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Distributionally Robust Learning

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Contents

1	Intro	Introduction				
	1.1	Robust Optimization	6			
	1.2	Distributionally Robust Optimization	8			
	1.3	Outline	11			
	1.4	Notational Conventions	14			
	1.5	Abbreviations	17			
2	The	Wasserstein Metric	20			
	2.1	Basics	20			
	2.2	A Distance Metric	22			
	2.3	The Dual Problem	25			
	2.4	Some Special Cases	28			
	2.5	The Transport Cost Function	29			
	2.6	Robustness of the Wasserstein Ambiguity Set	33			
	2.7	Setting the Radius of the Wasserstein Ball	37			
3	Solv	ing the Wasserstein DRO Problem	48			
	3.1	Dual Method	48			
	3.2	The Extreme Distribution	54			
	3.3	A Discrete Empirical Nominal Distribution	55			
	3.4	Finite Sample Performance	59			
	3.5	Asymptotic Consistency	61			

4	Dist	ributionally Robust Linear Regression	64		
	4.1	The Problem and Related Work	64		
	4.2	The Wasserstein DRO Formulation for			
		Linear Regression	66		
	4.3	Performance Guarantees for the DRO Estimator	72		
	4.4	Experiments on the Performance of			
		Wasserstein DRO	87		
	4.5	An Application of Wasserstein DRO to			
		Outlier Detection	102		
	4.6	Summary	107		
5	Dist	ributionally Robust Grouped Variable Selection	108		
	5.1	The Problem and Related Work	108		
	5.2	The Groupwise Wasserstein Grouped LASSO	110		
	5.3	Performance Guarantees to the DRO			
		Groupwise Estimator	118		
	5.4	Numerical Experiments	124		
	5.5	Summary	139		
6	Dist	ributionally Robust Multi-Output Learning	140		
	6.1	The Problem and Related Work	140		
	6.2	Distributionally Robust Multi-Output			
		Learning Models	143		
	6.3	The Out-of-Sample Performance Guarantees	156		
	6.4	Numerical Experiments	161		
	6.5	Summary	173		
7	Optimal Decision Making via Regression				
	Info	rmed K-NN	174		
	7.1	The Problem and Related Work	174		
	7.2	Robust Nonlinear Predictive Model	177		
	7.3	Prescriptive Policy Development	185		
	7.4	Developing Optimal Prescriptions for Patients	190		
	7.5	Summary	200		

8	Advanced Topics in DistributionallyRobust Learning201		
	8.1	Distributionally Robust Learning with Unlabeled Data	202
	8.2	Distributionally Robust Reinforcement Learning	211
9	Discussion and Conclusions		221
Ac	know	vledgments	224
Re	ferer	ices	226

Distributionally Robust Learning

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ABSTRACT

This monograph develops a comprehensive statistical learning framework that is robust to (distributional) perturbations in the data using Distributionally Robust Optimization (DRO) under the Wasserstein metric. Beginning with fundamental properties of the Wasserstein metric and the DRO formulation, we explore duality to arrive at tractable formulations and develop finite-sample, as well as asymptotic, performance guarantees. We consider a series of learning problems, including (i) distributionally robust linear regression; (ii) distributionally robust regression with group structure in the predictors; (iii) distributionally robust multi-output regression and multiclass classification, (iv) optimal decision making that combines distributionally robust regression with nearest-neighbor estimation; (v) distributionally robust semi-supervised learning, and (vi) distributionally robust reinforcement learning. A tractable DRO relaxation for each problem is being derived, establishing a connection between robustness and regularization, and obtaining bounds on the prediction and estimation errors of the solution. Beyond theory, we include numerical experiments and case studies using synthetic and real data. The real data experiments are all associated with various health informatics problems, an application area which provided the initial impetus for this work.

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1

Introduction

A central problem in machine learning is to learn from data ("big" or "small") how to predict outcomes of interest. Outcomes can be binary or discrete, such as an event or a category, or continuous, e.g., a real value. In either case, we have access to a number N of examples from which we can learn; each example is associated with a potentially large number p of predictor variables and the "ground truth" discrete or continuous outcome. This form of learning is called supervised, because it relies on the existence of known examples associating predictor variables with the outcome. In the case of a binary/discrete outcome the problem is referred to as classification, while for continuous outcomes we use the term regression.

There are many methods to solve such supervised learning problems, from ordinary (linear) least squares regression, to logistic regression, Classification And Regression Trees (CART) [1], ensembles of decision trees [2], [3], to modern deep learning models [4]. Whereas the nonlinear models (random forests, gradient boosted trees, and deep learning) perform very well in many specific applications, they have two key drawbacks: (i) they produce predictive models that lack *interpretability* and (ii) they are hard to analyze and do not give rise to rigorous mathematical results characterizing their performance and important properties. In this monograph, we will mainly focus on the more classical linear models, allowing for some nonlinear extensions.

