Covariance-Robust Minimax Probability Machines for Algorithmic Recourse

Abstract

Algorithmic recourse is rising as a prominent technique to promote the explainability and transparency of the predictive model in ethical machine learning. Existing approaches to algorithmic recourse often assume an invariant predictive model; however, this model, in reality, is usually updated temporally upon the input of new data. Thus, a recourse that is valid respective to the present model may become *in*valid for the future model. To resolve this issue, we propose a pipeline to generate a model-agnostic recourse that is robust to model shifts. Our pipeline first estimates a linear surrogate of the *non*linear (black-box) model using covariance-robust minimax probability machines (MPM); then, the recourse is generated with respect to this robust linear surrogate. We show that the covariance-robust MPM recovers popular regularization schemes, including ℓ_2-regularization and class-reweighting. We also show that our covariance-robust MPM pushes the decision boundary in an intuitive manner, which facilitates an interpretable generation of a robust recourse. The numerical results demonstrate the usefulness and robustness of our pipeline.

1 Introduction

Recent prevalence of machine learning (ML) in supporting consequential decisions involving humans such as loan approval (Moscato et al., 2021), job hiring (Cohen et al., 2019; Schumann et al., 2020), and criminal justice (Brayne & Christin, 2021) urges the need of transparent ML systems with explanations and feedback to users (Doshi-Velez & Kim, 2017; Miller, 2019). One popular and emerging approach to providing feedback is the algorithmic recourse (Ustun et al., 2019). A *recourse* suggests how the input instance should be modified to alter the outcome of a predictive model. Consider a specific scenario in which an individual is rejected from receiving a loan by a financial institution's ML model. Recently, it has become a legal necessity to provide explanations and recommendations to the individual so that they can improve their situation and are able to obtain a loan in the future (GDPR, Voigt & Von dem Bussche (2017)). For example, such an explanation can be of the form "increase the income to $5000" or "reduce the debt/asset ratio to below 20%". Leveraging the recourses, financial institutions can assess the reliability of their ML predictive model and increase user engagement through actionable feedback and acceptance guarantee if they fulfill the requirements.

To construct plausible and meaningful recourses, one must assess and strike a balance between conflicting criteria. They can be: (1) *validity*, a recourse should effectively reverse the unfavorable prediction of the model into a favorable one, (2) *proximity*, recourse should be close to the original input instance to alleviate the efforts required, and thus to encourage the adoption of the recourse, (3) *actionability*, prescribed modifications should follow causal laws of our society (Ustun et al., 2019; Karimi et al., 2021); for example, one can not modify their race or decrease their age.

Various techniques were proposed to devise algorithmic recourses for a given predictive model, extensive surveys are provided in (Karimi et al., 2020a; Stepin et al., 2021; Pawelczyk et al., 2021; Verma et al., 2020). Wachter et al. (2017) introduced the definition of counterfactual explanations and proposed a gradient-based approach to find the nearest instance that yields a favorable outcome. Ustun et al. (2019) proposed a mixed integer programming formulation (AR) that can find recourses for a linear classifier with a flexible design of the actionability constraints. Alternatively, Karimi et al. (2021; 2020b) investigated the nearest recourse through the lens of minimal intervention to take causal relationships between features into account. Some recent works including Russell (2019)

and Mothilal et al. (2020) also studied the problem of generating a menu of diverse recourses to provide multiple possibilities that users might choose.

The aforementioned methods rely on an assumption of an invariant predictive model. Nevertheless, machine learning models are usually re-trained or re-calibrated as new data arrive. Thus, a valid recourse at present may become invalid in the future, leading to an exemplary case where a rejected applicant may spend efforts to improve their income and reapply for a loan, but then is rejected (again) simply because the ML model has been updated. This leads to a potential inefficiency due to the waste of resources and loss of trust in the recommendation and in the ML system (Rudin, 2019).

Studying this phenomenon, Rawal et al. (2020) described several types of model shifts related to the correction, temporal, and geospatial shifts from data. They pointed out that the recourses, even constructed with state-of-the-art algorithms, are vulnerable to distributional shifts in the model's parameters. Pawelczyk et al. (2020) study counterfactual explanations under predictive multiplicity and its relation to the difference in the way two classifiers treat predicted individuals. Black et al. (2021) then show that the constructed recourses might be invalid even for the model retrained with different initial conditions such as weight initialization and leave-one-out variations in data. Recently, Upadhyay et al. (2021) leveraged robust optimization to propose ROAR - a framework for generating recourses that are robust to shifts in the predictive model, which is assumed to be a linear classifier.

Despite the promising results, existing methods are often restricted to the linear classifiers setting to be able to introduce actionability or robustness (Ustun et al., 2019; Russell, 2019; Upadhyay et al., 2021; Rawal et al., 2020). For non-linear classifiers, a linear surrogate such as LIME (Ribeiro et al., 2016) is used to approximate the local decision boundary of the black-box classifiers; recourse is then generated respectively to the (linear) surrogate model rather than the nonlinear model. LIME is well-known for explaining predictions of black-box ML models by fitting a reweighted linear regression model to the perturbed samples around an input instance. It is commonly used in the recourse literature as the linear surrogate to approximate the local decision boundary of the black-box models (Ustun et al., 2019; Upadhyay et al., 2021).

However, LIME's surrogate has also known with several limitations. Firstly, Laugel et al. (2018) and White & Garcez (2019) showed that LIME may not be faithful to the underlying models since the local surrogate models of LIME might be influenced by input features at a global scale rather than a local scale. Secondly, explanations generated by perturbation-based methods are also well-known to be sensitive to the original input and the synthesized perturbations (Alvarez-Melis & Jaakkola, 2018; Ghorbani et al., 2019; Slack et al., 2020; 2021; Agarwal et al., 2021; Laugel et al., 2018).

Several works have been proposed to overcome these issues. Laugel et al. (2018) and Vlassopoulos et al. (2020) proposed alternative sampling procedures that generate sample instances in the neighborhood of the closest counterfactual to fit a local surrogate. White & Garcez (2019) integrated counterfactual explanation to local surrogate models to introduce a novel fidelity measure of an explanation. Later, Garreau & von Luxburg (2020) and Agarwal et al. (2021) analyzed theoretically the stability[1] of LIME, especially in the low sampling size regime. Zhao et al. (2021) leveraged Bayesian reasoning to improve the consistency in repeated explanations of a single prediction. Nevertheless, the impact and effectiveness of these surrogates on the recourse generation are still unknown.

Contributions. This paper revisits the recourse generation scheme through surrogate models. We propose a novel model-agnostic pipeline that facilitates generation of *robust* and *actionable* recourses. The core of our pipeline is the use of the covariance-robust minimax probability machines (MPM) as a linear surrogate of the nonlinear black-box ML model. Our paper contributes

- to the field of MPM and robust classifier: We propose and analyze in detail the covariance-robust MPMs in which the set of possible perturbations of the covariance matrices are prescribed using distances on the space of positive semidefinite matrices. Motivated by the statistical distances between Gaussian distributions, we show that the covariance-robustness induces and connects to two prominent regularization schemes of the nominal MPM:
  - if the distance is motivated by the Bures distance, we recover the ℓ_2-regularization,
  - if the distance is motivated by the Fisher-Rao distance, we recover class reweighting schemes.

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[1]Throughout, "robustness" is used in the algorithmic recourse setting with respect to the model shifts (Rawal et al., 2020). "Robustness" is also used to indicate the sensitivity of LIME to the sampling distribution. To avoid confusion, in what follows, we use "stability" to refer to the aforementioned sensitivity of LIME.

Figure 1: The sampler generates new instances around x_0 and queries the predicted labels from the black-box classifier f. The new labeled instances are used to estimate the moment information $(\widehat{\mu}_y, \widehat{\Sigma}_y)$, which serve as parameters for the MPM. The MPM surrogate θ^φ is the target classifier used to generate recourses that are robust to model shifts.

While prior works showed that distributionally robust optimization (DRO) with optimal transport distance recovers norm regularization (Shafieezadeh-Abadeh et al., 2019b) and f-divergence DRO leads to reweighting (Duchi & Namkoong, 2019), this paper extends the connections to the MPMs.

• to the field of robust algorithmic recourse: We propose an intuitive and interpretable approach to generate robust recourse. We show that, by calibrating the radii of the ambiguity sets in a proper manner, the covariance-robust MPM shifts the separation hyperplane towards the favorable class. As a consequence, our recourse exhibits robustness to model shifts and it is also lenient to incorporate mixed-integer constraints to promote actionability.

This paper unfolds as follows. In Section 2, we delineate our explanation framework using MPM. Section 3 dives deeper into the MPM problem and its robustification. Section 4-5 construct two types of covariance-robust MPM using the Bures and Fisher-Rao distance on the space of covariance matrices. In Section 6, we demonstrate empirically that the covariance-robust MPM provides a competitive approximation of the local decision boundary, and improves the robustness of the recourse subject to model shifts.

2   RECOURSE GENERATION FRAMEWORK

Throughout this paper, we assume that the covariate space is $\mathcal{X} = \mathbb{R}^d$ and we have a binary label space $\mathcal{Y} = \{-1, +1\}$. Without any loss of generality, we assume that label -1 encodes the unfavorable decision, while $+1$ encodes the favorable one. Given a specific classifier and an input x_0 with an unfavorable predicted outcome, the goal of this paper is to find a recourse recommendation for x_0 that has a high probability of being classified into a favorable group, subject to possible shifts in the parameters underlying the classifier. Such recourse is termed a robust recourse. Our robust recourse generator consists of three components (see Figure 1 for a schematic view):

(i) a local sampler: we use a similar sampling procedure as in Vlassopoulos et al. (2020) and Laugel et al. (2018). Given an instance x_0, we choose k nearest counterfactuals $x_1, \ldots, x_k$ from the training data that have opposite label to x_0. For each counterfactual x_i, we perform a line search to find a point $x_{b,i}$ that is on the decision boundary and the line segment between x_0 and x_i. Among $x_{b,i}$, we choose the nearest point x_b to x_0 and sample uniformly in a an ℓ_2-neighborhood with radius r_p around x_b. We then query the black-box classifier to obtain the predicted labels of the synthesized samples.

