Abstract

Many machine learning tasks that involve predicting an output response can be solved by training a weighted regression model. Unfortunately, the predictive power of this type of models may severely deteriorate under low sample sizes or under covariate perturbations. Reweighting the training samples has aroused as an effective mitigation strategy to these problems. In this paper, we propose a novel and coherent scheme for kernel-reweighted regression by reparametrizing the sample weights using a doubly non-negative matrix. When the weighting matrix is confined in an uncertainty set using either the log-determinant divergence or the Bures-Wasserstein distance, we show that the adversarially reweighted estimate can be solved efficiently using first-order methods. Numerical experiments show that our reweighting strategy delivers promising results on numerous datasets.

1 Introduction

We are interested in learning a parameter \( \beta \) that has a competitive predictive performance on a response variable \( Y \). Given \( N \) training samples \((\hat{z}_i, \hat{x}_i, \hat{y}_i)_{i=1}^N\) in which \((\hat{z}_i, \hat{x}_i)\) are the contexts that possess explanatory power on \( \hat{y}_i \), learning the parameter \( \beta \) can be posed as a weighted regression problem of the form

\[
\min_{\beta} \sum_{i=1}^N \omega(\hat{z}_i) \ell(\beta, \hat{x}_i, \hat{y}_i).
\]  

(1)

In problem (1), \( \omega \) is a weighting function that indicates the contribution of the sample-specific loss to the objective. By aligning the covariate \((\hat{z}_i, \hat{x}_i)\) appropriately to the weighting term \( \omega(\hat{z}_i) \) and the loss term \( \ell(\beta, \hat{x}_i, \hat{y}_i) \), the generic formulation of problem (1) can be adapted to many popular learning and estimation tasks in machine learning. For example, problem (1) encapsulates the family of kernel smoothers, including the Nadaraya-Watson estimator [18, 24, 42].

Example 1.1 (Nadaraya-Watson (NW) estimator for conditional expectation). Given the samples \((\hat{z}_i, \hat{y}_i)_{i=1}^N\), we are interested in estimating the conditional expectation of \( Y \) given \( Z = z_0 \) for some covariate \( z_0 \in Z \). The NW estimator is the optimizer of problem (1) with \( \ell(\beta, y) = \| \beta - y \|^2 \) and the weighting function \( \omega \) is given through a kernel \( K \) via \( \omega(\hat{z}_i) = K(z_0, \hat{z}_i) \). The NW estimate of \( E[Y|Z = z_0] \) admits a closed form expression

\[
\beta_{NW} = \frac{\sum_{i=1}^N K(z_0, \hat{z}_i)\hat{y}_i}{\sum_{i=1}^N K(z_0, \hat{z}_i)}.
\]
Moreover, the NW estimator utilizes a locally constant function to estimate the conditional expectation $E[Y|Z=z_0]$. Locally linear regression [3] [34] extends the NW estimator to reduce the noise produced by the linear component of a target function [29] §3.2.

**Example 1.2 (Locally linear regression (LLR)).** For univariate output and $z \equiv x$, the LLR minimizes the kernel-weighted loss with $f((\beta_1, \beta_2), z, y) = (\beta_1 + \beta_2^T z - y)^2$. The LLR estimate of $E[Y|Z=z_0]$ admits a closed form expression

$$\beta_{\text{LLR}} = \left( \left( \bar{Z}^T W \bar{Z} \right)^{-1} \bar{Z}^T W \bar{Y} \right)^\top \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

with $\bar{Y} = [\bar{y}_1, \ldots, \bar{y}_n]^\top \in \mathbb{R}^n$, $W = \text{diag}(K(z_0, \bar{z}_1), \ldots, K(z_0, \bar{z}_n)) \in \mathbb{R}^{n \times n}$ and

$$\bar{Z} = \begin{bmatrix} 1 & (\bar{z}_1 - z_0)^\top \\ \vdots & \vdots \\ 1 & (\bar{z}_n - z_0)^\top \end{bmatrix}.$$ 

Intuitively, the NW and LLR estimators are special instances of the larger family of local polynomial estimators with order zero and one, respectively. Problem (1) is also the building block for local learning algorithms [8], density ratio estimation [5], pp.152, risk minimization with covariate shift [19] §4, domain adaptation [39], geographically weighted regression [9], local interpretable machine learning [4, 35]. In addition, there also exists a family of positive definite kernels, which forms the backbone of kernel machine learning [4][35].

**Definition 1.3 (Non-negative kernel).** A function $K : Z \times Z \rightarrow \mathbb{R}$ is non-negative if $K(z, z') \geq 0$ for any $z, z' \in Z$.

In all of the aforementioned applications, a prevailing trait is that the weight $\omega$ is given through a kernel. To avoid any confusion in the terminologies, it is instructive to revisit and distinguish the relevant definitions of kernels. The first family is the non-negative kernels, which are popularly employed in nonparametric statistics [40].

**Definition 1.4 (Positive definite kernel).** A symmetric function $K : Z \times Z \rightarrow \mathbb{R}$ is positive definite if for any $n \in \mathbb{N}$ and any choices of $(z_i)_{i=1}^n \in Z$ and $(\alpha_i)_{i=1}^n \in \mathbb{R}$, we have

$$\sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j K(z_i, z_j) \geq 0. \quad (2)$$

Moreover, $K$ is strictly positive definite if we have in addition that for mutually distinct $(z_i)_{i=1}^n \in Z$, the equality in (2) implies $\alpha_1 = \ldots = \alpha_n = 0$.

Positive definite kernels are a powerful tool to model geographical interactions [9], to characterize the covariance structure in Gaussian processes [31] §4, and to construct non-linear kernel methods [35]. Interestingly, the two above-mentioned families of kernels have a significant overlap. Examples of kernels that are both non-negative and strictly positive definite include the Gaussian kernel with bandwidth $h > 0$ defined for any $z, z' \in Z$ as

$$K(z, z') = \exp(-\|z - z'\|^2 / h^2),$$

the Laplacian kernel, the Cauchy kernel, the Matérn kernel, the rational quadratic kernel, etc.

It is well-known that the non-parametric statistical estimator obtained by solving (1) is sensitive to the corruptions of the training data [11][23][50]. Similar phenomenon is also observed in machine learning where the solution of the risk minimization problem (1) is not guaranteed to be robust or generalizable [1][2][14][16][21][23][44][45][46]. The quality of the solution to (1) also deteriorates if the training sample size $N$ is small. Reweighting, obtained by modifying $\omega(z_i)$, is arising as an attractive resolution to improve robustness and enhance the out-of-sample performance in the test data [32][36][33]. At the same time, reweighting schemes have shown to produce many favorable effects: reweighting can increase fairness [17][22][41], and can also effectively handle covariate shift [12][19][47].
While reweighting has been successfully applied to the empirical risk minimization regime in which the weights are uniformly $1/N$, reweighting the samples when the weighting function $\omega$ is tied to a kernel is not a trivial task. In fact, the kernel captures inherently the relative positions of the relevant covariates $\hat{z}$, and any reweighting scheme should also reflect these relationships in a global viewpoint. Another difficulty also arises due to the lack of convexity or concavity, which prohibits the modifications of the kernel parameters. For example, the mapping $h \mapsto \exp(- \|z - z'\|_2^2/h^2)$ for the Gaussian kernel is neither convex nor concave if $z \neq z'$. Thus, it is highly challenging to optimize over $h$ in the bandwidth parameter space. Alternatively, modifying the covariates $(\hat{z}_i)_{i=1}^N$ will also result in reweighting effects. Nevertheless, optimizing over the covariates is intractable for sophisticated kernels such as the Matérn kernel.

**Contributions.** This paper relies fundamentally on an observation that the Gram matrix of a non-negative, (strictly) positive definite kernel is a non-negative, positive (semi)definite (also known as doubly non-negative) matrix. It is thus natural to modify the weights by modifying the corresponding matrix parametrization in an appropriate manner. Our contributions in this paper are two-fold:

- We propose a novel scheme for reweighting using a reparametrization of the sample weights as a doubly non-negative matrix. The estimate is characterized as the solution to a min-max optimization problem, in which the admissible values of the weights are obtained through a projection of an uncertainty set from the matrix space.

- We report in-depth analysis on two reweighting approaches based on the construction of the matrix uncertainty set with the log-determinant divergence and the Bures-Wasserstein distance. Exploiting strong duality, we show that the worst-case loss function and its gradient can be efficiently evaluated by solving the univariate dual problems. Consequently, the adversarially reweighted estimate can be found efficiently using first-order methods.

**Organization of the paper.** Section 2 introduces our generic framework of reweighting using doubly non-negative matrices. Sections 3 and 4 study two distinctive ways to customize our reweighting framework using the log-determinant divergence and the Bures-Wasserstein distance. Section 5 empirically illustrates that our reweighting strategy delivers promising results in the conditional expectation task based on numerous real life datasets.