Clearly, there is a plethora of application areas where such models have been developed and used. A common thread throughout this monograph is formed by applications in medicine and health care, broadly characterized by the term *predictive health analytics*. While in principle these applications are not substantially different from other domains, they have important salient features that need to be considered. These include:

- 1. Presence of outliers. Medical data often contain outliers, which may be caused by medical errors, erroneous or missing data, equipment and lab configuration errors, or even different interpretation/use of a variable by different physicians who enter the data.
- 2. Risk of "overfitting" from too many variables. For any individual and any outcome we wish to predict, using all predictor variables may lead to overfitting and large generalization errors (out-ofsample). The common practice is to seek sparse models, using the fewest variables possible without significantly compromising accuracy. In some settings, especially when genetic information is included in the predictors, the number of predictors can exceed the training sample size, further stressing the need for sparsity. Sparse regression models originated in the seminar work on the Least Absolute Shrinkage and Selection Operator, better known under the acronym LASSO [5].
- 3. Lack of linearity. In some applications, the linearity of regression or logistic regression may not fully capture the relationship between predictors and outcome. While kernel methods [6] can be used to employ linear models in developing nonlinear predictors, other choices include combining linear models with nearest neighbor ideas to essentially develop *piecewise linear* models.

To formulate the learning problems of interest more concretely, let $\mathbf{x} = (x_1, \ldots, x_p) \in \mathbb{R}^p$ denote a column vector with the predictors and

Introduction

let $y \in \mathbb{R}$ be the outcome or response. In the classification problem, we have $y \in \{-1, +1\}$. We are given training data $(\mathbf{x}_i, y_i), i \in [\![N]\!]$, where $[\![N]\!] \stackrel{\triangle}{=} 1, \ldots, N$, from which we want to "learn" a function $f(\cdot)$ so that $f(\mathbf{x}_i) = y_i$ for most *i*. Further, we want $f(\cdot)$ to generalize well to new samples (i.e., to have good out-of-sample performance).

In the regression problem, we view the \mathbf{x}_i 's as independent variables (predictor vectors) and y_i as the real-valued dependent variable. We still want to determine a function $f(\mathbf{x})$ that predicts y. In linear regression, $f(\mathbf{x}) = \boldsymbol{\beta}' \mathbf{x}$, where $\boldsymbol{\beta}$ is a coefficient vector, prime denotes transpose, and we assume one of the elements of \mathbf{x} is equal to one with the corresponding coefficient being the *intercept* (of the regression function at zero). Both classification and regression problems can be formulated as:

$$\min_{\beta} \mathbb{E}^{\mathbb{P}^*}[h_{\beta}(\mathbf{x}, y)], \tag{1.1}$$

where \mathbb{P}^* is the probability distribution of (\mathbf{x}, y) , $\mathbb{E}^{\mathbb{P}^*}$ stands for the expectation under \mathbb{P}^* , and $h_\beta(\mathbf{x}, y)$ is a loss function penalizing differences between $f(\mathbf{x})$ and y. This formulation is known as *expected* risk minimization. Ordinary Least Squares (OLS) uses a squared loss $h_\beta(\mathbf{x}, y) = (f(\mathbf{x}) - y)^2$ while logistic regression uses the logloss function $h_\beta(\mathbf{x}, y) = \log(1 + \exp\{-yf(\mathbf{x})\})$. Since \mathbb{P}^* is typically unknown, a common practice is to approximate it using the *empirical distribution* $\hat{\mathbb{P}}_N$ which assigns equal probability to each training sample, leading to the following *empirical risk minimization* formulation:

$$\min_{\beta} \frac{1}{N} \sum_{i=1}^{N} h_{\beta}(\mathbf{x}_i, y_i).$$

One of the well known issues of OLS regression is that the regression function can be particularly sensitive to outliers. To illustrate this with a simple example, consider a case of regression with a single predictor; see Figure 1.1. Points in the training set are shown as blue dots. Suppose we include in the training set some outliers depicted as magenta stars. OLS regression results in the black line. Notice how much the slope of this line has shifted away from the blue dots to accommodate the outliers. This skews future predictions but also our ability to identify new outlying observations. Several approaches have been introduced to address this issue [7], [8] and we discuss them in more detail in Section 4.



Figure 1.1: Regression example.

The main focus of this monograph is to develop robust learning methods for a variety of learning problems. To introduce robustness into the generic problem, we will use ideas from robust optimization and formulate a robust version of the expected risk minimization Problem (1.1). We will further focus on distributional robustness. The problems we will formulate are min-max versions of Problem (1.1) where one minimizes a worst case estimate of the loss over some appropriately defined ambiguity set. Such min-max formulations have a long history, going back to the origins of game theory [9], where one can view the problem as a game between an adversary who may affect the training set and the optimizer who responds to the worst-case selection by the adversary. They also have strong connections with \mathcal{H}_{∞} and robust control theory [10], [11].

To avoid being overly broad, we will restrict our attention to the intersection of statistical learning and *Distributionally Robust Optimiza*tion (DRO) under the Wasserstein metric [12]–[14]. Even this more narrow area has generated a lot of interest and recent work. While we will cover several aspects, we will not cover a number of topics, including:

• the integration of DRO with different optimization schemes, e.g., inverse optimization [15], polynomial optimization [16], multi-stage optimization [17], [18], and chance-constrained optimization [19], [20];

Introduction

- the application of DRO to stochastic control problems, see, e.g., [21]–[23], and statistical hypothesis testing [24];
- the combination of DRO with general estimation techniques, see, e.g., [25] for distributionally robust Minimum Mean Square Error Estimation, and [26] for distributionally robust Maximum Likelihood Estimation.