(ii) a linear surrogate using (covariance-robust) MPM: We use the samples previously synthesized to estimate the moment information $(\widehat{\mu}_y, \widehat{\Sigma}_y)$ of the covariate conditional on each predicted class y. We then train a covariance-robust MPM parametrized by θ^φ to approximate the local decision boundary of the ML model.

(iii) a recourse search: Basically, we can apply any existing recourse search for linear models on top of the linear surrogate θ^φ dictated by the covariance-robust MPMs to find a robust recourse. In this paper, we use a simple projection onto the hyperplane prescribed by θ^φ for simplicity and AR (Ustun et al., 2019), which is a MIP-based framework, to promote actionable recourses.

Center to the success of our pipeline is the possibility of shifting the MPM classification hyperplane toward the region of the favorable class, which induces robust recourse with respect to model shifts in a geometrically-intuitive manner (see Remark 4.6 for a detailed discussion). It is imperative to

note a clear distinction between our pipeline and the existing method of ROAR (Upadhyay et al., 2021): ROAR uses a non-robust surrogate in Step (ii) and then formulates a min-max optimization problem in Step (iii) for recourse search, whilst our pipeline uses a *robust* surrogate in Step (ii) and then employs a simple recourse search in Step (iii). Note that mixed-integer formulations can be injected in Step (iii) to generate more realistic robust recourses in our pipeline. On the contrary, mixed-integer constraints are not easy to be integrated into the min-max formulation of ROAR.

Subsequently, Sections 3-5 describe in detail different methods to build robust surrogates in Step (ii). The application of recourse research in Step (iii) is provided in the experiment section (Section 6.2).

3 (COVARIANCE-ROBUST) MPM

MPM is a binary classification framework pioneered by Lanckriet et al. (2001) and extended further to Quadratic MPM in (Lanckriet et al., 2003). For each class $y \in \mathcal{Y}$, the MPM makes no assumption on the specific parametric form of the (conditional) distribution $\widehat{\mathbb{P}}_y$ of $X|Y = y$. Instead, MPM assumes that we can identify $\widehat{\mathbb{P}}_y$ only up to the first two moments, *i.e.*, it assumes that $\widehat{\mathbb{P}}_y$ has mean vector $\widehat{\mu}_y \in \mathbb{R}^d$ and covariance matrix $\widehat{\Sigma}_y \in \mathbb{S}_+^d$, denoted $\widehat{\mathbb{P}}_y \sim (\widehat{\mu}_y, \widehat{\Sigma}_y)$. These moments can be estimated from the samples synthesized from the boundary sampler. The goal of MPM is to find a (non-trivial) linear classifier that minimizes the maximum misclassification rate among classes. To this end, let us consider the following family of linear classifiers parametrized by $\theta = (w, b) \in \mathbb{R}^{d+1}$, $w \neq 0$ with classification rule

$$\mathcal{C}_\theta(x) = \text{sign}(w^\top x - b),$$

where (w, b) is the slope and intercept. The MPM solves the min-max optimization problem

$$\min_{\theta \in \Theta} \max_{y \in \mathcal{Y}} \max_{\widehat{\mathbb{P}}_y \sim (\widehat{\mu}_y, \widehat{\Sigma}_y)} \widehat{\mathbb{P}}_y(\mathcal{C}_\theta(X) \neq y), \tag{1}$$

where we define the feasible set $\Theta \triangleq \{\theta = (w, b) \in \mathbb{R}^{d+1} : w \neq 0\}$. Notice that the constraints $w \neq 0$ eliminate trivial solutions to the classification problem.

To derive the MPM, we define the set of feasible slopes $\mathcal{W} = \left\{ w \in \mathbb{R}^d \backslash \{0\} : \sum_{y \in \mathcal{Y}} y w^\top \widehat{\mu}_y = 1 \right\}$, which is a hyperplane in $\mathbb{R}^d$. The main instrument for solving (1) is the following result from (Lanckriet et al., 2001, §2) which provides the form of its optimal solution.

Lemma 3.1 (Optimal solution). *Let $\widehat{w}$ be an optimal solution to the second-order cone program*

$$\min_{w \in \mathcal{W}} \sum_{y \in \mathcal{Y}} \sqrt{w^\top \widehat{\Sigma}_y w}, \tag{2}$$

then $\widehat{\theta} = (\widehat{w}, \widehat{b})$ solves the MPM problem (1)*, where*

$$\widehat{\kappa} = \left(\sum_{y \in \mathcal{Y}} \sqrt{w^\top \widehat{\Sigma}_y w} \right)^{-1}, \quad \text{and} \quad \widehat{b} = \widehat{w}^\top \widehat{\mu}_{+1} - \widehat{\kappa} \sqrt{\widehat{w}^\top \widehat{\Sigma}_{+1} \widehat{w}}.$$

In this paper, we refer to the second-order cone program (2) as the *nominal* MPM problem, because the MPM is fully determined by the solution to (2). We next discuss the covariance-robust MPM.

3.1 QUADRATIC MPM

In a practical setting, it is likely that the covariance matrices $\widehat{\Sigma}_y$ are misspecified, for example, due to low sample size, statistical estimation error, or corrupted data. To hedge against these mismatches, Lanckriet et al. (2003) proposed to add another layer of robustness by allowing the mean vectors and the covariance matrices of the conditional distributions to be chosen (adversarially) in a prescribed set, which we call the ambiguity set. They showed that perturbing the mean vectors does not change the optimal classifier. In this paper, we, therefore, perturb only the covariance matrices. More specifically, we allow the conditional distribution $\mathbb{P}_y$ to be in the ambiguity set

$$\mathbb{U}_y^\varphi(\widehat{\mathbb{P}}_y) = \{\mathbb{P}_y : \mathbb{P}_y \sim (\widehat{\mu}_y, \Sigma_y), \ \varphi(\Sigma_y \parallel \widehat{\Sigma}_y) \leq \rho_y\},$$

where φ is a measure of dissimilarity between covariance matrices. The distributionally robust minimax probability machine is formulated as

$$\min_{\theta \in \Theta} \max_{y \in \mathcal{Y}} \max_{\mathbb{P}_y \in \mathbb{U}_y^{\varphi}(\widehat{\mathbb{P}}_y)} \mathbb{P}_y(\mathcal{C}_{\theta}(X) \neq y). \tag{3}$$

Previously, Lanckriet et al. (2003) considered the robust MPM with moment uncertainty, in which the covariance matrix is perturbed using the quadratic divergence.

Definition 3.2 (Quadratic divergence). *Given two positive semidefinite matrices Σ, $\widehat{\Sigma} \in \mathbb{S}_+^d$, the quadratic divergence between them is $\mathbb{Q}(\Sigma \parallel \widehat{\Sigma}) = \mathrm{Tr}\left[(\Sigma - \widehat{\Sigma})^2\right]$.*

By definition, $\mathbb{Q}$ is non-negative and equals zero if and only if $\Sigma = \widehat{\Sigma}$, so it is a divergence on $\mathbb{S}_+^d$. More, $\mathbb{Q}$ is the *squared* Frobenius norm of $\Sigma - \widehat{\Sigma}$. The Quadratic MPM has the following form (Lanckriet et al., 2003).

Theorem 3.3 (Quadratic MPM). *Suppose that $\varphi \equiv \mathbb{Q}$. Let $w^{\mathbb{Q}}$ be a solution to the problem*

$$\min_{w \in \mathcal{W}} \sum_{y \in \mathcal{Y}} \sqrt{w^{\top}(\widehat{\Sigma}_y + \sqrt{\rho_y}I)w}. \tag{4}$$

Then $\theta^{\mathbb{Q}} = (w^{\mathbb{Q}}, b^{\mathbb{Q}})$ solves the distributionally robust MPM problem (3)*, with*

$$\kappa^{\mathbb{Q}} = \left(\sum_{y \in \mathcal{Y}} \sqrt{(w^{\mathbb{Q}})^{\top}(\widehat{\Sigma}_y + \sqrt{\rho_y}I)w^{\mathbb{Q}}}\right)^{-1}, \quad b^{\mathbb{Q}} = (w^{\mathbb{Q}})^{\top}\widehat{\mu}_{+1} - \kappa^{\mathbb{Q}}\sqrt{(w^{\mathbb{Q}})^{\top}(\widehat{\Sigma}_{+1} + \sqrt{\rho_{+1}}I)w^{\mathbb{Q}}}.$$

The Quadratic MPM can be considered as a regularization of the nominal problem (2): each matrix $\widehat{\Sigma}_y$ is added with a diagonal matrix $\sqrt{\rho_y}I$, making the matrix better conditioned. This is equivalently known as inverse regularization, which ensures invertibility when $\widehat{\Sigma}_y$ is low-rank and $\rho_y > 0$.

3.2 Covariance-Robust MPM

While Lanckriet et al. (2003) focused only on the quadratic divergence, their results can be generalized to the covariance-robust MPM with a general divergence φ. For any $y \in \mathcal{Y}$, define $\tau_y : \mathbb{R}^d \to \mathbb{R}$ as

$$\tau_y^{\varphi}(w) \triangleq \max_{\Sigma_y \in \mathbb{S}_+^d : \varphi(\Sigma_y \parallel \widehat{\Sigma}_y) \leq \rho_y} \sqrt{w^{\top}\Sigma w}. \tag{5}$$

We are now ready to give a generalized reformulation of problem (3). The proof follows similar steps as in Lanckriet et al. (2003) and is omitted.