**Notations.** The identity matrix is denoted by $I$. For any $A \in \mathbb{R}^{p \times p}$, $\text{Tr} [A]$ denotes the trace of $A$, $A \geq 0$ means that all entries of $A$ are nonnegative. Let $S^p$ denote the vector space of $p$-by-$p$ real and symmetric matrices. The set of positive (semi)-definite matrices is denoted by $S^p_+$ (respectively, $S^p_+$). For any $A, B \in \mathbb{R}^{p \times p}$, we use $\langle A, B \rangle = \text{Tr} [A^\top B]$ to denote the Frobenius inner product between $A$ and $B$, and $\|v\|_2$ to denote the Euclidean norm of $v \in \mathbb{R}^p$.

## 2 A Reweighting Framework with Doubly Non-negative Matrices

We delineate in this section our reweighting framework using doubly non-negative matrices. This framework relies on the following observation: we can reparametrize the weights in \( \hat{\Omega} \) into a matrix $\hat{\Omega}$ and the loss terms in (1) into a matrix $V(\beta)$, and the solution to the estimation problem (1) can be equivalently characterized as the minimizer of the problem

$$
\min_{\beta} \langle \hat{\Omega}, V(\beta) \rangle.
$$

Notice that there may exist multiple equivalent reparametrizations of the form (3). However, in this paper, we focus on one specific parametrization where $\hat{\Omega}$ is the nominal matrix of weights

$$
\hat{\Omega} = \begin{bmatrix}
\hat{\Omega}_{00} & \hat{\Omega}_{01} & \cdots & \hat{\Omega}_{0N} \\
\hat{\Omega}_{10} & \hat{\Omega}_{11} & \cdots & \hat{\Omega}_{1N} \\
\vdots & \vdots & \ddots & \vdots \\
\hat{\Omega}_{N0} & \hat{\Omega}_{N1} & \cdots & \hat{\Omega}_{NN}
\end{bmatrix} \in S^{N+1}
$$
with the elements being given by the weighting function $\omega$ as $\hat{\Omega}_{0 i} = \hat{\Omega}_{i 0} = \omega(\hat{z}_i)$ for $i = 1, \ldots, N$, and the matrix-valued mapping $V : \beta \mapsto V(\beta) \in \mathbb{S}^{N+1}$ satisfies
\[
V(\beta) = \begin{bmatrix}
0 & \ell(\beta, \hat{x}_1, \hat{y}_1) & \cdots & \ell(\beta, \hat{x}_N, \hat{y}_N) \\
\ell(\beta, \hat{x}_1, \hat{y}_1) & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
\ell(\beta, \hat{x}_N, \hat{y}_N) & 0 & \cdots & 0 \\
\end{bmatrix}.
\]

A simple calculation reveals that the objective function of (3) is equivalent to that of (1) up to a positive constant factor of 2. As a consequence, their solutions coincide.

Problem (3) is an overparametrized reformulation of the weighted risk minimization problem (1). Indeed, the objective function of problem (3) involves an inner product of two symmetric matrices, while problem (1) can be potentially reformulated using an inner product of two vectors. While lifting the problem to the matrix space is not necessarily the most efficient approach, it endows us with more flexibility to perturb the weights in a coherent manner. This flexibility comes from the following two observations: (i) there may exist multiple matrices that can be used as the nominal matrix $\hat{\Omega}$, and one can potentially choose $\hat{\Omega}$ to improve the quality of the estimator, (ii) the geometry of the space of positive (semi)definite matrices is richer than the space of vectors.

To proceed, we need to make the following assumption.

**Assumption 2.1** (Regularity conditions). The following assumptions hold throughout the paper.

(i) The function $\ell$ is nonnegative, and $\ell(\cdot, x, y)$ is convex, continuously differentiable for any $(x, y)$.

(ii) The nominal weighting matrix $\hat{\Omega}$ is symmetric positive definite and nonnegative.

In this paper, we propose to find an estimate $\beta^*$ that solves the following adversarially reweighted estimation problem
\[
\min_{\beta} \max_{\Omega \in \mathcal{U}_{\varphi, \rho}(\hat{\Omega})} \langle \Omega, V(\beta) \rangle
\]
for some set $\mathcal{U}_{\varphi, \rho}(\hat{\Omega})$ of feasible weighting matrices. The estimate $\beta^*$ thus minimizes the worst-case loss uniformly over all possible perturbations of the weight $\Omega \in \mathcal{U}_{\varphi, \rho}(\hat{\Omega})$. In particular, we explore the construction of the uncertainty set $\mathcal{U}_{\varphi, \rho}(\hat{\Omega})$ that is motivated by the Gram matrix obtained via some non-negative and positive definite kernels. In this way, the weighting matrix can capture more information on the pair-wise relation among training data. Hence, it is reasonable to consider the set $\mathcal{U}_{\varphi, \rho}(\hat{\Omega})$ of the form
\[
\mathcal{U}_{\varphi, \rho}(\hat{\Omega}) \triangleq \left\{ \Omega \in \mathbb{S}^{N+1}_+ : \Omega \succeq 0, \, \varphi(\Omega, \hat{\Omega}) \leq \rho \right\}.
\]

By definition, any $\Omega \in \mathcal{U}_{\varphi, \rho}(\hat{\Omega})$ is a symmetric, positive semidefinite matrix and all elements of $\Omega$ are nonnegative. A matrix with these properties is called *doubly nonnegative*. From a high level perspective, the set $\mathcal{U}_{\varphi, \rho}(\hat{\Omega})$ is defined as a ball of radius $\rho$ centered at the nominal matrix $\hat{\Omega}$ and this ball is prescribed by a pre-determined measure of dissimilarity $\varphi$. Throughout this paper, we prescribe the uncertainty set $\mathcal{U}_{\varphi, \rho}(\hat{\Omega})$ using some divergence $\varphi$ on the space of symmetric, positive semidefinite matrices $\mathbb{S}^{N+1}_+$.

**Definition 2.2** (Divergence). For any $N \in \mathbb{N}$, $\varphi$ is a divergence on the symmetric positive semidefinite matrix space $\mathbb{S}^{N+1}_+$ if it is: (i) **non-negative**: $\varphi(\Omega_1, \Omega_2) \geq 0$ for all $\Omega_1, \Omega_2 \in \mathbb{S}^{N+1}_+$, and (ii) **indiscernable**: if $\varphi(\Omega_1, \Omega_2) = 0$ then $\Omega_1 = \Omega_2$.

If we denote the adversarially reweighted loss function associated with $\mathcal{U}_{\varphi, \rho}(\hat{\Omega})$ by
\[
F_{\varphi, \rho}(\beta) \triangleq \max_{\Omega \in \mathcal{U}_{\varphi, \rho}(\hat{\Omega})} \langle \Omega, V(\beta) \rangle,
\]
then $\beta^*$ can be equivalently rewritten as
\[
\beta^* = \arg\min_{\beta} F_{\varphi, \rho}(\beta).
\]
A direct consequence is that the function $F_{\varphi,\rho}$ is convex in $\beta$ as long as the loss function $\ell$ satisfies the convex property of Assumption 2.1. Hence, the estimate $\beta^*$ can be found efficiently using convex optimization provided that the function $F_{\varphi,\rho}$ and its gradient can be efficiently evaluated. Moreover, because $\varphi$ is a divergence, $U_{\varphi,\rho}(\hat{\Omega}) = \{\Omega\}$. Hence by setting $\rho = 0$, we will recover the nominal estimate that solves (1). In Section 3 and 4, we will subsequently specify two possible choices of $\varphi$ that lead to the desired efficiency in computing $F_{\varphi,\rho}$ as well as its gradient. Further discussion on Assumption 2.1 is relegated to the appendix. We close this section by discussing the robustness effects of our weighting scheme (4) on the conditional expectation estimation problem.

Remark 2.3 (Connection to distributionally robust optimization). Consider the conditional expectation estimation setting, in which $E[Y|Z = z_0]$ is the solution of the minimum mean square error estimation problem

$$E[Y|Z = z_0] = \arg\min_{\beta} \ E[(\beta - Y)^2|Z = z_0].$$

In this setting, our reweighting scheme (4) coincides with the following distributionally robust optimization problem

$$\min_{\beta} \ \max_{Q_Y|Z = z_0 \in B(\hat{P}_Y|Z = z_0)} \ E_{Q_Y|Z = z_0}[((\beta - Y)^2],$$

with the nominal conditional distribution defined as $\hat{P}_Y|Z = z_0(dy) \propto \sum_{i=1}^N K(z_0, \hat{z}_i)\delta_{\hat{y}_i}(dy)$. The ambiguity set $B(\hat{P}_Y|Z = z_0)$ is a set of conditional probability measures of $Y|Z = z_0$ constructed specifically as

$$B(\hat{P}_Y|Z = z_0) = \left\{ Q_Y|Z = z_0 : \exists \Omega \in U_{\varphi,\rho}(\hat{\Omega}) \text{ so that } \Omega_0 = \Omega_{\hat{y}_i} = \rho(\hat{z}_i) \ \forall i \right\}.$$

Remark 2.4 (Choice of the nominal matrix). The performance of the estimate may depend on the specific choice of the nominal matrix $\Omega$. However, in this paper, we do not study this dependence in details. When the weights $\omega(\hat{z}_i)$ are given by a kernel, it is advised to choose $\Omega$ as the Gram matrix.