Most of the learning problems we consider, except for Section 8.2, are static *single-period* problems where the data are assumed to be independently and identically distributed. For extensions of DRO to a dynamic setting where the data come in a sequential manner, we refer to [27] for a distributionally robust Kalman filter model [23], [28], and [29] for robust dynamic programming, and [30] for a distributionally robust online adaptive algorithm.

In this monograph, we focus mainly on linear predictive models, with the exception of Section 7, where the non-linearity is captured by a non-parametric *K*-Nearest Neighbors (K-NN) model. For extensions of robust optimization to non-linear settings, we refer to [31] for robust kernel methods, [32] for distributionally robust graphical models, and [33] for distributionally robust deep neural networks.

In the remainder of this Introduction, we will present a brief outline of robust optimization in Section 1.1 and distributionally robust optimization in Section 1.2. In Section 1.3 we provide an outline of the topics covered in the rest of the monograph. Section 1.4 summarizes our notational conventions and Section 1.5 collects all abbreviations we will use.

1.1 Robust Optimization

Robust optimization [34], [35] provides a way of modeling uncertainty in the data without the use of probability distributions. It restricts data perturbations to be within a deterministic uncertainty set, and seeks a solution that is optimal for the worst-case realization of this uncertainty. Consider a general optimization problem:

$$\min_{\beta} h_{\beta}(\mathbf{z}), \tag{1.2}$$

1.1. Robust Optimization

where β is a vector of decision variables, \mathbf{z} is a vector of given parameters, and h is a real-valued function. Assuming that the values of \mathbf{z} lie within some uncertainty set \mathcal{Z} , a robust counterpart of Problem (1.2) can be written in the following form:

$$\min_{\beta} \max_{\mathbf{z} \in \mathcal{Z}} h_{\beta}(\mathbf{z}).$$
(1.3)

Problem (1.3) is computationally tractable for many classes of uncertainty sets \mathcal{Z} . For a detailed overview of robust optimization we refer to [34]–[36].

There has been an increasing interest in using robust optimization to develop machine learning algorithms that are immunized against data perturbations; see, for example, [37]–[44] for classification methods. [41] considered both feature uncertainties:

$$\mathcal{Z}_{\mathbf{x}} \triangleq \{ \mathbf{\Delta} \mathbf{X} \in \mathbb{R}^{N \times p} \colon \| \mathbf{\Delta} \mathbf{x}_i \|_q \le \rho, i \in [\![N]\!] \},\$$

where $\Delta \mathbf{X}$ can be viewed as a feature perturbation matrix on N samples with p features, $\|\cdot\|_q$ is the ℓ_q norm, and $\Delta \mathbf{x}_i \in \mathbb{R}^p, i \in [N]$, are the rows of $\Delta \mathbf{X}$, as well as label uncertainties:

$$\mathcal{Z}_{y} \triangleq \left\{ \Delta \mathbf{y} \in \{0,1\}^{N} \colon \sum_{i=1}^{N} \Delta y_{i} \leq \Gamma \right\},$$

where $\Delta y_i \in \{0, 1\}$, with 1 indicating that the label was incorrect and has in fact been flipped, and 0 otherwise, and Γ is an integer-valued parameter controlling the number of data points that are allowed to be mislabeled. They solved various robust classification models under these uncertainty sets. As an example, the robust Support Vector Machine (SVM) [45] problem was formulated as:

$$\min_{\mathbf{w},b} \max_{\mathbf{\Delta y} \in \mathcal{Z}_y} \max_{\mathbf{\Delta X} \in \mathcal{Z}_x} \sum_{i=1}^N \max\{1 - y_i(1 - 2\Delta y_i)(\mathbf{w}'(\mathbf{x}_i + \mathbf{\Delta x}_i) - b), 0\}.$$

[39] studied a robust linear regression problem with feature-wise disturbance:

$$\min_{\boldsymbol{\beta}} \max_{\boldsymbol{\Delta X} \in \mathcal{Z}_{\mathbf{x}}} \|\mathbf{y} - (\mathbf{X} + \boldsymbol{\Delta X})\boldsymbol{\beta}\|_2$$

where β is the vector of regression coefficients, and the uncertainty set

$$\mathcal{Z}_{\mathbf{x}} \triangleq \{ \mathbf{\Delta} \mathbf{X} \in \mathbb{R}^{N \times p} \colon \| \mathbf{\Delta} \tilde{\mathbf{x}}_i \|_2 \le c_i, \ i \in \llbracket p \rrbracket \},\$$

Introduction

where $\Delta \tilde{\mathbf{x}}_i \in \mathbb{R}^N, i \in [\![p]\!]$, are the columns of $\Delta \mathbf{X}$. They showed that such a robust regression problem is equivalent to the following ℓ_1 -norm regularized regression problem:

$$\min_{\boldsymbol{\beta}} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2 + \sum_{i=1}^p c_i |\beta_i|.$$

1.2 Distributionally Robust Optimization

Different from robust optimization, Distributionally Robust Optimization (DRO) treats the data uncertainty in a probabilistic way. It minimizes a worst-case expected loss function over a probabilistic ambiguity set that is constructed from the observed samples and characterized by certain known properties of the true data-generating distribution. DRO has been an active area of research in recent years, due to its probabilistic interpretation of the uncertain data, tractability when assembled with certain metrics, and extraordinary performance observed on numerical examples, see, for example, [12]–[14], [46], [47]. DRO can be interpreted in two related ways: it refers to (i) a robust optimization problem where a worst-case loss function is being hedged against; or, alternatively, (ii) a stochastic optimization problem where the expectation of the loss function with respect to the probabilistic uncertainty of the data is being minimized. Figure 1.2 provides a schematic comparison of various optimization frameworks.