Proposition 3.4 (Covariance-robust MPM). *Let w^{φ} be the optimal solution to the problem*

$$\min_{w \in \mathcal{W}} \sum_{y \in \mathcal{Y}} \tau_y^{\varphi}(w),$$

then $\theta^{\varphi} = (w^{\varphi}, b^{\varphi})$ solves the distributionally robust MPM problem (3)*, where*

$$\kappa^{\varphi} = \left(\sum_{y \in \mathcal{Y}} \tau_y^{\varphi}(w^{\varphi})\right)^{-1}, \quad and \quad b^{\varphi} = (w^{\varphi})^{\top}\widehat{\mu}_{+1} - \kappa^{\varphi}\tau_{+1}^{\varphi}(w^{\varphi}).$$

3.3 Equivalence under Gaussian Assumptions

While the quadratic divergence $\mathbb{Q}$ in Definition 3.2 is attractive for its tractability, it is not statistically meaningful. More specifically, it does not coincide with any distance between probability distributions with the corresponding covariance information. In this paper, we consider discrepancy measures φ that arise as a statistical distance between Gaussian distributions. To this goal, we first need to show that the covariance-robust MPM is invariant with the Gaussian assumption. Define a parametric ambiguity set constructed on the space of Gaussian distribution of the form

$$\mathcal{U}_y^{\mathcal{N}}(\widehat{\mathbb{P}}_y) = \left\{\mathbb{P}_y \in \mathcal{P}(\mathcal{X}) : \mathbb{P}_y \sim \mathcal{N}(\widehat{\mu}_y, \Sigma_y), \varphi(\Sigma_y \parallel \widehat{\Sigma}_y) \leq \rho_y\right\},$$

wherein any distribution is Gaussian. Consider the Gaussian distributionally robust MPM problem

$$\min_{\theta} \max_{y \in \mathcal{Y}} \max_{\mathbb{P}_y \in \mathcal{U}_y^{\mathcal{N}}(\widehat{\mathbb{P}}_y)} \mathbb{P}_y(\mathcal{C}_{\theta}(X) \neq y). \tag{6}$$

Proposition 3.5 (Gaussian equivalence). *The optimizer $\theta^{\varphi} = (w^{\varphi}, b^{\varphi})$ in Proposition 3.4 also solves the Gaussian parametric covariance-robust MPM problem* (6)*.*

Proposition 3.5 justifies the use of divergences induced by a distance between normal distributions. We study several constructions of the covariance-robust MPM in the subsequent sections.

4 BURES MPM

We first explore the case where φ is the Bures divergence whose definition is as follows.

Definition 4.1 (Bures divergence). *Given two positive semi-definite matrices $\Sigma, \widehat{\Sigma} \in \mathbb{S}_+^d$, the Bures divergence between them is $\mathbb{B}(\Sigma \| \widehat{\Sigma}) = \mathrm{Tr}\left[\Sigma + \widehat{\Sigma} - 2(\widehat{\Sigma}^{\frac{1}{2}}\Sigma\widehat{\Sigma}^{\frac{1}{2}})^{\frac{1}{2}}\right]$.*

It can be shown that $\mathbb{B}$ is symmetric and non-negative, and it vanishes to zero if and only if $\Sigma = \widehat{\Sigma}$. As such, $\mathbb{B}$ is a divergence on the space of positive semidefinite matrices. Moreover, $\mathbb{B}$ also equals the *squared* type-2 Wasserstein distance between two Gaussian distributions with the same mean vector and covariance matrices Σ and $\widehat{\Sigma}$ (Olkin & Pukelsheim, 1982; Givens & Shortt, 1984; Gelbrich, 1990). Next, we assert the form of the Bures MPM.

Theorem 4.2 (Bures MPM). *Suppose that $\varphi \equiv \mathbb{B}$. Let $w^{\mathbb{B}}$ be the solution of the following problem*

$$\min_{w \in \mathcal{W}} \sum_{y \in \mathcal{Y}} \sqrt{w^\top \widehat{\Sigma}_y w} + \left(\sum_{y \in \mathcal{Y}} \rho_y\right)\|w\|_2. \tag{7}$$

Then $\theta^{\mathbb{B}} = (w^{\mathbb{B}}, b^{\mathbb{B}})$ is the optimal solution of the distributionally robust MPM problem (3), *where*

$$\kappa^{\mathbb{B}} = \left(\sum_{y \in \mathcal{Y}} \sqrt{(w^{\mathbb{B}})^\top \widehat{\Sigma}_y w^{\mathbb{B}}} + \left(\sum_{y \in \mathcal{Y}} \rho_y\right)\|w^{\mathbb{B}}\|_2\right)^{-1}, \quad and$$

$$b^{\mathbb{B}} = (w^{\mathbb{B}})^\top \widehat{\mu}_{+1} - \kappa^{\mathbb{B}}\left(\sqrt{(w^{\mathbb{B}})^\top \widehat{\Sigma}_{+1} w^{\mathbb{B}}} + \rho_{+1}\|w^{\mathbb{B}}\|_2\right).$$

Theorem 4.2 unveils a fundamental connection between robustness and regularization: if we construct the ambiguity sets for the covariance matrices using the Bures divergence, the resulting optimization problem (7) is an l_2-regularization of the nominal problem (2). This connection aligns with previous observations highlighting the equivalence between regularization schemes and optimal transport robustness (Shafieezadeh-Abadeh et al., 2019a; Blanchet et al., 2019).

To prove Theorem 4.2, we provide a result that asserts the analytical form of $\tau_y^{\mathbb{B}}(w)$.

Proposition 4.3 (Bures divergence). *If $\varphi \equiv \mathbb{B}$, then $\tau_y^{\mathbb{B}}(w) = \rho_y\|w\|_2 + \sqrt{w^\top \widehat{\Sigma}_y w}$ for all $y \in \mathcal{Y}$.*

The proof of Theorem 4.2 follows by combining Propositions 3.4 and 4.3, the details are omitted.

Next, we study the asymptotic form of the Bures MPM as the radii of the ambiguity sets grow. Note that problem (7) depends only on the *sum* of the radii, but not on the individual values of each radius. Let $\rho = \sum_{y \in \mathcal{Y}} \rho_y$ be their sum, it suffices to study when ρ grows to infinity. To this end, denoted by $w_\rho^{\mathbb{B}}$ the optimal solution of problem (7) parametrized by ρ. The next result provides the analysis of the asymptotic value of $w_\rho^{\mathbb{B}}$ as $\rho \to \infty$.

Proposition 4.4 (Bures asymptotic hyperplane). *Fix a label $y \in \mathcal{Y}$ and suppose that the radius ρ_{-y} is a constant.[2] Let $w_{\rho_y}^{\mathbb{B}}$ be the optimal solution of* (7) *parametrized by ρ_y. As $\rho_y \to \infty$ then*

$$w_{\rho_y}^{\mathbb{B}} \to w_\infty^{\mathbb{B}} \triangleq \left(\sum_{y \in \mathcal{Y}} y\widehat{\mu}_y\right) \Big/ \Big\| \sum_{y \in \mathcal{Y}} y\widehat{\mu}_y \Big\|_2^2.$$

Notice that as $\rho_y \to \infty$, $\kappa^{\mathbb{B}}\tau_y^{\mathbb{B}}(w_{\rho_y}^{\mathbb{B}}) \to 1$. Thus, $b_\infty^{\mathbb{B}} = (w_\infty^{\mathbb{B}})^\top \widehat{\mu}_y - y$ for any $y \in \mathcal{Y}$. The asymptotic hyperplane defined by $w_\infty^{\mathbb{B}}$ is thus characterized by the linear equation $w_\infty^{\mathbb{B}} x - w_\infty^{\mathbb{B}} \widehat{\mu}_y + y = 0$, which identifies a hyperplane passing through $\widehat{\mu}_{-y}$ as $\sum_{y \in \mathcal{Y}} yw^\top \mu_y = 1$.

Figure 2: A 2D example of the Bures MPM hyperplanes with fixed $\rho_{+1} = 0$. The red line is for $\rho_1 = 0.01$, the green line is for $\rho_{-1} = 10$. The green dashed line is pushed towards the favorable region (predicted as +1).

Remark 4.5 (Asymptotic hyperplane for Quadratic MPM). *It is provable that the solution of problem* (4) *converges to $w_\infty^{\mathbb{B}}$ as $\rho = \sum_y \rho_y$ tends to infinity. Thus, Quadratic MPM* (4) *and Bures MPM* (7) *are asymptotically equivalent even though they induce different regularizations of the nominal MPM* (2).

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[2] As $\mathcal{Y} = \{-1, +1\}$, $-y$ denotes the opposite class of y

Remark 4.6 (Geometric intuition for robust recourse). *Figure 2 visualizes the Bures MPM hyperplanes by varying the radii. Notice that the hyperplane drifts toward the favorable (+1) class as the uncertainty of the unfavorable (-1) covariance matrix increases. Thus, the recourse generated w.r.t. the green hyperplane is more robust compared to that generated w.r.t. the red one. By calibrating the radii, we shift the hyperplane and obtain robust recourses at different robustness-cost trade-offs.*

5 FISHER-RAO MPM

We now explore the case where φ is the Fisher-Rao distance which is defined as follows.

Definition 5.1 (Fisher-Rao distance). *Given two positive definite matrices $\Sigma, \widehat{\Sigma} \in \mathbb{S}_{++}^d$, the Fisher-Rao distance between them is $\mathbb{F}(\Sigma, \widehat{\Sigma}) = \|\log(\widehat{\Sigma}^{-\frac{1}{2}} \Sigma \widehat{\Sigma}^{-\frac{1}{2}})\|_2$, where $\log(\cdot)$ is the matrix logarithm.*

The Fisher-Rao distance enjoys many nice properties. In particular, it is invariant to inversion and congruence, *i.e.*, for any $\Sigma, \widehat{\Sigma} \in \mathbb{S}_{++}^d$ and invertible $A \in \mathbb{R}^{d \times d}$, $\mathbb{F}(\Sigma, \widehat{\Sigma}) = \mathbb{F}(\Sigma^{-1}, \widehat{\Sigma}^{-1}) = \mathbb{F}(A\Sigma A^\top, A\widehat{\Sigma}A^\top)$. Such invariances are especially statistically meaningful as it implies that the results remain unchanged if we reparametrize the problem with an inverse covariance matrix (instead of the covariance matrix) or apply a change of basis to the data space $\mathcal{X}$. It is shown that $\mathbb{F}$ is the unique Riemannian distance (up to scaling) on the cone $\mathbb{S}_{++}^d$ with such invariances (Savage, 1982). Next, we assert the form of the Fisher-Rao MPM.