3 Adversarial Reweighting Scheme using the Log-Determinant Divergence

We here study the adversarially reweighting scheme when the $\varphi$ is the log-determinant divergence.

Definition 3.1 (Log-determinant divergence). For any positive integer $p \in \mathbb{N}$, the log-determinant divergence from $\Omega_1 \in S_{++}^p$ to $\Omega_2 \in S_{++}^p$ amounts to

$$D(\Omega_1, \Omega_2) \triangleq \text{Tr} \left[ \Omega_1 \Omega_2^{-1} \right] - \log \det(\Omega_1 \Omega_2^{-1}) - p.$$ 

The divergence $D$ is the special instance of the log-determinant $\alpha$-divergence with $\alpha = 1$. Being a divergence, $D$ is non-negative and it vanishes to zero if and only if $\Omega_1 = \Omega_2$. It is important to notice that the divergence $D$ is only well-defined when both $\Omega_1$ and $\Omega_2$ are positive definite. Moreover, $D$ is non-symmetric and $D(\Omega_1, \Omega_2) \neq D(\Omega_2, \Omega_1)$ in general. The divergence $D$ is also tightly connected to the Kullback-Leibler divergence between two Gaussian distributions, and that $D(\Omega_1, \Omega_2) = \text{KL}(\mathcal{N}(0, \Omega_1) \| \mathcal{N}(0, \Omega_2))$, where $\mathcal{N}(0, \Omega)$ is a normal distribution with mean $0$ and covariance matrix $\Omega$.

Suppose that $\hat{\Omega}$ is invertible. Define the uncertainty set

$$U_{\Omega, \rho}(\hat{\Omega}) = \{ \Omega \in S_{++}^{N+1} : \Omega \succeq 0, \ D(\Omega, \hat{\Omega}) \leq \rho \}.$$

For any positive definite matrix $\hat{\Omega}$, the function $D(\cdot, \hat{\Omega})$ is convex, thus the set $U_{\Omega, \rho}(\hat{\Omega})$ is also convex. For this section, we examine the following optimal value function

$$F_{D, \rho}(\beta) = \max_{\Omega \in U_{\Omega, \rho}(\hat{\Omega})} \langle \Omega, V(\beta) \rangle, \quad (7)$$

\[ \]
which corresponds to the worst-case reweighted loss using the divergence $D$. The maximization problem \( \mathbf{7} \) constitutes a nonlinear, convex semidefinite program. Leveraging a strong duality argument, the next theorem asserts that the complexity of evaluating $F_{D,\rho}(\beta)$ is equivalent to the complexity of solving a univariate convex optimization problem.

**Theorem 3.2** (Primal representation). For any $\Omega \in S_{++}^{N+1}$ and $\rho \in (0, +\infty)$, the function $F_{D,\rho}$ is convex. Moreover, for any $\beta$ such that $V(\beta) \neq 0$, let $\gamma^*$ be the unique solution of the convex univariate optimization problem

$$
\inf_{\gamma \geq 0} \gamma \rho - \gamma \log \det(I - \gamma^{-1} \Omega^{\frac{1}{2}} V(\beta) \Omega^{\frac{1}{2}}),
$$

then $F_{D,\rho}(\beta) = \langle \Omega^*, V(\beta) \rangle$, where $\Omega^* = \Omega^{\frac{1}{2}} (I - (\gamma^*)^{-1} \Omega^{\frac{1}{2}} V(\beta) \Omega^{\frac{1}{2}})^{-1} \Omega^{\frac{1}{2}}$. Moreover, the symmetric matrix $\Omega^*$ is unique and doubly nonnegative.

Notice that the condition $V(\beta) \neq 0$ is not restrictive: if $V(\beta) = 0$, then Assumption \( 2.1 \)[1] implies that the incumbent solution $\beta$ incurs zero loss with $\ell(\beta, \tilde{x}_i, \tilde{y}_i) = 0$ for all $i$. In this case, $\beta$ is optimal and reweighting will produce no effect whatsoever. Intuitively, the infimum problem \( 8 \) is the dual counterpart of the supremum problem \( 7 \). The objective function of \( 8 \) is convex in the dual variable $\gamma$, and thus problem \( 8 \) can be efficiently solved using a gradient descent algorithm.

The gradient of $F_{D,\rho}$ is also easy to compute, as asserted in the following lemma.

**Lemma 3.3** (Gradient of $F_{D,\rho}$). The function $F_{D,\rho}$ is continuously differentiable at $\beta$ with

$$
\nabla_{\beta} F_{D,\rho}(\beta) = 2 \sum_{i=1}^{N} \Omega_{ii}^* \nabla_{\beta} \ell(\beta, \tilde{x}_i, \tilde{y}_i),
$$

where $\Omega^*$ is defined as in Theorem 3.2 using the parametrization

$$
\Omega^* = \begin{bmatrix}
\Omega_{00}^* & \Omega_{01}^* & \cdots & \Omega_{0N}^* \\
\Omega_{10}^* & \Omega_{11}^* & \cdots & \Omega_{1N}^* \\
\vdots & \vdots & \ddots & \vdots \\
\Omega_{N0}^* & \Omega_{N1}^* & \cdots & \Omega_{NN}^*
\end{bmatrix}.
$$

The proof of Lemma 3.3 exploits Danskin’s theorem and the fact that $\Omega^*$ is unique in Theorem 3.2. Minimizing $F_{D,\rho}$ is now achievable by applying state-of-the-art first-order methods.

**Sketch of Proof of Theorem 3.2**. The difficulty in deriving the dual formulation \( 8 \) lies in the non-negativity constraint $\Omega \succeq 0$. In fact, this constraint imposes $(N + 1)(N + 2)/2$ individual component-wise constraints, and as such, simply dualizing problem \( 7 \) using a Lagrangian multiplier will entail a large number of auxiliary variables. To overcome this difficulty, we consider the relaxed set $V_{D,\rho}(\Omega) = \{ \Omega \in S_{++}^{N+1} : D(\Omega, \hat{\Omega}) \leq \rho \}$. By definition, we have $\hat{V}_{D,\rho}(\hat{\Omega}) \subseteq V_{D,\rho}(\Omega)$, and $V_{D,\rho}(\hat{\Omega})$ omits the nonnegativity requirement $\Omega \succeq 0$. The set $V_{D,\rho}(\hat{\Omega})$ is also more amenable to optimization thanks to the following proposition.

**Proposition 3.4** (Properties of $V_{D,\rho}(\hat{\Omega})$). For any $\hat{\Omega} \in S_{++}^{N+1}$ and $\rho \geq 0$, the set $V_{D,\rho}(\hat{\Omega})$ is convex and compact. Moreover, the support function of $V_{D,\rho}(\hat{\Omega})$ satisfies

$$
\delta^*_{V_{D,\rho}(\hat{\Omega})}(T) \triangleq \sup_{\Omega \in V_{D,\rho}(\hat{\Omega})} \text{Tr}[\Omega T] = \inf_{\gamma > 0} \gamma \rho - \gamma \log \det(I - \gamma^{-1} \hat{\Omega}^{\frac{1}{2}} T \hat{\Omega}^{\frac{1}{2}} / \gamma)
$$

for any symmetric matrix $T \in S_{++}^{N+1}$.

Moreover, we need the following lemma which asserts some useful properties of the matrix $V(\beta)$.

**Lemma 3.5** (Properties of $V(\beta)$). For any $\beta$, the matrix $V(\beta)$ is symmetric, nonnegative, and it has only two non-zero eigenvalues of value $\pm \sqrt{\sum_{i=1}^{N} \ell(\beta, \tilde{x}_i, \tilde{y}_i)^2}$.

The proof of Theorem 3.2 proceeds by first constructing a tight upper bound for $F_{D,\rho}(\beta)$ as

$$
F_{D,\rho}(\beta) \leq \max_{\hat{\Omega} \in V_{D,\rho}(\hat{\Omega})} \langle \hat{\Omega}, V(\beta) \rangle = \inf_{\gamma \geq 0} \gamma \rho - \gamma \log \det(I - \frac{1}{\gamma} \hat{\Omega}^{\frac{1}{2}} V(\beta) \hat{\Omega}^{\frac{1}{2}}),
$$

where $\hat{\Omega}$ is the unique solution to the optimization problem \( 9 \).
where the inequality in (10) follows from the fact that $U_{D,\rho}(\hat{\Omega}) \subseteq V_{D,\rho}(\hat{\Omega})$, and the equality follows from Proposition 3.4. Notice that $V(\beta)$ has one nonnegative eigenvalue by virtue of Lemma 3.5 and thus the constraint $\gamma\hat{\Omega}^{-1} - V(\beta)$ already implies the condition $\gamma > 0$. Next, we argue that the optimizer $\Omega^*$ of problem (10) can be constructed from the optimizer $\gamma^*$ of the infimum problem via

$$\Omega^* = \hat{\Omega}^{\frac{1}{2}} [I - (\gamma^*)^{-1} \hat{\Omega}^{\frac{1}{2}} V(\beta) \hat{\Omega}^{\frac{1}{2}}]^{-1} \hat{\Omega}^{\frac{1}{2}}.$$ 

The last step involves proving that $\Omega^*$ is a nonnegative matrix, and hence $\Omega^* \in U_{D,\rho}(\hat{\Omega})$. As a consequence, the inequality (10) holds as an equality, which leads to the postulated result. The proof is relegated to the Appendix.