To formulate a DRO version of the expected risk minimization problem (1.1), consider the stochastic optimization problem:

$$\inf_{\beta} \mathbb{E}^{\mathbb{P}^*}[h_{\beta}(\mathbf{z})], \tag{1.4}$$

where we set $\mathbf{z} = (\mathbf{x}, y) \in \mathcal{Z} \subseteq \mathbb{R}^d$ in (1.1), $\boldsymbol{\beta} \in \mathbb{R}^p$ is a vector of coefficients to be learned, $h_{\boldsymbol{\beta}}(\mathbf{z}): \mathcal{Z} \times \mathbb{R}^p \to \mathbb{R}$ is the loss function of applying $\boldsymbol{\beta}$ on a sample $\mathbf{z} \in \mathcal{Z}$, and \mathbb{P}^* is the underlying true probability distribution of \mathbf{z} . The DRO formulation for (1.4) minimizes the worst-case expected loss over a probabilistic ambiguity set Ω :

$$\inf_{\beta} \sup_{\mathbb{Q} \in \Omega} \mathbb{E}^{\mathbb{Q}}[h_{\beta}(\mathbf{z})].$$
(1.5)

1.2. Distributionally Robust Optimization



Figure 1.2: Comparison of robust optimization with distributionally robust optimization.

The existing literature on DRO can be split into two main branches, depending on the way in which Ω is defined. One is through a moment ambiguity set, which contains all distributions that satisfy certain moment constraints [48]–[53]. In many cases it leads to a tractable DRO problem but has been criticized for yielding overly conservative solutions [54]. The other is to define Ω as a ball of distributions:

$$\Omega \triangleq \{ \mathbb{Q} \in \mathcal{P}(\mathcal{Z}) \colon D(\mathbb{Q}, \mathbb{P}_0) \le \epsilon \},\$$

where \mathcal{Z} is the set of possible values for \mathbf{z} ; $\mathcal{P}(\mathcal{Z})$ is the space of all probability distributions supported on \mathcal{Z} ; ϵ is a pre-specified radius of the set Ω ; and $D(\mathbb{Q}, \mathbb{P}_0)$ is a probabilistic distance function that measures the distance between \mathbb{Q} and a nominal distribution \mathbb{P}_0 .

The nominal distribution \mathbb{P}_0 is typically chosen as the empirical distribution on the observed samples $\{\mathbf{z}_1, \ldots, \mathbf{z}_N\}$:

$$\mathbb{P}_0 = \hat{\mathbb{P}}_N \triangleq \frac{1}{N} \sum_{i=1}^N \delta_{\mathbf{z}_i}(\mathbf{z}),$$

where $\delta_{\mathbf{z}_i}(\cdot)$ is the Dirac density assigning probability mass equal to 1 at \mathbf{z}_i ; see [12], [13], and [55]. There are also works employing a nonparametric kernel density estimation method to obtain a continuous density function for the nominal distribution, when the underlying true

Introduction

distribution is continuous, see [56], [57]. The kernel density estimator is defined as:

$$f_0(\mathbf{z}) = \frac{1}{N|\mathbf{H}|^{1/2}} \sum_{i=1}^N K(\mathbf{H}^{-1/2}(\mathbf{z} - \mathbf{z}_i)),$$

where f_0 represents the density function of the nominal distribution \mathbb{P}_0 , i.e., $f_0 = d\mathbb{P}_0/d\mathbf{z}$, $\mathbf{H} \in \mathbb{R}^{d \times d}$ represents a symmetric and positive definite bandwidth matrix, and $K(\cdot)$: $\mathbb{R}^d \to \mathbb{R}^+$ is a symmetric kernel function satisfying $K(\cdot) \geq 0$, $\int_{\mathbb{R}^d} K(\mathbf{z}) d\mathbf{z} = 1$, and $\int_{\mathbb{R}^d} K(\mathbf{z}) \mathbf{z} d\mathbf{z} = \mathbf{0}$.

An example of the probabilistic distance function $D(\cdot, \cdot)$ is the ϕ -divergence [58]:

$$D(\mathbb{Q}, \mathbb{P}_0) = \mathbb{E}^{\mathbb{P}_0} \left[\phi\left(\frac{\mathrm{d}\mathbb{Q}}{\mathrm{d}\mathbb{P}_0}\right) \right],$$

where $\phi(\cdot)$ is a convex function satisfying $\phi(1) = 0$. For example, if $\phi(t) = t \log t$, we obtain the Kullback-Leibler (KL) divergence [59], [60]. The definition of the ϕ -divergence requires that \mathbb{Q} is absolutely continuous with respect to \mathbb{P}_0 . If we take the empirical measure to be the nominal distribution \mathbb{P}_0 , this implies that the support of \mathbb{Q} must be a subset of the empirical examples. This constraint could potentially hurt the generalization capability of DRO.