Theorem 5.2 (Fisher-Rao MPM). *Suppose that $\varphi \equiv \mathbb{F}$. Let $w^{\mathbb{F}}$ be the solution of the problem*

$$\min_{w \in \mathcal{W}} \sum_{y \in \mathcal{Y}} \exp\left(\frac{\rho_y}{2}\right) \sqrt{w^\top \widehat{\Sigma}_y w}. \tag{8}$$

Then $\theta^{\mathbb{F}} = (w^{\mathbb{F}}, b^{\mathbb{F}})$ is the optimal solution of the distributionally robust MPM problem (3), where

$$\kappa^{\mathbb{F}} = \frac{1}{\sum_{y \in \mathcal{Y}} \exp\left(\frac{\rho_y}{2}\right) \sqrt{(w^{\mathbb{F}})^\top \widehat{\Sigma}_y w^{\mathbb{F}}}}, \quad \text{and } b^{\mathbb{F}} = (w^{\mathbb{F}})^\top \widehat{\mu}_{+1} - \kappa^{\mathbb{F}} \exp\left(\frac{\rho_{+1}}{2}\right) \sqrt{(w^{\mathbb{F}})^\top \widehat{\Sigma}_{+1} w^{\mathbb{F}}}.$$

Theorem 5.2 divulges another foundational connection between robustness and regularization: if we construct the ambiguity sets for the covariance matrices using the Fisher-Rao distance, the resulting optimization problem (8) is a *reweighted* version of the nominal problem (2). Each term $(w^\top \widehat{\Sigma}_y w)^{\frac{1}{2}}$ is assigned a weight $\exp(\rho_y/2)$, which is proportional to the radius ρ_y. This connection aligns with previous observations highlighting the equivalence between reweighting schemes and distributional robustness (Ben-Tal et al., 2013; Bayraksan & Love, 2015; Namkoong & Duchi, 2017; Hashimoto et al., 2018). To prove Theorem 5.2, we derive an analytical expression of $\tau_y^{\mathbb{F}}(w)$.

Proposition 5.3 (Fisher-Rao distance). *If $\varphi \equiv \mathbb{F}$, then $\tau_y^{\mathbb{F}}(w) = \exp\left(\frac{\rho_y}{2}\right)(w^\top \widehat{\Sigma} w)^{\frac{1}{2}}$ for all $y \in \mathcal{Y}$.*

The proof of Theorem 5.2 follows by combining the results from Proposition 3.4 and Proposition 5.3, the detailed proof is omitted. Next, we study the asymptotic form of the Fisher-Rao MPM.

Proposition 5.4 (Fisher-Rao asymptotic hyperplane). *Fix a label $y \in \mathcal{Y}$ and suppose that the radius ρ_{-y} is a constant. Let $w_{\rho_y}^{\mathbb{F}}$ be the optimal solution of (8) parametrized by ρ_y. Let $a \triangleq \sum_{y \in \mathcal{Y}} y\widehat{\mu}_y$, then as $\rho_y \to \infty$, $w_{\rho_y}^{\mathbb{F}} \to w_{\infty, y}^{\mathbb{F}} \triangleq (a^\top \widehat{\Sigma}_y^{-1} a)^{-1} \widehat{\Sigma}_y^{-1} a$.*

Similar to the Bures MPM, the boundary prescribed by the Fisher-Rao MPM can be shifted through an appropriate calibration of the radii ρ_y. Thus, Fisher-Rao MPM can generate a robust algorithmic recourse in a geometrically-intuitive manner.

6 NUMERICAL EXPERIMENTS

We conduct comprehensive experiments to highlight the performance of our models. We first compare the fidelity and stability of our surrogates with LIME. We then compare the quality of our recourses against two popular baselines: ROAR (Upadhyay et al., 2021) and AR (Ustun et al., 2019).

Classifier. We use three-layer MLP with 20, 50, 20 nodes and ReLU activation functions in each consecutive layer. We use a sigmoid function in the last layer to produce probabilities.

Dataset. We evaluate our framework using popular real-world datasets for algorithmic recourse: *German Credit* (Dua & Graff, 2017; Groemping, 2019), *Small Bussiness Administration (SBA)* (Li et al., 2018), and *Student performance* (Cortez & Silva, 2008). Each dataset contains two sets of data (the present data - D_1 and the shifted data D_2). The shifted dataset D_2 could capture the correction shift (German credit), the temporal shift (SBA), or the geospatial shift (Student). For each dataset, we use 80% of the instances in the present data D_1 to train an underlying predictive model and the remaining instances are used to generate and evaluate recourses. The shifted data D_2 is used to train future classifiers in Section 6.2. The main text contains the results for the German and Student datasets. Further results, including the SBA and the synthetic data, are provided in Appendix A.

6.1   Fidelity and Stability of the Surrogate Models

We evaluate the performance of different surrogate models with respect to the current classifier. We compare our methods: QUAD-MPM in (3.3), the BW-MPM in (4.2) and the FR-MPM in (5.2) against the popular linear surrogate LIME (Ribeiro et al., 2016) under the following metrics:

Stability. We use the procedure in Agarwal et al. (2021) to measure the stability of the surrogate models with respect to the location. For a given instance x, we sample 10 neighbors $x' \sim \mathcal{N}(x, 0.001I)$, then use the above-mentioned methods to find the linear surrogate $\theta_{x'} = (w_{x'}, b_{x'})$ at x'. We report the maximum distance of the explanations of x' to the explanation of x; precisely, the stability measure is

$$\text{Stability}(w_x) = \max_{x' \sim \mathcal{N}(x, 0.001I)} \|w_x - w_{x'}\|_2.$$

Fidelity. We use the LocalFid criterion as in Laugel et al. (2018) to measure the fidelity of a local surrogate model. Concretely, the local fidelity of a given instance x is measured as:

$$\text{LocalFid}(x, w_x) = \text{Acc}_{x' \in \mathcal{V}_x}(f(x'), s_x(x')),$$

where $f(\cdot)$ is the original classifier and $s_x(\cdot)$ is

Figure 3: Benchmarks of fidelity and stability on the German and Student dataset. Higher local fidelity and lower stability are better.

the local surrogate classifier. The function Acc returns the fraction of instances where the output class of f and s_x agree, where instances are drawn uniformly from an l_2-ball $\mathcal{V}_x$ of radius r_{fid} centered on x. Here, we set r_{fid} to 10% of the maximum distance between instances in the training data and generate 1000 samples $x' \in \mathcal{V}_x$. Note that $\mathcal{V}_x$ is for evaluation only and independent from the perturbation samples used to train the local surrogate.

To generate the MPM's surrogates, we choose 10 nearest counterfactuals of x_0 in training data to find x_b. We set the perturbation radius r_p to 5% of the maximum distance between instances in the training data and set $\rho_{+1} = 0$, $\rho_{-1} = 1.0$. For LIME, we use the default parameters recommended in the LIME source code and return $\theta = (w, b - 0.5)$ as the LIME's surrogate, similar to Laugel et al. (2018). We vary the number of perturbation samples in a range of $[500, 10000]$ to measure the fidelity and sensitivity of constructed surrogates under low sampling sizes. The results on German and Student datasets are shown in Figure 3. The results show the superiority of MPM's surrogates compared to LIME in both local fidelity and stability metrics. Meanwhile, FR-MPM provides higher-fidelity surrogates compared to QUAD-MPM and BW-MPM.

6.2   Robustness of Recourses

We now study the robustness to model shifts of recourses and its trade-off against the recourse cost.

Metrics. We use an ℓ_1-distance as the *cost* function. We define the *current validity* as the validity of the generated recourses with respect to the given classifier. To measure the validity of recourses under the model shifts, we sample 80% instances of the shifted data D_2 100 times to train 100 'future' MLP classifiers. We then report the *future validity* of recourse as the fraction of the future classifiers with respect to which the recourse is valid.

Baselines. The experiment in Section 6.1 suggests that the Fisher-Rao model can be used to represent the class of covariance-robust MPM. We use FR-MPM as the linear surrogate $\theta^{\mathbb{F}} = (w^{\mathbb{F}}, b^{\mathbb{F}})$ and a simple projection to generate recourse by finding $x_r = \arg\min\{\|x - x_0\|_1 : x^\top w^{\mathbb{F}} + b^{\mathbb{F}} \geq 0\}$.

We compare the above method, namely FR-MPM-PROJ, against strong baselines, including Wachter (Wachter et al., 2017) and ROAR (Upadhyay et al., 2021) using LIME (Ribeiro et al., 2016), CLIME (Agarwal et al., 2021), and LIMELS (Laugel et al., 2018)[3] as surrogates. Comparisons with ROAR using the vanilla MPM and SVM surrogates are in Appendix A.2.

