|_F^2 \right] + \frac{\lambda}{2} \|\theta\|_2^2$$
  
s.t. :  $\mathbf{P}_i \mathbf{1} = \mathbf{P}_i^\top \mathbf{1} = \mathbf{Q}_i \mathbf{1} = \mathbf{Q}_i^\top \mathbf{1} = \mathbf{1}, \quad \forall i$ 

#### **Optimization Techniques Used:**

- Outer (Q) : projected Quasi-Newton (Schmidt, et.al., 2009)
- Inner ( $\theta$ ) : closed-form solution
- Inner (P) : projection to doubly-stochastic matrix
- Projection to doubly-stochastic matrix : ADMM

### Consistency

#### **Empirical Risk Perspective of Adversarial Bipartite Matching**

$$\begin{split} \min_{\theta} \mathbb{E}_{\substack{x \sim P \\ \pi \mid x \sim \tilde{P}}} \left[ AL_{f_{\theta}}^{\text{perm}}(x, \pi) \right] \\ \text{where: } AL_{f_{\theta}}^{\text{perm}}(x, \pi) \triangleq \min_{\hat{P}(\hat{\pi} \mid x)} \max_{\substack{\check{P}(\check{\pi} \mid x) \\ \check{\pi} \mid x \sim \check{P}}} \mathbb{E}_{\hat{\pi} \mid x \sim \check{P}} \left[ \text{loss}(\hat{\pi}, \check{\pi}) + f_{\theta}(x, \check{\pi}) - f_{\theta}(x, \pi) \right] \end{split}$$

#### AL<sup>perm</sup> is consistent

when f is optimized over all measurable functions on the input space  $(x, \pi)$ 

#### ALperm is also consistent

*f* is optimized over a restricted set of functions:  $f(x, \pi) = \sum_i g_i(x, \pi_i)$ 

when g is allowed to be optimized over all measurable functions on the individual input space  $(x, \pi_i)$ 

### Experiments

#### Application: Video Tracking



#### Public Benchmark Datasets

*Table 3.* Dataset properties

DATASET	# Elements	# Examples
TUD-CAMPUS	12	70
TUD-STADTMITTE	16	178
ETH-SUNNYDAY	18	353
ETH-BAHNHOF	34	999
ETH-Pedcross2	30	836

#### Empirical runtime (until convergence)

Table 5. Running time (in seconds) of the model for various number of elements n with fixed number of samples (m = 50)

DATASET	# Elements	ADV MARG.	SSVM
CAMPUS	12 1.0	1.96 1.0	0.22
Stadtmitte	16 1.3	2.46 1.2	0.25
SUNNYDAY	18 1.5	2.75 1.4	0.15
Pedcross2	30 2.5	8.18 4.2	0.26
BAHNHOF	34 2.8	9.79 5.0	0.31

relative: 12=1.0 relative: 1.96=1.0

Adversarial. Marginal Formulation: grows (roughly) quadratically in *n* 

CRF: impractical even for n = 20(Petterson et. al., 2009)

### **Experiment Results**

Table 1: The mean and standard deviation (in parenthesis) of the average accuracy (1 - the average Hamming loss) for the adversarial bipartite matching model compared with Structured-SVM.

Training/ A: Testing	dv. Bipartite Matching	Structured SVM
Campus/ Stadtmitte	$0.662 \\ (0.08)$	$0.662 \\ (0.08)$
Stadtmitte/ Campus	0.667 (0.11)	$0.660 \\ (0.12)$
Bahnhof/ Sunnyday	<b>0.754</b> (0.10)	$0.729 \\ (0.15)$
Pedcross2/ Sunnyday	<b>0.750</b> (0.10)	$0.736 \\ (0.13)$
Sunnyday/ Bahnhof	<b>0.751</b> (0.18)	$0.739 \\ (0.20)$
Pedcross2/ Bahnhof	<b>0.763</b> (0.16)	$0.731 \\ (0.21)$
Bahnhof/ Pedcross2	<b>0.714</b> (0.16)	$0.701 \\ (0.18)$
Sunnyday/ Pedcross2	<b>0.712</b> (0.17)	$0.700 \\ (0.18)$

6 pairs of dataset significantly outperforms SSVM

2 pairs of dataset competitive with SSVM

### **Bipartite Matching in Graphs**



### Conclusion

### **Robust Adversarial Learning Algorithms**



Align better with the loss/performance metric (by incorporating the metric into its learning objective)







Ongoing and Future Works

### **Ongoing and Future Works (1)**

### 1. Fairness and Privacy in Machine Learning

Important issues in automated decision using ML algorithms.