Other choices for $D(\cdot, \cdot)$ include the Prokhorov metric [61], and the Wasserstein distance [13], [14], [18], [62], [63]. DRO with the Wasserstein metric has been extensively studied in the machine learning community; see, for example, [12] and [64] for robustified regression models, [33] for adversarial training in neural networks, and [55] for distributionally robust logistic regression. [46] and [47] provided a comprehensive analysis of the Wasserstein-based distributionally robust statistical learning problems with a scalar (as opposed to a vector) response. In recent work, [65] proposed a DRO formulation for convex regression under an absolute error loss.

In this monograph we adopt the Wasserstein metric to define a datadriven DRO problem. Specifically, the ambiguity set Ω is defined as:

$$\Omega \triangleq \{ \mathbb{Q} \in \mathcal{P}(\mathcal{Z}) \colon W_{s,t}(\mathbb{Q}, \hat{\mathbb{P}}_N) \le \epsilon \},$$
(1.6)

where $\hat{\mathbb{P}}_N$ is the uniform empirical distribution over N training samples $\mathbf{z}_i, i \in [\![N]\!]$, and $W_{s,t}(\mathbb{Q}, \hat{\mathbb{P}}_N)$ is the order-t Wasserstein distance $(t \ge 1)$

1.3. Outline

between \mathbb{Q} and $\hat{\mathbb{P}}_N$ defined as:

$$W_{s,t}(\mathbb{Q},\hat{\mathbb{P}}_N) \triangleq \left(\min_{\pi \in \mathcal{P}(\mathcal{Z} \times \mathcal{Z})} \int_{\mathcal{Z} \times \mathcal{Z}} (s(\mathbf{z}_1, \mathbf{z}_2))^t \mathrm{d}\pi(\mathbf{z}_1, \mathbf{z}_2) \right)^{1/t}, \quad (1.7)$$

where s is a metric on the data space \mathcal{Z} , and π is the joint distribution of \mathbf{z}_1 and \mathbf{z}_2 with marginals \mathbb{Q} and $\hat{\mathbb{P}}_N$, respectively. The Wasserstein distance between two distributions represents the cost of an optimal mass transportation plan, where the cost is measured through the metric s.

We choose the Wasserstein metric for two main reasons. On one hand, the Wasserstein ambiguity set is rich enough to contain both continuous and discrete relevant distributions, while other metrics such as the KL divergence, exclude all continuous distributions if the nominal distribution is discrete [13], [14]. Furthermore, considering distributions within a KL distance from the empirical, does not allow for probability mass outside the support of the empirical distribution.

On the other hand, measure concentration results guarantee that the Wasserstein set contains the true data-generating distribution with high confidence for a sufficiently large sample size [66]. Moreover, the Wasserstein metric takes into account the closeness between support points while other metrics such as the ϕ -divergence only consider the probabilities on these points. An image retrieval example in [14] suggests that the probabilistic ambiguity set constructed based on the KL divergence prefers the pathological distribution to the true distribution, whereas the Wasserstein distance does not exhibit such a problem. The reason lies in that the ϕ -divergence does not incorporate a notion of closeness between two points, which in the context of image retrieval represents the perceptual similarity in color.

1.3 Outline

The goal of this monograph is to develop a comprehensive robust statistical learning framework using a Wasserstein-based DRO as the modeling tool. Specifically,

• we provide background knowledge on the basics of DRO and the Wasserstein metric, and show its robustness inducing property

Introduction

through discussions on the Wasserstein ambiguity set and the property of the DRO solution;

- we cover a variety of predictive and prescriptive models that can be posed and solved using the Wasserstein DRO approach, and show novel problem-tailored theoretical results and real world applications, strengthening the notion of robustness through these discussions;
- we consider a variety of synthetic and real world case studies of the respective models, which validate the theory and the proposed DRO approach and highlight its advantages compared to several alternatives. This could potentially (i) ease the understanding of the model and approach; and (ii) attract practitioners from various fields to put these models into use.

Robust models can be useful when (i) the training data is contaminated with noise, and we want to learn a model that is immunized against the noise; or (ii) the training data is pure, but the test set is contaminated with outliers. In both scenarios we require the model to be insensitive to the data uncertainty/unreliability, which is characterized through a probability distribution that resides in a set consisting of all distributions that are within a pre-specified distance from a nominal distribution. The learning problems that are studied in this monograph include:

- Distributionally Robust Linear Regression (DRLR), which estimates a robustified linear regression plane by minimizing the worst-case expected absolute loss over a probabilistic ambiguity set characterized by the Wasserstein metric.
- Groupwise Wasserstein Grouped LASSO (GWGL), which aims at inducing sparsity at a group level when there exists a predefined grouping structure for the predictors, through defining a specially structured Wasserstein metric for DRO.
- Distributionally Robust Multi-Output Learning, which solves a DRO problem with a multi-dimensional response/label vector, generalizing the single-output model addressed in DRLR.