Cost-validity trade-off. We fix the number of perturbation samples to 1000 and vary the ambiguity size ($\rho_{+1} = 0$, $\rho_{-1} \in [0, 10]$ for FR-MPM-PROJ and $\delta_{\max} \in [0, 0.2]$ for the uncertainty size of ROAR). We then plot the Pareto frontiers of the cost-validity trade-off in Figure 4. Generally, increasing the ambiguity size will increase both the current and future validity of recourses, but induces a sacrifice in the cost. This result is consistent with the analysis in Rawal et al. (2020). However, the frontiers of FR-MPM-PROJ dominate the frontiers of LIME-ROAR, CLIME-ROAR, and LIMELS-ROAR. Note that we use CARLA's implementation with default parameters for Wachter and its higher cost compared to the linear surrogate's methods on the Student dataset is consistent with results in Upadhyay et al. (2021) and Pawelczyk et al. (2021). Table 1 shows the performance of FR-MPM-PROJ at radii $\rho_{+1} = 0$, $\rho_{-1} = 10$ and of ROAR-related methods at uncertainty size $\delta_{\max} = 0.2$. Here, the FR-MPM-PROJ has similar future validity compared to LIMELS-ROAR, but at a lower cost and higher current validity. Further results and discussion are in Appendix A.2.

Table 1: Performance of competing algorithms on real datasets. For the current and future validity, higher is better. For the cost, lower is better. Bold indicates the best performance.

Method	German credit		
	Cost	*Cur Validity*	*Fut Validity*
Wachter	**0.42** ± 0.02	**1.00** ± 0.00	0.52 ± 0.03
LIME-PROJ	0.45 ± 0.10	0.35 ± 0.11	0.51 ± 0.08
LIME-ROAR	1.09 ± 0.19	0.66 ± 0.15	0.64 ± 0.08
CLIME-ROAR	1.40 ± 0.45	0.76 ± 0.17	0.72 ± 0.11
LIMELS-ROAR	1.29 ± 0.07	0.88 ± 0.03	**0.79** ± 0.02
QUAD-MPM-PROJ	0.90 ± 0.02	0.89 ± 0.05	0.76 ± 0.03
BW-MPM-PROJ	1.03 ± 0.02	0.93 ± 0.04	0.78 ± 0.01
FR-MPM-PROJ	1.01 ± 0.02	0.94 ± 0.03	0.78 ± 0.01

Figure 4: Pareto frontier of the cost-validity trade-off on the German and Student datasets.

Actionability. By introducing robustness into the linear surrogate model, our method can use AR (Ustun et al., 2019) as a recourse search mechanism to promote flexible actionability constraints. In Table 2, we compare the AR performance using different surrogate models (LIME, CLIME, LIMELS, SVM, MPMs). We consider the recourse under some actionability constraints such as immutable race, gender, or non-decrease age (see Appendix A.1 for more details on the actionability constraints). The result shows that AR using FR-MPM as the linear surrogate increases both the current and future validity substantially compared to other surrogates. The results for other datasets are presented in Appendix A.2

Table 2: Performance of AR using different local surrogate models.

Method	German credit		
	Cost	*Cur Validity*	*Fut Validity*
LIME-AR	0.44 ± 0.08	0.15 ± 0.05	0.40 ± 0.07
CLIME-AR	0.73 ± 0.53	0.27 ± 0.12	0.45 ± 0.10
LIMELS-AR	0.36 ± 0.11	0.24 ± 0.09	0.44 ± 0.08
SVM-AR	0.39 ± 0.10	0.21 ± 0.08	0.42 ± 0.08
MPM-AR	**0.29** ± 0.06	0.19 ± 0.07	0.42 ± 0.06
QUAD-MPM-AR	1.25 ± 0.09	0.77 ± 0.05	0.73 ± 0.03
BW-MPM-AR	1.86 ± 0.08	0.79 ± 0.03	**0.74** ± 0.03
FR-MPM-AR	1.92 ± 0.10	**0.80** ± 0.05	**0.74** ± 0.03

Conclusions. This paper revisited and provided comprehensive evaluations of common surrogates for robust algorithmic recourse. We proposed a pipeline that shifts the surrogate boundary using the covariance-robust MPMs, leading to an intuitive and interpretable approach to enhance robustness. We showed that our surrogates are more stable and faithful to the underlying model. Consequentially, our recourses exhibit robustness with a better cost-validity trade-off and still promote actionability through mixed-integer constraints. Besides, statistical results of the covariance-robust MPMs also bridged the understanding of distributionally robust MPMs and two prominent regularization schemes. The derivation Logdet-MPM is provided in Appendix C.

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[3]LIMELS uses the same boundary sampling algorithm as the FR-MPM but trains a ridge regression instead.

REPRODUCIBILITY STATEMENT

In order to foster reproducibility, we have released all source code and scripts used to replicate our experimental results at `https://anonymous.4open.science/r/mpm-recourse`. The repository includes source code, datasets, configurations, and instructions; thus one could reproduce our results with several commands.

We use the original authors' implementations of for LIME[4] (Ribeiro et al., 2016) and AR[5] (Ustun et al., 2019). We use a well-known CARLA's implementation[6] for Wachter (Wachter et al., 2017). Since we cannot find the open-source code for CLIME (Agarwal et al., 2021), LIMELS (Laugel et al., 2018), and ROAR (Upadhyay et al., 2021), we implement according to their papers. CLIME and LIMELS are adapted from LIME's source code while ROAR is adapted from CARLA's source code for Wachter.

The hyperparameter configurations for our methods and other baseline are clearly stated in Section A, Appendix A.1 and Appendix A.2 and also stored in the repository. The surrogates sharing the same local sampler will be ensured to have the same random seed, therefore, having the same synthesized samples. The hyperparameters that affect baselines' performance such as λ and the probabilistic threshold of Wachter and ROAR will also be studied in Appendix A.2.

The remaining proofs and theoretical claims are provided in Appendix B.

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A EXPERIMENTS

A.1 EXPERIMENTAL DETAILS

Classifier. We use a three-layer MLP with 20, 50, and 20 nodes and a ReLU activation in each consecutive layer. We use the sigmoid function in the last layer to produce probabilities. To train this classifier, we use the binary cross-entropy, solved using the Adam optimizer and 1000 epochs.

Datasets. We provide more details about synthetic and real-world datasets. For synthetic data, we generate 2-dimensional data by sampling instances uniformly in a rectangle $x = (x_1, x_2) \in [-2, 4] \times [-2, 7]$. Each sample is labeled using the following function:

$$f(x) = \begin{cases} 1 & \text{if} \quad x_2 \geq 1 + x_1 + 2x_1^2 + x_1^3 - x_1^4 + \varepsilon, \\ 0 & \text{otherwise,} \end{cases}$$

where ε is random noise. We generate a present data set D_1 with $\varepsilon = 0$ and a shifted data set D_2 with $\varepsilon \sim \mathcal{N}(0, 1)$. The decision boundary of the MLP classifier for current synthetic data is illustrated in Figure 5.

Figure 5: An illustration of MLP's decision boundary for the synthetic data.

The detail of three real-world datasets are listed below:

i *German Credit* (Dua & Graff, 2017). The dataset contains the information (e.g. age, gender, financial status,...) of 1000 customers who took a loan from a bank. The classification task is to determine the risk (good or bad) of an individual. There is another version of this dataset regarding corrections of coding error (Groemping, 2019). We use the corrected version of this dataset as shifted data to capture the correction shift. The features we used in this dataset include 'duration', 'amount', 'personal_status_sex', and 'age'. When considering actionability constraints (Section 6.2), we set 'personal_status_sex' as immutable and 'age' to be non-decrease.

ii *Small Bussiness Administration (SBA)* (Li et al., 2018). This data includes 2,102 observations with historical data of small business loan approvals from 1987 to 2014. We divide this dataset into two datasets (one is instances from 1989 - 2006 and one is instances from 2006 - 2014) to capture temporal shifts. We use the following features: selected, 'Term', 'NoEmp', 'CreateJob', 'RetainedJob', 'UrbanRural', 'ChgOffPrinGr', 'GrAppv', 'SBA_Appv', 'New', 'RealEstate', 'Portion', 'Recession'. When considering actionability constraints, we set 'UrbanRural' as immutable.

iii *Student performance* (Cortez & Silva, 2008). This data includes the performance records of 649 students in two schools: Gabriel Pereira (GP) and Mousinho da Silveira (MS). The classification task is to determine if their final score is above average or not. We split this dataset into two sets in two schools to capture geospatial shifts. The features we used are: 'age', 'Medu', 'Fedu', 'studytime', 'famsup', 'higher', 'internet', 'romantic', 'freetime', 'goout', 'health', 'absences', 'G1', 'G2'. When considering actionability constraints, we set 'romantic' as immutable and 'age' to be non-decreased.

For categorical features, we use one-hot encoding to convert them to binary features, similar to Mothilal et al. (2020). We also normalize continuous features to zero mean and unit variance before training the classifier. The performance of the classifier is reported in Table 3.

Table 3: Accuracy and AUC results of the classifiers on the synthetic and three real-world datasets.

Classifier	Dataset	Present data D_1		Shift data D_2	
		Accuracy	*AUC*	*Accuracy*	*AUC*
MLP	Synthetic data	0.99 ± 0.00	1.00 ± 0.00	0.94 ± 0.01	0.99 ± 0.01
	German credit	0.67 ± 0.02	0.60 ± 0.03	0.66 ± 0.23	0.60 ± 0.04
	SBA	0.96 ± 0.00	0.99 ± 0.00	0.98 ± 0.01	0.96 ± 0.01
	Student	0.86 ± 0.02	0.93 ± 0.01	0.91 ± 0.04	0.97 ± 0.02

A.2 ADDITIONAL EXPERIMENTAL RESULTS

Local fidelity and stability experiments. Here, we provide benchmarks of local fidelity and stability (Section 6.1) on the synthetic and datasets in Figure 6.

Figure 6: Benchmarks of the local fidelity and stability on synthetic and SBA dataset.

The cost-validity trade-off. Here, we provide more detail about the settings of the baselines and the complementary results of the experiments in Section 6.2 in the main paper.

For Wachter's implementation, we use CARLA's source code[7] (Pawelczyk et al., 2021), which already has an adaptive scheme to adjust the hyperparameter (λ) if no valid recourse is found. We adopt this implementation for ROAR and set the initial λ to 0.1 as suggested in (Upadhyay et al., 2021).