4 Adversarial Reweighting Scheme using the Bures-Wasserstein Type Divergence

In this section, we explore the construction of the set of possible weighting matrices using the Bures-Wasserstein distance on the space of positive semidefinite matrices.

**Definition 4.1** (Bures-Wasserstein divergence). For any positive integer $p \in \mathbb{N}$, the Bures-Wasserstein divergence between $\Omega_1 \in \mathbb{S}^p_+$ and $\Omega_2 \in \mathbb{S}^p_+$ amounts to

$$W(\Omega_1, \Omega_2) \triangleq \text{Tr} [\Omega_1 + \Omega_2 - 2(\Omega_2^{\frac{1}{2}} \Omega_1 \Omega_2^{\frac{1}{2}})^{\frac{1}{2}}].$$

For any positive semidefinite matrices $\Omega_1$ and $\Omega_2$, the value $W(\Omega_1, \Omega_2)$ is equal to the square of the type-2 Wasserstein distance between two Gaussian distributions $\mathcal{N}(0, \Omega_1)$ and $\mathcal{N}(0, \Omega_2)$ [15]. As a consequence, $W$ is a divergence: it is non-negative and indiscernable. However, $W$ is not a proper distance because it may violate the triangle inequality. Compared to the divergence $D_2$ studied in Section 3, the Bures-Wasserstein divergence $W$ has several advantages as it is symmetric and is well-defined for all positive *semi*-definite matrices. This divergence has also been of interest in quantum information, statistics, and the theory of optimal transport.

Given the nominal weighting matrix $\hat{\Omega}$, we define the set of possible weighting matrices using the Bures-Wasserstein divergence $W$ as

$$U_{W,\rho}(\hat{\Omega}) \triangleq \{ \Omega \in \mathbb{S}^{N+1}_+ : \Omega \succeq 0, W(\Omega, \hat{\Omega}) \leq \rho \}.$$ 

Correspondingly, the worst-case loss function is

$$F_{W,\rho}(\beta) \triangleq \max_{\Omega \in U_{W,\rho}(\hat{\Omega})} \langle \Omega, V(\beta) \rangle.$$ 

(11)

**Theorem 4.2** (Primal representation). For any $\hat{\Omega} \in \mathbb{S}^{N+1}_+$ and $\rho \in (0, +\infty)$, the function $F_{W,\rho}$ is convex. Moreover, for any $\beta$ such that $V(\beta) \neq 0$, let $\gamma^*$ be the unique solution of the convex univariate optimization problem

$$\inf_{\gamma > V(\beta)} \gamma (\rho - \text{Tr} [\hat{\Omega}] + \gamma^2 \langle (\gamma I - V(\beta))^{-1}, \hat{\Omega} \rangle),$$

(12)

then $F_{W,\rho}(\beta) = \langle \gamma^*, V(\beta) \rangle$, where $\gamma^* = (\gamma^*)^2 [\gamma^* I - V(\beta)]^{-1} \hat{\Omega} [\gamma^* I - V(\beta)]^{-1}$. Moreover, the symmetric matrix $\gamma^*$ is unique and doubly nonnegative.

Thanks to the uniqueness of $\gamma^*$ and Danskin’s theorem, the gradient of $F_{W,\rho}$ is now a by-product of Theorem 4.2.

**Lemma 4.3** (Gradient of $F_{W,\rho}$). The function $F_{W,\rho}$ is continuously differentiable at $\beta$ with

$$\nabla_\beta F_{W,\rho}(\beta) = 2 \sum_{i=1}^{N} \Omega^*_{0i} \nabla_\beta \ell(\beta, \hat{x}_i, \hat{y}_i),$$

where $\Omega^*$ is defined as in Theorem 4.2 using the similar parametrization (9).

A first-order minimization algorithm can be used to find the robust estimate with respect to the loss function $F_{W,\rho}$. Notice that problem (12) is one-dimensional, and either a bisection search or a gradient descent subroutine can be employed to solve (12) efficiently.
We evaluate our adversarial reweighting schemes on the conditional expectation estimation task. Consider the relaxed set \( V_{W,\rho}(\Omega) \triangleq \{ \Omega \in \mathbb{S}^{N+1}_{+} : W(\Omega, \hat{\Omega}) \leq \rho \} \). By definition, \( V_{W,\rho}(\hat{\Omega}) \) omits the nonnegativity requirement \( \Omega \geq 0 \) and thus \( \mathcal{U}_{W,\rho}(\hat{\Omega}) \subseteq V_{W,\rho}(\hat{\Omega}) \). The advantage of considering \( V_{W,\rho}(\hat{\Omega}) \) arises from the fact that the support function of the set \( V_{W,\rho}(\hat{\Omega}) \) admits a simple form [26 Proposition A.4].

Proposition 4.4 (Properties of \( V_{W,\rho}(\hat{\Omega}) \)). For any \( \hat{\Omega} \in \mathbb{S}^{N+1} \) and \( \rho \geq 0 \), the set \( V_{W,\rho}(\hat{\Omega}) \) is convex and compact. Moreover, the support function of \( V_{W,\rho}(\hat{\Omega}) \) satisfies

\[
\delta_{V_{W,\rho}(\hat{\Omega})}(T) \triangleq \sup_{\Omega \in V_{W,\rho}(\hat{\Omega})} \mathrm{Tr}[\Omega T] = \inf_{\gamma > 0} \frac{1}{\gamma T} \gamma (\rho - \mathrm{Tr}[\hat{\Omega}]) + \gamma^2 \langle (\gamma I - T)^{-1}, \hat{\Omega} \rangle.
\]

The upper bound for \( F_{W,\rho}(\beta) \) can be constructed as

\[
F_{W,\rho}(\beta) \leq \max_{\Omega \in V_{W,\rho}(\hat{\Omega})} \langle \Omega, V(\beta) \rangle = \inf_{\gamma > 0} \gamma I - V(\beta) + \gamma^2 \langle (\gamma I - V(\beta))^{-1}, \hat{\Omega} \rangle,
\]

where the inequality in (13) follows from the fact that \( \mathcal{U}_{W,\rho}(\hat{\Omega}) \subseteq V_{W,\rho}(\hat{\Omega}) \), and the equality follows from Proposition 4.4. In the second step, we argue that the optimizer \( \Omega^* \) of problem (13) can be constructed from the optimizer \( \gamma^* \) of the infimum problem via

\[
\Omega^* = (\gamma^*)^2 (\gamma^* I - V(\beta))^{-1} \hat{\Omega} (\gamma^* I - V(\beta))^{-1}.
\]

The last step involves proving that \( \Omega^* \) is a nonnegative matrix by exploiting Lemma 3.5 and hence \( \Omega^* \in \mathcal{U}_{W,\rho}(\hat{\Omega}) \). Thus, inequality (13) is tight, leading to the desired result.

5 Numerical Experiments on Real Data

We evaluate our adversarial reweighting schemes on the conditional expectation estimation task. To this end, we use the proposed reweighted scheme on the NW estimator of Example 1.1. The robustification using the log-determinant divergence and the Bures-Wasserstein divergence are denoted by NW-LogDet and NW-BuresW, respectively. We compare our NW robust estimates against four popular baselines for estimating the conditional expectation: (i) the standard NW estimate in Example 1.1 with Gaussian kernel, (ii) the LLR estimate in Example 1.2 with Gaussian kernel, (iii) the intercepted \( \beta_1 \) of LLR estimate (i.e., only the first dimension of \( \beta_{\text{LLR}} \)), denoted as LLR-I, and (iv) the NW-Metric [29] which utilizes the Mahalanobis distance in the Gaussian kernel.

Datasets. We use 8 real-world datasets: (i) abalone (Abalone), (ii) bank-32fh (Bank), (iii) cpu (CPU), (iv) kin40k (KIN), (v) elevators (Elevator), (vi) pol (POL), (vii) pumadyn32nm (PUMA), and (viii) slice (Slice) from the Delve datasets, the UCI datasets, the KEEL datasets and datasets in Noh et al. [29]. Due to space limitation, we report results on the first 4 datasets and relegate the remaining datasets to the Appendix. Datasets characteristics can also be found in the supplementary material.