1.3. Outline

- Optimal decision making using *DRLR informed K-Nearest Neighbors* (*K-NN*) estimation, which selects among a set of actions the optimal one through predicting the outcome under each action using K-NN with a distance metric weighted by the DRLR solution.
- Distributionally Robust Semi-Supervised Learning, which estimates a robust classifier with partially labeled data, through (i) either restricting the marginal distribution to be consistent with the unlabeled data, (ii) or modifying the structure of DRO by allowing the center of the ambiguity set to vary, reflecting the uncertainty in the labels of the unsupervised data.
- Distributionally Robust Reinforcement Learning, which considers Markov Decision Processes (MDPs) and seeks to inject robustness into the probabilistic transition model, deriving a lower bound for the distributionally robust value function in a regularized form.

The remainder of this monograph is organized as follows. Section 2 presents basics and key properties for the Wasserstein metric. Section 3 discusses how to solve a general Wasserstein DRO problem, the structure of the worst-case distribution, and the performance guarantees of the DRO estimator. The rest of the sections are dedicated to specific learning problems that can be posed as a DRO problem.

In Section 4, we develop the Wasserstein DRO formulation for linear regression under an absolute error loss. Section 5 discusses distributionally robust grouped variable selection, and develops the *Groupwise Wasserstein Grouped LASSO (GWGL)* formulation under the absolute error loss and log-loss. In Section 6, we generalize the single-output model and develop distributionally robust multi-output learning models under Lipschitz continuous loss functions and the multiclass log-loss. Section 7 presents an optimal decision making framework which selects among a set of actions the best one, using predictions from *K-Nearest Neighbors (K-NN)* with a metric weighted by the Wasserstein DRO solution. Section 8 covers a number of active research topics in the domain of DRO under the Wasserstein metric, including (i) DRO in *Semi-Supervised Learning (SSL)* with partially labeled datasets; (ii) DRO in

Introduction

Reinforcement Learning (RL) with temporal correlated data. We close the monograph by discussing further potential research directions in Section 9.

1.4 Notational Conventions

Vectors

- Boldfaced lowercase letters denote vectors, ordinary lowercase letters denote scalars, boldfaced uppercase letters denote matrices, and calligraphic capital letters denote sets.
- **e**_i denotes the *i*-th unit vector, **e** or **1** the vector of ones, and **0** a vector of zeros.
- All vectors are column vectors. For space saving reasons, we write $\mathbf{x} = (x_1, \dots, x_{\dim(\mathbf{x})})$ to denote the column vector \mathbf{x} , where dim (\mathbf{x}) is the dimension of \mathbf{x} .

Sets and functions

- We use $\mathbb R$ to denote the set of real numbers, and $\mathbb R^+$ the set of non-negative real numbers.
- For a set \mathcal{X} , we use $|\mathcal{X}|$ to denote its cardinality.
- We write cone $\{\mathbf{v} \in \mathcal{V}\}$ for a cone that is generated from the set of vectors $\mathbf{v} \in \mathcal{V}$.
- $\mathbf{1}_{\mathcal{A}}(\mathbf{x})$ denotes the indicator function, i.e., $\mathbf{1}_{\mathcal{A}}(\mathbf{x}) = 1$ if $\mathbf{x} \in \mathcal{A}$, and 0 otherwise.
- For $\mathbf{z} \triangleq (\mathbf{x}, y) \in \mathcal{X} \times \mathcal{Y}$ and a function h, the notations $h(\mathbf{z})$ and $h(\mathbf{x}, y)$ are used interchangeably, and $\mathcal{Z} \triangleq \mathcal{X} \times \mathcal{Y}$.
- \$\mathcal{B}(\mathcal{Z})\$ denotes the set of Borel measures supported on \$\mathcal{Z}\$, and \$\mathcal{P}(\mathcal{Z})\$ denotes the set of Borel probability measures supported on \$\mathcal{Z}\$.
- For any integer n we write $[\![n]\!]$ for the set $\{1, \ldots, n\}$. Hence, $\mathcal{P}([\![n]\!])$ denotes the *n*-th dimensional probability simplex.

1.4. Notational Conventions

Matrices

- I denotes the identity matrix.
- Prime denotes transpose. Specifically, \mathbf{A}' denotes the transpose of a matrix \mathbf{A} .
- For a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$, we will denote by $\mathbf{A} = (a_{ij})_{i \in [m]}^{j \in [n]}$ the elements of \mathbf{A} , by $\mathbf{a}_1, \ldots, \mathbf{a}_m$ the rows of \mathbf{A} , and, with some abuse of our notation which denotes vectors by lowercase letters, we will denote by $\mathbf{A}_1, \ldots, \mathbf{A}_n$ the columns of \mathbf{A} .
- For a symmetric matrix \mathbf{A} , we write $\mathbf{A} \succ 0$ to denote a positive definite matrix, and $\mathbf{A} \succeq 0$ a positive semi-definite matrix.
- diag(**x**) denotes a diagonal matrix whose main diagonal consists of the elements of **x** and all off-diagonal elements are zero.
- tr(A) denotes the trace (i.e., sum of the diagonal elements) of a square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$.
- $|\mathbf{A}|$ denotes the determinant of a square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$.