Regarding the surrogate models, we use the open-source code with the default settings for LIME[8] (Ribeiro et al., 2016). We adapt this source code accordingly for CLIME's implementation (Agarwal et al., 2021). LIMELS, SVM, and MPM-related surrogates use the same boundary sampling procedure (with the same seed), in which we set the number of counterfactuals $k = 10$ and the number of perturbation samples is 1000.

Figure 7 shows the Pareto frontiers of the cost-validity trade-off on the real world datasets. Table 4 shows the performance of FR-MPM-PROJ at radii $\rho_{+1} = 0, \rho_{-1} = 10$ and of ROAR-related methods at uncertainty size $\delta_{\max} = 0.2$ on synthetic, SBA, and Student datasets. The hyperparameter λ is set to 0.1 for both Wachter and ROAR-related methods.

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[7]https://github.com/carla-recourse/CARLA

[8]https://github.com/marcotcr/lime

Figure 7: Pareto frontier of the cost-validity trade-off with the MLP classifier on the real-world datasets. For FR-MPM-PROJ, we vary the ambiguity size in a range of $\rho_- \in [0, 10]$. For the ROAR-related methods, we vary the uncertainty size in a range of $\delta_{\max} \in [0, 0.2]$. And for Wachter, we vary the hyperparameter $\lambda \in [0.05, 0.4]$.

In FR-MPM-PROJ and ROAR-related methods, the trade-off between cost and validity can be observed when increasing the ambiguity size (ρ_{-1} for FR-MPM and $\delta_{\max}$ for ROAR-related methods), similar to the analysis in (Rawal et al., 2020) and the experimental results in (Upadhyay et al., 2021; Black et al., 2021). Generally, the Pareto frontiers of FR-MPM-PROJ dominate the frontiers of ROAR-related methods on all evaluated datasets. In other words, with the same cost (or validity), our method will provide recourses with a higher validity (or lower cost) compared to ROAR. It can be seen in Table 4, our method has similar validity but a much smaller cost than ROAR on Synthetic and German datasets. Meanwhile, our method achieves higher validity with reasonable cost on SBA and Student datasets.

Comparing other baselines, LIMELS-ROAR performs slightly better compared to LIME-ROAR and CLIME-ROAR. Wachter provides the recourses with high current validity but is vulnerable to model shifts, resulting in poor future validity. Wachter has the lowest cost for the synthetic and German datasets but a higher cost in the SBA and Student datasets compared to the linear surrogate-based methods. This is consistent with the results in (Upadhyay et al., 2021) since the objective function of Wachter might be non-convex when the classifier is an MLP network.

Table 4: Performance of competing algorithms on synthetic, SBA, and Student datasets.

Method	Synthetic data			SBA			Student performance		
	Cost	Cur Validity	Fut Validity	Cost	Cur Validity	Fut Validity	Cost	Cur Validity	Fut Validity
Wachter	**1.01** ± 0.03	**1.00** ± 0.00	0.63 ± 0.04	1.74 ± 0.26	0.98 ± 0.01	0.13 ± 0.06	3.33 ± 0.11	**0.95** ± 0.03	0.29 ± 0.02
LIME-PROJ	2.13 ± 0.08	0.77 ± 0.01	0.76 ± 0.01	**0.81** ± 0.06	0.97 ± 0.01	0.79 ± 0.03	**1.07** ± 0.13	0.78 ± 0.04	0.37 ± 0.07
LIME-ROAR	2.59 ± 0.09	0.90 ± 0.01	0.89 ± 0.00	1.83 ± 0.16	**1.00** ± 0.00	0.87 ± 0.04	2.41 ± 0.31	**0.95** ± 0.03	0.74 ± 0.11
CLIME-ROAR	1.80 ± 0.07	0.81 ± 0.01	0.81 ± 0.01	1.50 ± 0.53	0.97 ± 0.04	0.78 ± 0.13	3.07 ± 0.75	**0.95** ± 0.04	0.81 ± 0.11
LIMELS-ROAR	1.30 ± 0.01	**1.00** ± 0.00	0.98 ± 0.01	1.63 ± 0.23	**1.00** ± 0.00	0.88 ± 0.05	2.47 ± 0.29	**0.95** ± 0.03	0.75 ± 0.09
QUAD-MPM-PROJ	1.09 ± 0.02	0.99 ± 0.01	0.98 ± 0.00	1.17 ± 0.11	**1.00** ± 0.00	0.85 ± 0.05	1.46 ± 0.13	**0.95** ± 0.03	0.54 ± 0.07
BW-MPM-PROJ	1.19 ± 0.02	**1.00** ± 0.00	0.99 ± 0.00	1.67 ± 0.13	**1.00** ± 0.00	0.95 ± 0.02	2.13 ± 0.18	**0.95** ± 0.03	0.76 ± 0.06
FR-MPM-PROJ	1.20 ± 0.02	**1.00** ± 0.00	**1.00** ± 0.00	1.83 ± 0.13	**1.00** ± 0.00	**0.97** ± 0.01	2.51 ± 0.21	**0.95** ± 0.03	**0.82** ± 0.05

Comparison with ROAR using the vanilla MPM and SVM as the surrogate model. Here, we compare the FR-MPM-PROJ with ROAR using the vanilla MPM and SVM as the surrogate model. Both vanilla MPM and SVM use the same boundary sample procedure (with the same seed number) as FR-MPM. The settings are similar to the experiment in Section 6.2. The result shown in Figure 8 demonstrates the merits of our method.

Actionability. We provide the complementary result of the actionability experiment on the synthetic, SBA, and Student datasets in Table 5. Using AR with FR-MPM produces the recourses with higher value in both the current and future validity compared to AR using other surrogates.

Figure 8: Pareto frontiers of our method compared with ROAR using vanilla MPM and SVM as the surrogate model. The recourses are generated with respect to the MLP classifier on synthetic and three real-world datasets.

Table 5: Performance of AR using different local surrogate models.

Method	Synthetic data			SBA			Student performance		
	Cost	Cur Validity	Fut Validity	Cost	Cur Validity	Fut Validity	Cost	Cur Validity	Fut Validity
LIME-AR	2.06 ± 0.07	0.67 ± 0.02	0.67 ± 0.01	4.50 ± 3.48	0.10 ± 0.07	0.04 ± 0.03	3.38 ± 0.24	0.45 ± 0.07	0.42 ± 0.06
CLIME-AR	1.34 ± 0.05	0.41 ± 0.02	0.43 ± 0.01	**4.10** ± 3.80	0.07 ± 0.07	0.01 ± 0.01	4.34 ± 1.24	0.63 ± 0.28	0.50 ± 0.15
LIMELS-AR	1.05 ± 0.05	0.62 ± 0.06	0.59 ± 0.04	4.97 ± 3.76	0.22 ± 0.15	0.06 ± 0.07	3.15 ± 0.16	0.49 ± 0.13	0.38 ± 0.03
SVM-AR	**1.02** ± 0.06	0.64 ± 0.04	0.61 ± 0.02	6.06 ± 4.06	0.26 ± 0.07	0.03 ± 0.02	3.07 ± 0.23	0.43 ± 0.13	0.36 ± 0.03
MPM-AR	1.08 ± 0.04	0.68 ± 0.04	0.62 ± 0.03	5.06 ± 3.33	0.39 ± 0.18	0.08 ± 0.05	**3.02** ± 0.19	0.40 ± 0.12	0.36 ± 0.02
QUAD-MPM-AR	1.65 ± 0.08	0.99 ± 0.01	0.98 ± 0.01	7.40 ± 3.36	0.97 ± 0.03	0.49 ± 0.19	5.60 ± 0.31	0.97 ± 0.04	0.69 ± 0.05
BW-MPM-AR	1.86 ± 0.09	**1.00** ± 0.00	0.99 ± 0.01	9.66 ± 3.21	0.98 ± 0.04	0.62 ± 0.03	8.62 ± 0.38	**1.00** ± 0.00	0.92 ± 0.05
FR-MPM-AR	2.03 ± 0.04	**1.00** ± 0.00	**0.99** ± 0.00	10.02 ± 3.09	**1.00** ± 0.00	**0.64** ± 0.03	9.63 ± 0.38	**1.00** ± 0.00	**0.95** ± 0.03

Ablation study. We conduct an ablation study to understand the contribution of each stage in our method. Figure 8 shows the comparison of our method with ROAR using vanilla MPM and SVM as the local surrogate. Figure 9 shows the Pareto frontiers of FR-MPM-PROJ compared to its ablations by alternating the FR-MPM with other surrogates (LIME, MPM) or alternating the projection with Wachter. Particularly, we compare our method with LIME-ROBUST-PROJ, which uses LIME as the surrogate model and then solves the robustified projection:

$$x_r = \arg\min\{\|x - x_0\|_1 \; : \; x^\top w + b - \delta_{\max}\|x\|_2 \geq 0\},$$

where (w, b) is the weight and bias of LIME's surrogate, $\delta_{\max}$ is similar to the uncertainty size of ROAR (Upadhyay et al., 2021). The recourses are generated with respect to the MLP classifier on synthetic and three real-world datasets. This result demonstrates the usefulness of the FR-MPM in promoting the generation of robust recourses. Note that, for $\rho_- = 0$ and $\rho_+ = 0$, the hyperplanes of the FR-MPM classifier recovers the vanilla MPM's hyperplane.

Comparison with the probabilistic shiftings. One might attempt to increase the probabilistic threshold (usually set to 0.5) at which a sample is considered 'favorable' to generate robust recourses. In Figure 10, we compare the proposed method with Wachter, LIME, and MPM with various probabilistic thresholds in the range [0.5, 0.9]. It can be seen that FR-MPM-PROJ consistently achieves the best performance compared to other baselines. Interestingly, Wachter improves its future validity significantly on the synthetic and German datasets as the threshold increases. However, our method still dominates Wachter in all datasets.