Setup. For each dataset, we randomly split 1200 samples for training, 500 samples for validation to choose the bandwidth \( h \) of the Gaussian kernel, and 800 samples for test. More specifically, we choose the squared bandwidth \( h^2 \) for the Gaussian kernel from a predefined set \( \{10^{-2}, 10^{-1.5}, 2 \times 10^{-2}, 10^{-1.5}, 5 \times 10^{-2} \} \). For a tractable estimation, we follow the approach in Brundson et al. [9] and Silverman [37] to restrict the relevant samples to \( N \) nearest neighbors of each test sample \( z_i \) with \( N \in \{10, 20, 30, 50\} \). The range of the radius \( \rho \) has 4 different values \( \rho \in \{0.01, 0.1, 1, 10\} \). Finally, the prediction error is measured by the root mean square error (RMSE),

\[
\text{RMSE} = \sqrt{\frac{1}{n_T} \sum_{i=1}^{n_T} (\hat{y}_i - \overline{y}_i)^2},
\]

where \( n_i \) is the test sample size (i.e., \( n_i = 800 \)) and \( \overline{y}_i \) is the conditional expectation estimate at the test sample \( z_i \). We repeat the above procedure 10 times to obtain the average RMSE. All our experiments are run on commodity hardware.

Ideal case: no sample perturbation. We first study how different estimators perform when there is no perturbation in the training data. In this experiment, we set the nearest neighbor size to \( N = 50 \), and our reweighted estimators are obtained with the uncertainty size of \( \rho = 0.1 \).

Figure 1 shows the average RMSE across the datasets. The NW-Metric estimator outperforms the standard NW, which agrees with the empirical observation in Noh et al. [29]. More importantly, we
Figure 1: Average RMSE for ideal case with no perturbation.

observe that our adversarial reweighting schemes perform competitively against the baselines on several datasets.

When training samples are perturbed. We next evaluate the estimation performances when \( \tau \in \{0.2N, 0.4N, 0.6N, 0.8N, N\} \) nearest samples from the \( N \) training neighbors of each test sample are perturbed. We specifically generate perturbations only in the response dimension by shifting \( y \mapsto \kappa y \), where \( \kappa \) is sampled uniformly from \([1.8, 2.2]\). We set \( N = 50 \) and \( \rho = 0.1 \) as the experiment for the ideal case (no sample perturbation).

Figure 2 shows the average RMSE for with varying perturbation level \( \tau \). The performance of the NW, LLR, LLR-I, and NW-Metric baselines severely deteriorate, while both NW-LogDet and NW-BuresW can alleviate the effect of data perturbation. Our adversarial reweighting schemes consistently outperform all baselines in all datasets for the perturbed training data, across all 5 perturbations \( \tau \).

We then evaluate the effects of the uncertainty size \( \rho \) and the nearest neighbor size \( N \) on NW-LogDet and NW-BuresW.

Figure 3: Average RMSE as a function of the ambiguity size \( \rho \). Errors at \( \rho = 0 \) indicate the performance of the vanilla NW estimator.

Effects of the uncertainty size \( \rho \). In this experiment, we set the nearest neighbor size to \( N = 50 \), the perturbation \( \tau = N \). Figure 3 illustrates the effects of the uncertainty size \( \rho \) for the adversarial reweighting schemes. Errors at \( \rho = 0 \) indicate the performance of the vanilla NW estimator. We observe that the adversarial reweighting schemes perform well at some certain \( \rho \) and when that \( \rho \) is increased more, the performances decrease. The uncertainty size \( \rho \) plays an important role for the adversarial reweighting schemes in applications. Tuning \( \rho \) may consequently improve the performances of the adversarial reweighting schemes.

Effects of the nearest neighbor size \( N \). In this experiment, we set the uncertainty size to \( \rho = 0.1 \).
Figure 4 shows the effects of the nearest neighbor size $N$ for the adversarial reweighting schemes under varying perturbation $\tau$ in the KIN dataset. We observe that the performances of the adversarial reweighting schemes with $N \in \{20, 30\}$ perform better than those with $N \in \{10, 50\}$. Note that when $N$ is increased, the computational cost is also increased (see Equation (1) and Figure 4). Similar to the cases of the uncertainty size $\rho$, tuning $N$ may also help to improve performances of the adversarial reweighting schemes.

**Under varying shifting w.r.t. $\kappa$.** In this experiment, we set the nearest neighbor size to $N = 50$. Figure 5 illustrates the performances of NW-LogDet under varying shifting w.r.t. $\kappa$ in the KIN dataset. For the left plots of the Figures 5 we set the uncertainty size to $\rho = 0.1$ when varying the perturbation $\tau$. We observe that the adversarial reweighting schemes provide different degrees of mitigation for the perturbation under varying shifting w.r.t. $\kappa$. For the right plots of the Figures 5 we set the perturbation to $\tau = 0.2N$ when varying the uncertainty size $\rho$. We observe that the reweighting schemes under varying shifting w.r.t. $\kappa$ have the same behaviors as in Figure 3 when we consider the effects of the original weights are given through kernel functions. Note that the adversarial reweighting with Bures-Wasserstein distance $W$ can be generalized to cases where the nominal weighting matrix $\Omega$ is singular, unlike the reweighting with the log-determinant divergence $D$.

**Time consumption.** In Figure 6 we illustrate the time consumption for the adversarial reweighting schemes under varying neighbor size $N$ and uncertainty size $\rho$ in the KIN dataset. The adversarial reweighting schemes averagely take about 10 seconds for their estimation. When $N$ and/or $\rho$ increases, the computation of the adversarial reweighting schemes take longer. This is intuitive because the dimension of the weight matrix $\Omega$ scales quadratically in the neighbor size $N$. Bigger uncertainty size $\rho$ implies a larger feasible set $U_{\phi, \rho}(\Omega)$, which leads to longer computing time to evaluate $F_{\phi, \rho}$ and its gradient.

**Concluding Remarks.** We introduce two novel schemes for sample reweighting using matrix reparametrization. These two invariants are particularly attractive when the original weights are given through kernel functions. Note that the adversarial reweighting with Bures-Wasserstein distance $W$ can be generalized to cases where the nominal weighting matrix $\Omega$ is singular, unlike the reweighting with the log-determinant divergence $D$.

**Remark 5.1 (Invariant under permutation).** Our results hold under any simultaneous row and column permutation of the nominal weighting matrix $\hat{\Omega}$ and the mapping $V(\beta)$. To see this, let $P$ be any $(N + 1)$-dimensional permutation matrix, and let $\Omega_P = P\hat{\Omega}P$ and $V_P(\beta) = PV(\beta)P$. Then

$$\max_{\Omega \in U_{\phi, \rho}(\Omega_P)} \langle \Omega, V_P(\beta) \rangle = \langle \Omega^*, V_P(\beta) \rangle = \langle \Omega^*, V(\beta) \rangle,$$

where $\Omega^*$ is calculated as in Theorem 3.2 for $\phi = D$, and as in Theorem 4.2 for $\phi = W$. The proof relies on the fact that $P^\top P = PP^\top = I$, that both $D$ and $W$ are permutation invariant (in the sense that $\phi(\Omega_1, \Omega_2) = \phi(P\Omega_1P, P\Omega_2P)$), and that the inner product is also permutation invariant. Similar results hold for the gradient information, and hence the optimal solution of $\beta$ is preserved under row and column permutations of $\Omega$ and $V(\beta)$. 
Acknowledgements. Material in this paper is based upon work supported by the Air Force Office of Scientific Research under award number FA9550-20-1-0397. Support is gratefully acknowledged from NSF grants 1915967, 1820942, 1838676, Simons Foundation grant (#318995), JSPS KAKENHI grant 20K19873, and MEXT KAKENHI grants 20H04243, 21H04874. We thank the anonymous referees for their constructive feedbacks that helped improve and clarify this paper.

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A Proofs and Additional Discussions

A.1 Proofs of Section 3

In the following, the symbol \( \langle \cdot, \cdot \rangle \) will be used to represent both Frobenius norm of matrices and standard Euclidean norm of vectors. Also for a \( p \times p \) matrix \( A \), we let \( \|A\|_2 = \sqrt{A^\top A} \) to denote its Frobenius norm and let \( \lambda_{\max}(A) \) to represent its maximum eigenvalue. In order to prove Proposition 3.4, we begin by computing the support function of the convex cone of symmetric positive definite (SPD) matrices.