Norms

- $\|\mathbf{x}\|_p \triangleq (\sum_i |x_i|^p)^{1/p}$ denotes the ℓ_p norm with $p \ge 1$, and $\|\cdot\|$ the general vector norm that satisfies the following properties:
 - 1. $\|\mathbf{x}\| = 0$ implies $\mathbf{x} = \mathbf{0}$;
 - 2. $||a\mathbf{x}|| = |a|||\mathbf{x}||$, for any scalar a;
 - 3. $\|\mathbf{x} + \mathbf{y}\| \le \|\mathbf{x}\| + \|\mathbf{y}\|;$
 - 4. $\|\mathbf{x}\| = \||\mathbf{x}\|\|$, where $|\mathbf{x}| = (|x_1|, \dots, |x_{\dim(\mathbf{x})}|);$
 - 5. $\|(\mathbf{x}, \mathbf{0})\| = \|\mathbf{x}\|$, for an arbitrarily long vector $\mathbf{0}$.
- Any **W**-weighted ℓ_p norm defined as

$$\|\mathbf{x}\|_p^{\mathbf{W}} \triangleq ((|\mathbf{x}|^{p/2})'\mathbf{W}|\mathbf{x}|^{p/2})^{1/p}$$

with a positive definite matrix **W** satisfies the above conditions, where $|\mathbf{x}|^{p/2} = (|x_1|^{p/2}, \dots, |x_{\dim(\mathbf{x})}|^{p/2}).$

Introduction

• For a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$, we use $\|\mathbf{A}\|_p$ to denote its induced ℓ_p norm that is defined as $\|\mathbf{A}\|_p \triangleq \sup_{\mathbf{x} \neq \mathbf{0}} \|\mathbf{A}\mathbf{x}\|_p / \|\mathbf{x}\|_p$.

Random variables

- For two random variables w_1 and w_2 , we say that w_1 is stochastically dominated by w_2 , denoted by $w_1 \stackrel{\scriptscriptstyle D}{\leq} w_2$, if $\mathbb{P}(w_1 \geq x) \leq \mathbb{P}(w_2 \geq x)$ for all $x \in \mathbb{R}$.
- For a dataset $\mathcal{D} \triangleq \{\mathbf{z}_1, \dots, \mathbf{z}_N\}$, we use $\hat{\mathbb{P}}_N$ to denote the empirical measure supported on \mathcal{D} , i.e., $\hat{\mathbb{P}}_N \triangleq \frac{1}{N} \sum_{i=1}^N \delta_{\mathbf{z}_i}(\mathbf{z})$, where $\delta_{\mathbf{z}_i}(\mathbf{z})$ denotes the Dirac delta function at point $\mathbf{z}_i \in \mathcal{Z}$.
- The N-fold product of a distribution \mathbb{P} on \mathcal{Z} is denoted by \mathbb{P}^N , which represents a distribution on the Cartesian product space \mathcal{Z}^N . We write \mathbb{P}^∞ to denote the limit of \mathbb{P}^N as $N \to \infty$.
- $\mathbb{E}^{\mathbb{P}}$ denotes the expectation under a probability distribution \mathbb{P} .
- For a random vector \mathbf{x} , $cov(\mathbf{x})$ will denote its covariance.
- *N_p*(**0**, **Σ**) denotes the *p*-dimensional Gaussian distribution with mean **0** and covariance matrix **Σ**.
- For a distribution $\mathbb{P} \in \mathcal{P}(\mathcal{X} \times \mathcal{Y}), \mathbb{P}_{\mathcal{X}}(\cdot) \triangleq \sum_{y \in \mathcal{Y}} \mathbb{P}(\cdot, y)$ denotes the marginal distribution over \mathcal{X} , and $\mathbb{P}_{|\mathbf{x}|} \in \mathcal{P}^{\mathcal{X}}(\mathcal{Y})$ is the conditional distribution over \mathcal{Y} given $\mathbf{x} \in \mathcal{X}$, where $\mathcal{P}^{\mathcal{X}}(\mathcal{Y})$ denotes the set of all conditional distributions supported on \mathcal{Y} , given features in \mathcal{X} .
- $W_{s,t}(\mathbb{P}, \mathbb{Q})$ denotes the order-*t* Wasserstein distance between measures \mathbb{P}, \mathbb{Q} under a cost metric *s*. For ease of notation and when the cost metric is clear from the context we will be writing $W_t(\mathbb{P}, \mathbb{Q})$.
- $\Omega_{\epsilon}^{s,t}(\mathbb{P})$ denotes the set of probability distributions whose order-t Wasserstein distance under a cost metric s from the distribution \mathbb{P} is less than or equal to ϵ , i.e.,

$$\Omega^{s,t}_{\epsilon}(\mathbb{P}) \triangleq \{ \mathbb{Q} \in \mathcal{P}(\mathcal{Z}) \colon W_{s,t}(\mathbb{Q}, \mathbb{P}) \le \epsilon \}.$$

For ease of notation, when the cost metric is clear from the context and t = 1, we will be writing $\Omega_{\epsilon}(\mathbb{P})$, or simply Ω when the center distribution \mathbb{P} is clear from the context.