Comparison of MPM-related methods with different distances. We compare FR-MPM-PROJ with QUAD-MPM-PROJ and BW-MPM-PROJ. The settings are similar in the cost-validity trade-off experiments. The results are shown in Figure 11. Generally, all three MPM-related methods perform better than LIME-ROAR and Wachter. However, FR-MPM-PROJ is better than QUAD-MPM-PROJ and BW-MPM-PROJ, especially in synthetic and Student datasets. Together with the superiority in the stability and fidelity experiment in Section 6.1, it suggests that FR-MPM is more suitable for generating recourses.

Figure 9: Ablation study: Pareto frontiers of FR-MPM-PROJ compared to its ablations by alternating the FR-MPM by common local surrogates. The recourses are generated with respect to the MLP classifier on synthetic and three real-world datasets.

Figure 10: Comparison with the probabilistic shiftings.

Figure 11: The comparison among MPM-related methods with different distances.

B PROOFS

B.1 PROOFS OF SECTION 3

Proof of Proposition 3.4. Following from Lanckriet et al. (2001, Equation (2)), the covariance-robust MPM problem

$$\min_{\theta \in \Theta} \max_{y \in \mathcal{Y}} \max_{\mathbb{P}_y \in \mathbb{U}_y^\varphi(\widehat{\mathbb{P}}_y)} \mathbb{P}_y(\mathcal{C}_\theta(X) \neq y)$$

is equivalent to

$$
\begin{aligned}
\max \quad & \alpha \\
\text{s.t.} \quad & \alpha \in \mathbb{R}_+, \ w \in \mathbb{R}^d, \ b \in \mathbb{R} \\
& 1 - \alpha \geq \max_{\mathbb{P}_y \in \mathbb{U}_y^\varphi(\widehat{\mathbb{P}}_y)} \mathbb{P}_y(y(w^\top X - b) \leq 0) \qquad \forall y \in \mathcal{Y}.
\end{aligned}
\tag{9}
$$

Notice that here, equivalency means the optimal solution $(w^\star, b^\star)$ of (9) will constitute the optimal solution $\theta^\star = (w^\star, b^\star)$ of the original min-max-max problem. Moreover, note that the worst-case probability admits a two-layer decomposition

$$\max_{\mathbb{P}_y \in \mathbb{U}_y^\varphi(\widehat{\mathbb{P}}_y)} \mathbb{P}_y(y(w^\top X - b) \leq 0) = \max_{\Sigma_y \in \mathbb{S}_+^d : \varphi(\Sigma_y \| \widehat{\Sigma}_y) \leq \rho_y} \max_{\mathbb{P}_y \sim (\widehat{\mu}_y, \Sigma_y)} \mathbb{P}_y(y(w^\top X - b) \leq 0).$$

As a consequence, using a similar argument as in Lanckriet et al. (2001), problem (9) is equivalent to

$$
\begin{aligned}
\max \quad & \kappa \\
\text{s.t.} \quad & \kappa \in \mathbb{R}_+, \ w \in \mathbb{R}^d, \ b \in \mathbb{R} \\
& y(-b + w^\top \widehat{\mu}_y) \geq \kappa \times \max_{\Sigma_y \in \mathbb{S}_+^d : \varphi(\Sigma_y \| \widehat{\Sigma}_y) \leq \rho_y} \sqrt{w^\top \Sigma_y w} \qquad \forall y \in \mathcal{Y}.
\end{aligned}
$$

The results now follow by applying the same line of arguments using the quantity $\tau_y^\varphi(w)$ in place of $\sqrt{w^\top \Sigma_y w}$. □

Proof of Proposition 3.5. Under the Gaussian parametric assumption, we have

$$\max_{\mathbb{P}_y \in \mathcal{U}_y^{\mathcal{N}}(\widehat{\mathbb{P}}_y)} \mathbb{P}_y(y(w^\top X - b) \leq 0) = \max_{\Sigma_y \in \mathbb{S}_+^d : \varphi(\Sigma_y \| \widehat{\Sigma}_y) \leq \rho_y} \max_{\mathbb{P}_y \sim \mathcal{N}(\widehat{\mu}_y, \Sigma_y)} \mathbb{P}_y(y(w^\top X - b) \leq 0).$$

In this case, using the same argument as in Lanckriet et al. (2001), the covariance-robust MPM with Gaussian assumption

$$\min_{\theta \in \Theta} \max_{y \in \mathcal{Y}} \max_{\mathbb{P}_y \in \mathcal{U}_y^{\mathcal{N}}(\widehat{\mathbb{P}}_y)} \mathbb{P}_y(\mathcal{C}_\theta(X) \neq y)$$

is equivalent to

$$
\begin{aligned}
\max \quad & \alpha \\
\text{s.t.} \quad & \alpha \in \mathbb{R}_+,\ w \in \mathbb{R}^d,\ b \in \mathbb{R} \\
& y(-b + w^\top \widehat{\mu}_y) \geq \Phi^{-1}(\alpha) \times \max_{\Sigma_y \in \mathbb{S}_+^d : \varphi(\Sigma_y \| \widehat{\Sigma}_y) \leq \rho_y} \sqrt{w^\top \Sigma_y w} \qquad \forall y \in \mathcal{Y},
\end{aligned}
$$

where Φ is the cumulative distribution function of the standard Gaussian distribution. Because Φ is a monotonically increasing function, the covariance-robust MPM with Gaussian assumption is further equivalent to

$$
\begin{aligned}
\max \quad & \kappa \\
\text{s.t.} \quad & \kappa \in \mathbb{R}_+,\ w \in \mathbb{R}^d,\ b \in \mathbb{R} \\
& y(-b + w^\top \widehat{\mu}_y) \geq \kappa \times \max_{\Sigma_y \in \mathbb{S}_+^d : \varphi(\Sigma_y \| \widehat{\Sigma}_y) \leq \rho_y} \sqrt{w^\top \Sigma_y w} \qquad \forall y \in \mathcal{Y},
\end{aligned}
$$

with $\kappa \leftarrow \Phi^{-1}(\alpha)$. The results now follow by applying the same line of arguments using the quantity $\tau_y^\varphi(w)$ in place of $\sqrt{w^\top \Sigma_y w}$.

$\square$

B.2 PROOFS OF SECTION 4

Proof of Proposition 4.3. By Nguyen et al. (2021, Proposition 2.8), we have

$$
\tau_y^{\mathbb{B}}(w)^2 = \inf_{\gamma I \succ ww^\top} \gamma(\rho_y - \text{Tr}\left[\widehat{\Sigma}_y\right]) + \gamma^2 \langle (\gamma I - ww)^{-1}, \widehat{\Sigma}_y \rangle.
$$

Using the Sherman-Morrison formula (Bernstein, 2009, Corollary 2.8.8), we find

$$
(I - \frac{1}{\gamma}ww)^{-1} = I + \frac{ww^\top}{\gamma - \|w\|_2^2}.
$$

Notice that the constraint $\gamma I \succ ww^\top$ is equivalent to $\gamma > \|w\|_2^2$ by Schur complement. Thus, we have

$$
\tau_y^{\mathbb{B}}(w)^2 = \inf_{\gamma > \|w\|_2^2} \gamma \rho_y + \gamma \frac{w^\top \widehat{\Sigma}_y w}{\gamma - \|w\|_2^2}.
$$

The optimal solution in the variable γ is

$$
\gamma^\star = \|w\|_2^2 + \sqrt{\frac{w^\top \widehat{\Sigma}_y w \|w\|_2^2}{\rho_y}},
$$

with the corresponding optimal value

$$
\tau_y^{\mathbb{B}}(w)^2 = (\rho_y \|w\|_2 + \sqrt{w^\top \widehat{\Sigma}_y w})^2.
$$

We thus have the necessary result. $\square$

Proof of Proposition 4.4. Note that problem (7) has an unique solution because the objective function is strictly convex and coercive. Moreover, the optimal solution of (7) coincides with the optimal solution $w^\star(\lambda)$ of the following second-order cone program

$$
\min_{w \in \mathcal{W}} \frac{1}{\lambda} \sum_{y \in \mathcal{Y}} \sqrt{w^\top \widehat{\Sigma}_y w} + \|w\|_2,
$$

where $\lambda = 1/\rho$. By a compactification of $\mathcal{W}$ and applying Berge's maximum theorem (Berge, 1963, pp. 115-116), the function $w^\star(\lambda)$ is continuous on a non-negative compact range of λ, and converges to $w^\star(0)$ as $\lambda \to 0$. The optimal solution $w^\star(0)$ coincides with the solution of

$$
\min_{w \in \mathcal{W}} \|w\|_2, \tag{10}
$$

which is the Euclidean projection of the origin onto the hyperplane $\mathcal{W}$. An elementary computation confirms that

$$
w^\star(0) = \frac{\sum_{y \in \mathcal{Y}} y \widehat{\mu}_y}{\| \sum_{y \in \mathcal{Y}} y \widehat{\mu}_y \|_2^2}.
$$

Letting $w_\infty^{\mathbb{B}} = w^\star(0)$ completes the proof. $\square$

B.3 PROOFS OF SECTION 5

Proof of Proposition 5.3. Notice that

$$\tau_y^{\mathbb{F}}(w)^2 = \begin{cases} \max & w^\top \Sigma_y w \\ \text{s.t.} & \|\log(\widehat{\Sigma}_y^{-\frac{1}{2}} \Sigma_y \widehat{\Sigma}_y^{-\frac{1}{2}})\|_F \le \rho_y. \end{cases}$$