**Lemma A.1** (Support function of SPD matrices). For any matrices \( A \in S^{N+1} \) and \( \Omega \in S^{N+1} \), we have \( \text{Tr} [A\Omega] \leq \lambda_{\max}(A) \text{Tr} [\Omega] \), and \( \text{Tr} [A\Omega] < 0 \) if in addition \( A \preceq 0 \) and \( A \neq 0 \). Also for each \( A \in S^{N+1} \),

\[
\sup_{\Omega > 0} \text{Tr} [A\Omega] = \begin{cases} +\infty & \text{if } \lambda_{\max}(A) > 0, \\ 0 & \text{if } \lambda_{\max}(A) \leq 0. \end{cases}
\]

*Proof of Lemma A.1* Since \( A \) is symmetric, we can decompose it as \( D = Q^\top A Q \) with \( D \) being a diagonal matrix formed by eigenvalues of \( A \) and \( Q \) being an orthogonal matrix whose columns are normalized eigenvectors of \( A \). Then \( Q^\top A = DQ^\top \) and hence

\[
\text{Tr} [A\Omega] = \text{Tr} [Q^\top \Omega Q^\top A Q] = \text{Tr} [DQ^\top \Omega Q] \leq \lambda_{\max}(D) \text{Tr} [Q^\top \Omega Q] = \lambda_{\max}(A) \text{Tr} [\Omega],
\]

where we have used the fact \( Q^\top \Omega Q \succ 0 \) to obtain the inequality. In case \( A \preceq 0 \) and \( A \neq 0 \), then as all diagonal elements of \( D \) are nonpositive with at least one negative element we have \( \text{Tr} [A\Omega] = \text{Tr} [DQ^\top \Omega Q] < 0 \). These give the first part of the lemma.

For the second part, let \( v \) be an eigenvector of \( A \) corresponding to eigenvalue \( \lambda_{\max}(A) \). In case \( \lambda_{\max}(A) > 0 \), by taking \( \Omega_t = I + tvv^\top \) with \( t \in (0, +\infty) \) and letting \( t \to +\infty \) we see that \( \text{Tr} [A\Omega_t] = \text{Tr} [A] + t\lambda_{\max}(A) \text{Tr} [vv^\top] \) tends to \( +\infty \). This implies that \( \sup_{\Omega > 0} \text{Tr} [A\Omega] = +\infty \).

For the case \( \lambda_{\max}(A) \leq 0 \), we instead take \( \Omega_t = tI + tvv^\top \) with \( t \in (0, 1) \) and let \( t \to 0^+ \) to conclude that \( \sup_{t > 0} \text{Tr} [A\Omega_t] \geq 0 \). On the other hand, due to the first part of the lemma we always have \( \sup_{\Omega > 0} \text{Tr} [A\Omega] \leq 0 \). Therefore, the desired result follows.

*For Proposition 3.4*

**Proof of Proposition 3.4** The set \( \calV_{\Omega, \rho}(\overline{\Omega}) \) is bounded. Indeed, if \( \rho = 0 \) then \( \calV_{\Omega, \rho}(\overline{\Omega}) = \{\overline{\Omega}\} \) which is trivially bounded. If \( \rho > 0 \), then any \( \Omega \in \calV_{\Omega, \rho}(\overline{\Omega}) \) satisfies \( \text{Tr} [\Omega^{-1} - \log \det(\Omega^{-1})] - (N + 1) \leq \rho \). Since \( \Omega^{-1} \) is similar to the matrix \( \overline{\Omega}^{-\frac{1}{2}} \Omega^{-\frac{1}{2}} \), we can rewrite this as

\[
\text{Tr} [\overline{\Omega}^{-\frac{1}{2}} \Omega^{-\frac{1}{2}} - \log \det(\overline{\Omega}^{-\frac{1}{2}} \Omega^{-\frac{1}{2}})] - (N + 1) \leq \rho. \quad (14)
\]

We claim that this implies that \( \Omega \) is bounded in the sense that there exist numbers \( 0 < \underline{\sigma} \leq \bar{\sigma} < \infty \) depending only on \( \rho, \overline{\Omega} \), and \( N \) such that \( \underline{\sigma} I \preceq \Omega \preceq \bar{\sigma} I \). To see this, let \( \sigma_i \) (\( i = 1, \ldots, N + 1 \)) be the eigenvalues of \( \overline{\Omega}^{-\frac{1}{2}} \Omega^{-\frac{1}{2}} \). Then (14) gives

\[
\sum_{i = 1}^{N + 1} [\sigma_i - \log \sigma_i - 1] \leq \rho.
\]

Because the function \( \sigma \to \sigma - \log \sigma - 1 \) is non-negative for every \( \sigma > 0 \), we then find that \( \{\sigma_i - \log \sigma_i - 1\}_{i = 1}^{N + 1} \) is bounded. Therefore, \( \sigma_i \) must be bounded between two positive constants depending only on \( \rho \) and \( N \). Now let \( \lambda \) be an eigenvalue of \( \Omega \) and let \( v \) be its associated eigenvector. Then \( \lambda \|v\|^2 = \langle v, \Omega v \rangle = \langle (\overline{\Omega}^{-\frac{1}{2}} v), \overline{\Omega}^{-\frac{1}{2}} \Omega^{-\frac{1}{2}} (\overline{\Omega}^{-\frac{1}{2}} v) \rangle \), and so

\[
\sigma_* \|\overline{\Omega}^{-\frac{1}{2}} v\|^2 \leq \lambda \|v\|^2 \leq \sigma^* \|\overline{\Omega}^{-\frac{1}{2}} v\|^2,
\]

where \( \sigma_* \) and \( \sigma^* \) respectively denote the smallest and largest eigenvalues of \( \overline{\Omega}^{-\frac{1}{2}} \Omega^{-\frac{1}{2}} \). It follows that \( \sigma_* \lambda_{\min}(\overline{\Omega}) \leq \lambda \leq \sigma^* \lambda_{\max}(\overline{\Omega}) \). Thus all eigenvalues of \( \Omega \) are bounded between two positive constants, and the claim is proved.
One now can rewrite $\mathcal{V}_{D,\rho}(\hat{\Omega})$ as

$$
\mathcal{V}_{D,\rho}(\hat{\Omega}) = \left\{ \Omega \in S_+^{N+1} : \sigma I \preceq \Omega \preceq \sigma I, \; \text{Tr} \left[ \hat{\Omega}^{-1} \right] - \log \det(\hat{\Omega}^{-1}) - (N + 1) \leq \rho \right\}.
$$

The function $\Omega \mapsto \text{Tr} \left[ \hat{\Omega}^{-1} \right] - \log \det(\hat{\Omega}^{-1})$ is convex and continuous on the set $\{ \Omega : \sigma I \preceq \Omega \preceq \sigma I \}$, and the last equality follows from strong duality \cite[Proposition 5.3.1]{ref}.

We now proceed to provide the support function of $\mathcal{V}_{D,\rho}(\hat{\Omega})$. One can verify that $\hat{\Omega}$ is the Slater point of the convex set $\mathcal{V}_{D,\rho}(\hat{\Omega})$. Assume momentarily that $T \neq 0$, using a duality argument, we find

$$
\sup_{\Omega \in \mathcal{V}_{D,\rho}(\hat{\Omega})} \text{Tr} \left[ T \hat{\Omega} \right] = \sup_{\Omega > 0} \inf_{\gamma \geq 0} \text{Tr} \left[ T \hat{\Omega} \right] + \gamma \left( \rho - \text{Tr} \left[ \hat{\Gamma}^{-1} \hat{\Omega} \right] + \log \det \hat{\Omega} \right)
$$

$$
= \inf_{\gamma \geq 0} \left\{ \gamma \rho + \sup_{\Omega > 0} \left\{ \text{Tr} \left[ (T - \gamma \hat{\Omega}^{-1}) \Omega \right] + \gamma \log \det \hat{\Omega} \right\} \right\},
$$

where the last equality follows from strong duality \cite[Proposition 5.3.1]{ref}, and $\rho \triangleq \rho + (N + 1) - \log \det \hat{\Omega} \in \mathbb{R}$. Note that $\gamma = 0$ is not an optimal solution to the minimization problem (15). Indeed, if the maximum eigenvalue of $T$ is strictly positive, then the objective value of problem (15) evaluated at $\gamma = 0$ is $+\infty$ by Lemma \ref{lem:A.1}. However, because $\mathcal{V}_{D,\rho}(\hat{\Omega})$ is compact and bounded, we have $\sup_{\Omega \in \mathcal{V}_{D,\rho}(\hat{\Omega})} \text{Tr} \left[ T \hat{\Omega} \right] < \infty$. In case the maximum eigenvalue of $T$ is nonpositive, then from Lemma \ref{lem:A.1}, we see that the objective value of problem (15) evaluated at $\gamma = 0$ is $0$, while $\sup_{\Omega \in \mathcal{V}_{D,\rho}(\hat{\Omega})} \text{Tr} \left[ T \hat{\Omega} \right] < 0$. Thus, the infimum in problem (15) can be restricted to $\gamma > 0$.

If $T - \gamma \hat{\Omega}^{-1} \neq 0$, then the inner supremum problem in (15) becomes unbounded according to Lemma \ref{lem:A.1}.