1.5. Abbreviations

1.5 Abbreviations

ACE		Angiotensin-Converting Enzyme
ACS		American College of Surgeons
AD		Absolute Deviation
ARB		Angiotensin Receptor Blockers
a.s.		almost surely
AUC		Area Under the ROC Curve
BMI		Body Mass Index
CART		Classification And Regression Trees
CCA		Canonical Correlation Analysis
CCR		Correct Classification Rate
CI		Confidence Interval
CT		Computed Tomography
CTDI		CT Dose Index
CVaR		Conditional Value at Risk
C&W		The Curds and Whey procedure
DRLR		Distributionally Robust Linear
		Regression
DRO		Distributionally Robust Optimization
EHRs		Electronic Health Records
EN		Elastic Net
FA		False Association
FD		
ТD		False Disassociation
FES		False Disassociation Factor Estimation and Selection
FES GLASSO	· · · · · · · · · · · · · · · · · · ·	False Disassociation Factor Estimation and Selection Grouped LASSO
FES GLASSO GSRL	· · · · · · · · · · · · · · · · · · ·	False Disassociation Factor Estimation and Selection Grouped LASSO Grouped Square Root LASSO
FES GLASSO GSRL GWGL	·····	False Disassociation Factor Estimation and Selection Grouped LASSO Grouped Square Root LASSO Groupwise Wasserstein Grouped
FES GLASSO GSRL GWGL	· · · · · · · · · · · · · · · · · · ·	False Disassociation Factor Estimation and Selection Grouped LASSO Grouped Square Root LASSO Groupwise Wasserstein Grouped LASSO
FES GLASSO GSRL GWGL HbA _{1c}	······	False Disassociation Factor Estimation and Selection Grouped LASSO Grouped Square Root LASSO Groupwise Wasserstein Grouped LASSO hemoglobin A1c
FES GLASSO GSRL GWGL HbA _{1c} HIPAA	······	False Disassociation Factor Estimation and Selection Grouped LASSO Grouped Square Root LASSO Groupwise Wasserstein Grouped LASSO hemoglobin A1c Health Insurance Portability and
FES GLASSO GSRL GWGL HbA _{1c} HIPAA	· · · · · · · · · · · · · · · · · · ·	False Disassociation Factor Estimation and Selection Grouped LASSO Grouped Square Root LASSO Groupwise Wasserstein Grouped LASSO hemoglobin A1c Health Insurance Portability and Accountability Act
FES GLASSO GSRL GWGL HbA _{1c} HIPAA ICD-9	· · · · · · · · · · · · · · · · · · ·	False Disassociation Factor Estimation and Selection Grouped LASSO Grouped Square Root LASSO Groupwise Wasserstein Grouped LASSO hemoglobin A1c Health Insurance Portability and Accountability Act International Classification of
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FES GLASSO GSRL GWGL HbA _{1c} HIPAA ICD-9 i.i.d.	· · · · · · · · · · · · · · · · · · ·	False Disassociation Factor Estimation and Selection Grouped LASSO Grouped Square Root LASSO Groupwise Wasserstein Grouped LASSO hemoglobin A1c Health Insurance Portability and Accountability Act International Classification of Diseases, Ninth Revision independently and identically

Introduction

IRB	 Institutional Review Board
IRLS	 Iteratively Reweighted Least Squares
KL	 Kullback–Leibler
K-NN	 K-Nearest Neighbors
LAD	 Least Absolute Deviation
LASSO	 Least Absolute Shrinkage and
	Selection Operator
LG	 Logistic Regression
LHS	 Left Hand Side
LMS	 Least Median of Squares
LOESS	 LOcally Estimated Scatterplot
	Smoothing
LTS	 Least Trimmed Squares
MAD	 Median Absolute Deviation
MCC	 MultiClass Classification
MDP	 Markov Decision Process
MeanAE	 Mean Absolute Error
min-max	 minimization-maximization
MLE	 Maximum Likelihood Estimator
MLG	 Multiclass Logistic Regression
MLR	 Multi-output Linear Regression
MPD	 Minimal Perturbation Distance
MPI	 Maximum Percentage Improvement
MPMs	 Minimax Probability Machines
MSE	 Mean Squared Error
NPV	 Negative Predictive Value
NSQIP	 National Surgical Quality
	Improvement Program
OLS	 Ordinary Least Squares
PCR	 Principal Components Regression
PPV	 Positive Predictive Value
PVE	 Proportion of Variance Explained
RBA	 Robust Bias-Aware
RHS	 Right Hand Side
RL	 Reinforcement Learning

1.5. Abbreviations

ROC	 Receiver Operating Characteristic
RR	 Relative Risk
RRR	 Reduced Rank Regression
RTE	 Relative Test Error
SNR	 Signal to Noise Ratio
\mathbf{SR}	 Squared Residuals
SSL	 Semi-Supervised Learning
std	 standard deviation
SVM	 Support Vector Machine
ТА	 True Association
TD	 True Disassociation
TAR	 True Association Rate
TDR	 True Disassociation Rate
WGD	 Within Group Difference
w.h.p.	 with high probability
WMSE	 Weighed Mean Squared Error
w.p.1	 with probability 1
w.r.t.	 with respect to

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