Using the transformation $Z_y \leftarrow \widehat{\Sigma}_y^{-\frac{1}{2}} \Sigma_y \widehat{\Sigma}_y^{-\frac{1}{2}}$, we have

$$\tau_y^{\mathbb{F}}(w)^2 = \max \left\{ v^\top Z_y v \ : \ \|\log Z_y\|_F \le \rho_y \right\}$$

with $v = \widehat{\Sigma}^{\frac{1}{2}} w$. We now proceed to show that the above optimization problem admits the maximizer

$$Z_y^\star = UU^\top + \exp(\rho_y)\frac{vv^\top}{\|v\|_2^2},$$

where U is an $d \times (d-1)$ orthonormal matrix whose columns are orthogonal to v. First, by Nguyen et al. (2019, Lemma C.1), the feasible region is compact. Since the objective function $v^\top Z_Y v$ is continuous in Z_y, an optimal solution $Z_y^\star$ exists. Next, we first claim that the constraint holds with equality at optimality. Suppose that $\|\log Z_y^\star\|_F < \rho_y$. Then, for some small $\delta > 0$, the matrix $Z_y^\star + \delta\, vv^\top$ is feasible due to the continuity of the constraint function $\|\log Z_y\|_F$ and has a strictly better objective value than the optimal solution $Z_y^\star$. This violates the optimality of $Z_y^\star$. Hence, $\|\log Z_y^\star\|_F = \rho_y$ for any optimal solution $Z_y^\star$, and the problem is equivalent to

$$\begin{aligned} \max \quad & v^\top Q\mathrm{Diag}(\lambda)Q^\top v \\ \text{s.t.} \quad & \textstyle\sum_{i=1}^d (\log \lambda_i)^2 = \rho_y^2, \\ & \lambda_1 \ge \cdots \ge \lambda_d > 0, \ Q \in \mathcal{O}(d), \end{aligned}$$

where $\mathcal{O}(d)$ is the set of $d \times d$ orthogonal matrices. For any orthogonal matrix Q, the objective function

$$v^\top Q\mathrm{Diag}(\lambda)Q^\top v \le \lambda_1 \|v\|_2^2,$$

the right-hand side of which can be attained by setting

$$Q = \left(\frac{v}{\|v\|_2}, \ U \right) \in \mathcal{O}(d).$$

Therefore, our problem is further reduced to

$$\begin{aligned} \max \quad & \lambda_1 \|v\|_2^2 \\ \text{s.t.} \quad & \textstyle\sum_{i=1}^d (\log \lambda_i)^2 = \rho_y^2, \ \lambda_1 \ge \cdots \ge \lambda_d > 0. \end{aligned}$$

It is then easy to see that at optimality, the optimal $\lambda \in \mathbb{R}_{++}^d$ must satisfy $\lambda_2 = \cdots = \lambda_d = 1$ and $(\log \lambda_1)^2 = \rho_y^2$. Since $\lambda_1 \ge \lambda_2 = 1$, we have $\log \lambda_1 = \rho_y$ and hence $\lambda_1 = \exp(\rho_y)$. In other words,

$$\begin{aligned} Z_y^\star &= \left(\frac{v}{\|v\|_2}, U \right) \begin{pmatrix} \exp(\rho_y) & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{pmatrix} \left(\frac{v}{\|v\|_2}, U \right)^\top \\ &= UU^\top + \exp(\rho_y)\frac{vv^\top}{\|v\|_2^2}. \end{aligned}$$

The corresponding optimal value is

$$\tau_y^{\mathbb{F}}(w)^2 = v^\top Z_y^\star v = \exp(\rho_y)\,\|v\|_2^2 = \exp(\rho_y)\,w^\top \widehat{\Sigma}_y w.$$

This completes the proof. $\qquad\square$

Proof of Proposition 5.4. Note that problem (8) has a unique solution because the objective function is strictly convex and coercive. Also, the optimal solution of (8) coincides with the solution $w^\star(\lambda)$ of

$$\min_{w \in \mathcal{W}} \ \sqrt{w^\top \widehat{\Sigma}_y w} + \lambda\sqrt{w^\top \widehat{\Sigma}_{-y} w},$$

where $\lambda = \exp\left(\frac{\rho_{-y} - \rho_y}{2}\right)$. By a compactification of $\mathcal{W}$ and applying Berge's maximum theorem (Berge, 1963, pp. 115-116), the function $w^\star(\lambda)$ is continuous on a non-negative compact range of λ, and converges to $w^\star(0)$ as $\lambda \to 0$. The optimal solution $w^\star(0)$ coincides with the solution of

$$\min_{w \in \mathcal{W}} \sqrt{w^\top \widehat{\Sigma}_y w}.$$

Because the square-root function is monotonically increasing, $w^\star(0)$ also solves

$$\min_{w \in \mathcal{W}} w^\top \widehat{\Sigma}_y w,$$

which is a convex, quadratic program with a single linear constraint. If a is defined as in the statement, then a convex optimization argument implies

$$w^\star(0) = \frac{1}{a^\top \widehat{\Sigma}_y^{-1} a} \widehat{\Sigma}_y^{-1} a,$$

which completes the proof. $\square$

C   LogDet MPM

In this appendix, we consider when φ is the Log-Determinant (LogDet) divergence. The LogDet divergence is formally defined as follows.

Definition C.1 (LogDet divergence). *Given two positive definite matrices $\Sigma, \widehat{\Sigma} \in \mathbb{S}_{++}^d$, the log-determinant divergence between them is*

$$\mathbb{D}(\Sigma \parallel \widehat{\Sigma}) = \mathrm{Tr}\left[\Sigma \widehat{\Sigma}^{-1}\right] - \log \det(\Sigma \widehat{\Sigma}^{-1}) - d.$$

It can be shown that $\mathbb{D}$ is a divergence because it is non-negative, and it vanishes to zero if and only if $\Sigma = \widehat{\Sigma}$. However, $\mathbb{D}$ is not symmetric, and in general we have $\mathbb{D}(\Sigma \parallel \widehat{\Sigma}) = \mathbb{D}(\widehat{\Sigma} \parallel \Sigma)$. The LogDet divergence $\mathbb{D}$ is related to the relative entropy: it is equal to the Kullback-Leibler divergence between two Gaussian distributions with the same mean vector and covariance matrices Σ and $\widehat{\Sigma}$.

We now provide the form of the LogDet MPM problem.

Theorem C.2 (LogDet MPM). *Suppose that $\varphi \equiv \mathbb{D}$. Let $w^{\mathbb{D}}$ be the optimal solution of the following second-order cone problem*

$$\min_{w \in \mathcal{W}} \sum_{y \in \mathcal{Y}} \sqrt{c_y} \sqrt{w^\top \widehat{\Sigma}_y w}, \tag{11}$$

where $c_y = -W_{-1}(-\exp(-\rho_y - 1))$ and W_{-1} is the Lambert-W function for the branch -1. Let $\kappa^{\mathbb{D}}$ and $b^{\mathbb{D}}$ be calculated as

$$\kappa^{\mathbb{D}} = \frac{1}{\sum_{y \in \mathcal{Y}} \sqrt{c_y} \sqrt{(w^{\mathbb{D}})^\top \widehat{\Sigma}_y w^{\mathbb{D}}}},$$

$$b^{\mathbb{D}} = (w^{\mathbb{D}})^\top \widehat{\mu}_{+1} - \kappa^{\mathbb{D}} \sqrt{c_{+1}} \sqrt{(w^{\mathbb{D}})^\top \widehat{\Sigma}_{+1} w^{\mathbb{D}}},$$

then $\theta^{\mathbb{D}} = (w^{\mathbb{D}}, b^{\mathbb{D}})$ is the optimal solution of the distributionally robust MPM problem (3).

Theorem C.2 shows that the LogDet divergence induces a similar reweighting scheme as the Fisher-Rao MPM. The asymptotic analysis of the LogDet MPM follows similarly from the Fisher-Rao MPM and is omitted. The proof of Theorem C.2 follows trivially from the below result, which provides the analytical form of $\tau_y^{\mathbb{D}}(w)$.

Proposition C.3 (LogDet divergence). *Suppose that $\varphi \equiv \mathbb{D}$, then for any $y \in \mathcal{Y}$, we have*

$$\tau_y^{\mathbb{D}}(w) = \sqrt{-W_{-1}(-\exp(-\rho_y - 1))} \sqrt{w^\top \widehat{\Sigma}_y w},$$

where W_{-1} is the Lambert-W function for the branch -1.

Proof of Proposition C.3. By Le et al. (2021, Proposition 3.4), we have

$$\tau_y^{\mathrm{D}}(w)^2 = \inf_{\substack{\gamma > 0 \\ \gamma \widehat{\Sigma}_y^{-1} \succ ww^\top}} \gamma \rho_y - \gamma \log \det(I - \widehat{\Sigma}_y^{\frac{1}{2}} ww^\top \widehat{\Sigma}_y^{\frac{1}{2}}/\gamma).$$

Using the matrix determinant formula (Bernstein, 2009), we have

$$\det(I - \widehat{\Sigma}_y^{\frac{1}{2}} ww^\top \widehat{\Sigma}_y^{\frac{1}{2}}/\gamma) = (1 - w^\top \widehat{\Sigma}_y w/\gamma).$$

Notice that the constraint $\gamma \widehat{\Sigma}_y^{-1} \succ ww^\top$ is translated into $\gamma > w^\top \widehat{\Sigma}_y w$. Thus, we have

$$\tau_y^{\mathrm{D}}(w)^2 = \inf_{\gamma > w^\top \widehat{\Sigma}_y w} \gamma \rho_y - \gamma \log(1 - w^\top \widehat{\Sigma}_y w/\gamma).$$

The first-order optimality condition for γ is

$$\rho - \log\left(1 - \frac{w^\top \widehat{\Sigma}_y w}{\gamma}\right) - \frac{w^\top \widehat{\Sigma}_y w}{\gamma - w^\top \widehat{\Sigma}_y w} = 0,$$

and the optimal solution for γ is

$$\gamma^\star = \frac{w^\top \widehat{\Sigma}_y w}{1 + 1/W_{-1}(-\exp(-\rho_y - 1))}.$$

Replacing the value of $\gamma^\star$ into the objective function leads to the necessary result. □