If $T - \gamma \hat{\Omega}^{-1} < 0$ then the inner supremum problem admits the unique optimal solution

$$
\hat{\Omega}^*(\gamma) = \gamma (\hat{\Omega}^{-1} - T)^{-1},
$$

which is obtained by solving the first-order optimality condition. By placing this optimal solution into the objective function and arranging terms together with using the definition of $\hat{\rho}$, we have

$$
\sup_{\Omega \in \mathcal{V}_{D,\rho}(\hat{\Omega})} \text{Tr} \left[ T \hat{\Omega} \right] = \inf_{\gamma > 0} \gamma \rho - \gamma \log \det(I - \gamma^{-1} \hat{\Omega}^{1/2} T \hat{\Omega}^{1/2}).
$$

To complete the proof, we show that the reformulation (17) holds even for $T = 0$ or $\rho = 0$. Notice that if $T = 0$ or $\rho = 0$, then the left-hand side of (17) evaluates to $0$. If $T = 0$, the infimum problem on the right-hand side of (17) also attains the optimal value of 0 asymptotically as $\gamma$ decreases to $0$. If $\rho = 0$ and $T \neq 0$, then the infimum problem on the right-hand side of (17) also attains the optimal value of 0 asymptotically as $\gamma$ increases to $+\infty$ by the l'Hopital rule

$$
\lim_{\gamma \uparrow +\infty} - \gamma \log \det(I - \hat{\Omega}^{1/2} T \hat{\Omega}^{1/2} / \gamma) = \text{Tr} \left[ T \hat{\Omega} \right].
$$

This observation completes the proof.

For an $p \times p$ real matrix $A$, its spectral radius $R(A)$ is defined as the largest absolute value of its eigenvalues. The following elementary fact is well known.

**Lemma A.2** (Nonnegativity of inverse). Let $A$ be an $p \times p$ real matrix such that $R(A) < 1$ and all its entries are nonnegative. Then the matrix $I - A$ is invertible and all entries of $(I - A)^{-1}$ are nonnegative.

**Proof of Lemma A.2** For completeness, we include a proof here. By Gelfand’s formula, we have

$$
\lim_{k \to +\infty} \| A^k \|_2^{1/2} = R(A) < 1.
$$
Thus there exist constants \( \tau \in (0, 1) \) and \( k_0 \in \mathbb{N} \) such that \( \|A^k\|_2 < \tau^k \) for every \( k \geq k_0 \). Therefore, the Neumann series

\[
\sum_{k=0}^{\infty} A^k = (I - A)^{-1}
\]

converges. This together with the assumption about the nonnegativity of \( A \) implies that all entries of \( (I - A)^{-1} \) are nonnegative.

**For Theorem 3.2**

**Proof of Theorem 3.2** We find

\[
F_{D, \rho}(\beta) = \max_{\Omega \in \mathcal{U}_{D, \rho}(\hat{\Omega})} \langle \Omega, V(\beta) \rangle
\]

(18a)

\[
\leq \max_{\Omega \in \mathcal{V}_{D, \rho}(\hat{\Omega})} \langle \Omega, V(\beta) \rangle
\]

(18b)

\[
= \inf_{\gamma > 0} \gamma \rho - \log \det(I - \gamma^{-1} \hat{\Omega}^{1/2} V(\beta) \hat{\Omega}^{1/2}),
\]

(18c)

where equality (18a) is the definition of \( F_{D, \rho} \) as in [7], inequality (18b) follows from the fact that \( \mathcal{U}_{D, \rho}(\hat{\Omega}) \subseteq \mathcal{V}_{D, \rho}(\hat{\Omega}) \), and equality (18c) follows from Proposition 3.4. Notice that \( V(\beta) \) has one nonnegative eigenvalue by virtue of Lemma 3.5 and thus the constraint \( \gamma I \succ \hat{\Omega}^{1/2} \Omega V(\beta) \hat{\Omega}^{1/2} \) implies the condition \( \gamma > 0 \).

The strictly positive radius condition \( \rho \in (0, +\infty) \) implies the existence of a Slater point \( \hat{\Omega} \) of the set \( \mathcal{U}_{D, \rho}(\hat{\Omega}) \). By [6] Proposition 5.5.4, the existence of a solution \( \gamma^* > 0 \) that minimizes the dual problem (18c) is guaranteed. Moreover, the objective function of problem (18c) is strictly convex, and thus the solution \( \gamma^* \) is unique. By inspecting (16), the solution

\[
\Omega^*(\gamma^*) = (\hat{\Omega}^{-1} - 1/\gamma^* V(\beta))^{-1}
\]

thus solves the primal problem (18b) by [6] pp. 178].

Assumption 2.1 implies that both \( \hat{\Omega} \) and \( V(\beta)/\gamma^* \) are nonnegative matrices. Also the spectral radius of \( (\gamma^*)^{-1} \hat{\Omega}^{1/2} \Omega V(\beta) \hat{\Omega}^{-1/2} \) is smaller than 1 by the feasibility of \( \gamma^* \) in problem (18c). Hence the matrix \( [I - (\gamma^*)^{-1} \hat{\Omega}^{1/2} \Omega V(\beta) \hat{\Omega}^{-1/2}]^{-1} \) is nonnegative by Lemma A.2

As \( \Omega^*(\gamma^*) = \hat{\Omega}^{1/2} [I - (\gamma^*)^{-1} \hat{\Omega}^{1/2} \Omega V(\beta) \hat{\Omega}^{-1/2}]^{-1} \hat{\Omega}^{-1/2} \), we conclude that \( \Omega^*(\gamma^*) \) is a matrix with nonnegative entries. Moreover, \( \Omega^*(\gamma^*) \) is also positive semidefinite. Thus \( \Omega^*(\gamma^*) \) is doubly nonnegative. This observation completes the proof.

**For Lemma 3.3**

**Proof of Lemma 3.3** Because \( \mathcal{U}_{D, \rho}(\hat{\Omega}) \) is compact, by [7] Proposition A.22, the subdifferential of \( F_{D, \rho} \) is

\[
\partial F_{D, \rho}(\beta) = \text{ConvexHull} \left( 2 \sum_{i=1}^{N} \Omega^*_{i} \nabla_{\beta} \ell(\beta, \hat{x}_i, \hat{y}_i) \bigg\vert \Omega^* \in \mathcal{O}^*(\beta) \right),
\]

where \( \mathcal{O}^*(\beta) = \{ \Omega \in \mathcal{U}_{D, \rho}(\hat{\Omega}) : \langle \Omega, V(\beta) \rangle = F_{D, \rho}(\beta) \} \) is the optimal solution set. By Theorem 3.2, the optimal solution set \( \mathcal{O}^*(\beta) \) is a singleton, which leads to the postulated result.

**For Lemma 3.5**

**Proof of Lemma 3.5** The symmetry of \( V(\beta) \) follows from definition. The nonnegativity of \( V(\beta) \) follows from Assumption 2.1. Let \( \lambda \) be an eigenvalue of \( V(\beta) \), then \( \lambda \) solves the characteristic equation \( \det(V(\beta) - \lambda I) = 0 \). By exploiting the form of \( V(\beta) \) and by the determinant formula for the arrowhead matrix, the eigenvalue \( \lambda \) then solves the algebraic equation \( \lambda^{N-1} \left[ 2 - \sum_{i=1}^{N} \ell(\beta, \hat{x}_i, \hat{y}_i)^2 \right] = 0 \). This completes the proof.
A.2 Proofs of Section 4

For Theorem 4.2

Proof of Theorem 4.2 The statement regarding $\gamma^*$ and the expression of $F_{W,\rho}$ and $\Omega^*$ follows from [26, Proposition A.4]. It remains to show that $\Omega^*$ is nonnegative. Indeed, the constraint $\gamma^* I > V(\beta)$ implies that the spectral radius of $(\gamma^*)^{-1} V(\beta)$ is smaller than 1. Therefore, the inverse matrix $[I - (\gamma^*)^{-1} V(\beta)]^{-1}$ is nonnegative according to Lemma A.2. The matrix $\Omega^*$ is thus the product of three nonnegative matrices and thus it is also nonnegative.

For Lemma 4.3

Proof of Lemma 4.3 The proof of this lemma is similar to that of Lemma 3.3 with the optimal set is now given by $\mathcal{O}^*(\beta) = \{ \Omega \in \mathcal{U}_{W,\rho}(\hat{\Omega}) : \langle \Omega, V(\beta) \rangle = F_{W,\rho}(\beta) \}$. The singleton of this $\mathcal{O}^*(\beta)$ is guaranteed by Theorem 3.2.

A.3 Discussions on Assumption 2.1

Assumption 2.1(i) is standard in the machine learning literature and it holds naturally in many classification and regression tasks. Regarding Assumption 2.1(ii), the non-negativity of $\hat{\Omega}$ follows directly if the weighting function $\omega$ is also non-negative. As shown below, positive definiteness holds under mild conditions of the training data and the weighting kernel.