Require the algorithm to produce fair prediction / privacy-preserving prediction.

Our formulation only enforces constraints on the adversary.

 $\min_{\hat{P}(\hat{Y}|\mathbf{X})} \max_{\check{P}(\check{Y}|\mathbf{X})} \mathbb{E}_{\mathbf{X},Y\sim\tilde{P};\hat{Y}|\mathbf{X}\sim\hat{P};\check{Y}|\mathbf{X}\sim\check{P}} \left[ \operatorname{loss}(\hat{Y},\check{Y}) \right]$ s.t.  $\mathbb{E}_{\mathbf{X}\sim\tilde{P};\check{Y}|\mathbf{X}\sim\check{P}} [\phi(\mathbf{X},\check{Y})] = \mathbb{E}_{\mathbf{X},Y\sim\tilde{P}} [\phi(\mathbf{X},Y)]$ 

Add fairness / privacy constraints to the predictor?

### 2. Multivariate Performance Metrics

Many ML applications uses multivariate performance metrics to evaluate the prediction.

- $F_{\beta}$ -score
- Precision/Recall @k
- Area under ROC curve (AOC)

How will the optimization techniques change to accommodate these metrics?

What if we have both structure in the label interactions as well as structure in the loss metrics?

e.g. Bipartite Matching with F1-score

### Ongoing and Future Works (2)

## 3. Structured Prediction & Graphical Models

More complex graphical structures are popular in some applications, e.g. computer vision.

Exact learning algorithms for AGM in this case may be intractable.

Can we develop learning algorithms for general graphical models?

What kind of approximation algorithms can be applicable?

#### 4. Deep Learning

Deep learning has been successfully applied to many prediction problems.

Most of deep learning architectures are not designed to optimize customized loss metrics.

How can the robust adversarial learning approach help designing deep learning architectures?

### Ongoing and Future Works (3)

### 5. Multitask Learning

In some problems, learning multiple tasks with different metrics simultaneously is desirable.

What if we want to optimize multiple different loss metrics simultaneously?

How will it change the optimization?

### 6. Statistical Theory of Loss Functions

In multiclass classification problem, both AL<sup>0-1</sup> and SVM-LLW are Fisher consistent. However, their performances are quite different.

Is there any stronger statistical guarantee that can separate high-performing Fisher consistent algorithm from the low-performing ones?

### Collaborators





### **Publications**

- Consistent Robust Adversarial Prediction for General Multiclass Classification Rizal Fathony, Kaiser Asif, Anqi Liu, Mohammad Bashiri, Xinhua Zhang, Brian D. Ziebart. JMLR submission in preparation.
- Distributionally Robust Graphical Models
   Rizal Fathony, Ashkan Rezaei, Mohammad Bashiri, Xinhua Zhang, Brian D. Ziebart.
   Advances in Neural Information Processing Systems 31 (NIPS), 2018.
- Efficient and Consistent Adversarial Bipartite Matching Rizal Fathony\*, Sima Behpour\*, Xinhua Zhang, Brian D. Ziebart. International Conference on Machine Learning (ICML), 2018.
- Adversarial Surrogate Losses for Ordinal Regression
   Rizal Fathony, Mohammad Bashiri, Brian D. Ziebart.
   Advances in Neural Information Processing Systems 30 (NIPS), 2017.
- Adversarial Multiclass Classification: A Risk Minimization Perspective Rizal Fathony, Anqi Liu, Kaiser Asif, Brian D. Ziebart. Advances in Neural Information Processing Systems 29 (NIPS), 2016.
- Kernel Robust Bias-Aware Prediction under Covariate Shift Anqi Liu, Rizal Fathony, Brian D. Ziebart. ArXiv Preprints, 2016.

### Thank You