Lemma A.3 (Positive definite nominal weighting matrix). Suppose that the weighting function $\omega$ can be represented by a strictly positive definite kernel $K : \mathcal{Z} \times \mathcal{Z} \rightarrow \mathbb{R}$ in the sense that $\omega(\hat{z}_i) = K(z_0, \hat{z}_i)$ for $i = 1, \ldots, N$ and for some distinct covariates $(z_0, \hat{z}_1, \ldots, \hat{z}_N) \in \mathcal{Z}^{N+1}$. Then

$$\hat{\Omega} \triangleq \begin{bmatrix}
K(z_0, z_0) & K(z_0, \hat{z}_1) & \cdots & K(z_0, \hat{z}_N) \\
K(\hat{z}_1, z_0) & K(\hat{z}_1, \hat{z}_1) & \cdots & K(\hat{z}_1, \hat{z}_N) \\
\vdots & \vdots & \ddots & \vdots \\
K(\hat{z}_N, z_0) & K(\hat{z}_N, \hat{z}_1) & \cdots & K(\hat{z}_N, \hat{z}_N)
\end{bmatrix}$$

is positive definite with $\hat{\Omega}_{i0} = \hat{\Omega}_{0i} = \omega(\hat{z}_i)$ for $i = 1, \ldots, N$.

The proof of Lemma A.3 follows by noticing that $\hat{\Omega}$ is the Gram matrix of a kernel $K$, and hence $\hat{\Omega}$ is a positive definite matrix [38, pp. 2392].

The next result shows that given any weight $\omega(\hat{z}_i)$, there exists a matrix $\hat{\Omega}$ satisfying Assumption 2.1(ii). Notice that it is always possible to choose the numbers $d_k$ satisfying the specified conditions below.

Lemma A.4 (Existence of $\hat{\Omega}$). Given any nonnegative weights $\omega(\hat{z}_i)$ for $i = 1, \ldots, N$, let $A$ be a symmetric matrix with all entries zero except for those on the first row and first column, and on the diagonal as follows

$$A \triangleq \begin{bmatrix}
d_0 & \omega(\hat{z}_1) & \cdots & \omega(\hat{z}_N) \\
\omega(\hat{z}_1) & d_1 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
\omega(\hat{z}_N) & 0 & \cdots & d_N
\end{bmatrix}.$$

Then $A$ is positive definite and nonnegative if $d_k$ are chosen such that $d_0 > 0$, $d_1 \Delta_1 > \omega(\hat{z}_1)^2$, and $d_k \Delta_k > d_1 \ldots d_{k-1} \omega(\hat{z}_k)^2$ for $k = 2, \ldots, N+1$, where $\Delta_k$ denotes the $k$th leading principal minor of the matrix $A$ which is independent of $d_k, \ldots, d_{N+1}$.

Proof of Lemma A.4 It is clear that $A$ is symmetric and nonnegative. The conditions on $d_k$ also ensures that $\Delta_k > 0$ for every $k = 1, \ldots, N + 1$. Thus $A$ is positive definite as well.

For the given non-negative weights $\omega(\hat{z}_i)$, Lemma A.4 shows that there are infinitely many doubly non-negative matrices $\hat{\Omega}$ that satisfy the condition $\Omega_{i0} = \hat{\Omega}_{0i} = \omega(\hat{z}_i)$ for $i = 1, \ldots, N$. 
In practice, the choice of \( \hat{\Omega} \) can impact the performance of our robust estimate, and fine-tuning the elements of \( \hat{\Omega} \) may improve the predictive power. For the scope of this paper, we aim to improve the robustness of NW and LLR estimators and therefore will mainly focus on the scenario described in Lemma A.3 where \( \hat{\Omega} \) is given by a strictly positive definite kernel.

\section{Implementation Details}

\subsection{Gradient Information}

We provide here the gradient information for the convex problems (8) and (12). This information can be exploited to derive fast numerical routines to find the optimal dual solution \( \gamma^* \).

Denote by \( g \) the objective function of problem (8). The gradient of \( g \) is

\[ \nabla g(\gamma) = \rho - \log \det(\gamma^{-1} \hat{\Omega}^{1/2} V(\beta) \hat{\Omega}^{1/2}) - \frac{1}{\gamma} \langle (\gamma^{-1} \hat{\Omega}^{1/2} V(\beta) \hat{\Omega}^{1/2})^{-1}, \hat{\Omega}^{1/2} V(\beta) \hat{\Omega}^{1/2} \rangle. \]

Let \( h \) be the objective function of problem (12). The gradient of \( h \) is

\[ \nabla h(\gamma) = \rho - \langle \hat{\Omega}, (\gamma^* \gamma^* I - V(\beta))^{-1} \rangle. \]

\subsection{Implementation}

Following Lemma 3.5, for a fixed value of \( \beta \), we can rewrite the low-rank matrix \( V(\beta) \) using the eigenvalue decomposition \( V(\beta) = Q \Lambda Q^\top \), where \( \Lambda \in \mathbb{R}^{2 \times 2} \) is a diagonal matrix and \( Q \in \mathbb{R}^{(N+1) \times 2} \) is an orthonormal matrix. Therefore, we can leverage the Woodbury matrix identity to implement the inverse in gradient computation (e.g., \( \nabla g \) and \( \nabla h \)) efficiently. For examples, (i)

\[ (\gamma I - V(\beta))^{-1} = \gamma^{-1} I - \gamma^{-2} Q (\Lambda^{-1} + \gamma^{-1} I_2)^{-1} Q^\top, \]

where we have exploited the fact that \( Q^\top Q = I_2 \) with \( I_2 \) being the \( 2 \times 2 \) identity matrix; and (ii)

\[ (I - \gamma^{-1} \hat{\Omega}^{1/2} V(\beta) \hat{\Omega}^{1/2})^{-1} = I - \hat{\Omega}^{1/2} Q (\Lambda^{-1} + Q^\top \hat{\Omega} Q)^{-1} Q^\top \hat{\Omega}^{1/2}. \]

Therefore, the inverse in gradient (e.g., \( \nabla g \) and \( \nabla h \)) is computed on \( 2 \times 2 \) matrices.

\section{Additional Empirical Results}

\textbf{Details of datasets.} Table 1 lists the detailed statistical characteristics of the datasets used in our experiments.

|                | Abalone | Bank | CPU | Elevators | KIN | POL | Puma | Slice |
|----------------|---------|------|-----|-----------|-----|-----|------|-------|
| #samples       | 4177    | 8192 | 8192| 16599     | 40000| 15000| 8192 | 53500 |
| #features      | 17      | 32   | 21  | 17        | 8   | 26  | 32   | 384   |

\textbf{Further results for the ideal case: no sample perturbation.} We illustrate further empirical results for all 8 datasets and with different nearest neighbor size \( N \) (e.g., similar to Figure 1 with the nearest neighbor size \( N = 50 \)).

- For \( N = 50 \), we illustrate results in Figure 7
- For \( N = 30 \), we illustrate results in Figure 8
- For \( N = 20 \), we illustrate results in Figure 9
- For \( N = 10 \), we illustrate results in Figure 10
Figure 7: Average RMSE for ideal case with no perturbation when $N = 50$ for all 8 datasets.

Figure 8: Average RMSE for ideal case with no perturbation when $N = 30$ for all 8 datasets.

Figure 9: Average RMSE for ideal case with no perturbation when $N = 20$ for all 8 datasets.
Further results for the cases when training samples are perturbed. We illustrate further empirical results for all 8 datasets with different nearest neighbor size $N$ (e.g., similar to Figure 2 where the nearest neighbor size $N = 50$).

- For $N = 50$, we illustrate results in Figure 11.
- For $N = 30$, we illustrate results in Figure 12.
- For $N = 20$, we illustrate results in Figure 13.
- For $N = 10$, we illustrate results in Figure 14.

Figure 11: RMSE for varying perturbation levels $\tau$ where $N = 50$. 
Figure 12: RMSE for varying perturbation levels $\tau$ where $N = 30$.

Figure 13: RMSE for varying perturbation levels $\tau$ where $N = 20$.

Figure 14: RMSE for varying perturbation levels $\tau$ where $N = 10$. 
Further results for the effects of the uncertainty size $\rho$. We illustrate further empirical results for different nearest neighbor size $N$ in all 8 datasets (e.g., similar to Figure 3 where the nearest neighbor size $N = 50$ and the perturbation $\tau = N$). Note that when $\rho = 0$, the reweighting schemes are equivalent to the vanilla NW estimator.

- For $N = 50$, we illustrate results for NW-LogDet and NW-BuresW in Figure 15 and Figure 16, respectively.
- For $N = 30$, we illustrate results for NW-LogDet and NW-BuresW in Figure 17 and Figure 18, respectively.
- For $N = 20$, we illustrate results for NW-LogDet and NW-BuresW in Figure 19 and Figure 20, respectively.
- For $N = 10$, we illustrate results for NW-LogDet and NW-BuresW in Figure 21 and Figure 22, respectively.

![Figure 15: Effects of the uncertainty size $\rho$ on RMSE for NW-LogDet when $N = 50$.](image1)

![Figure 16: Effects of the uncertainty size $\rho$ on RMSE for NW-BuresW when $N = 50$.](image2)
Figure 17: Effects of the uncertainty size $\rho$ on RMSE for NW-LogDet when $N = 30$.

Figure 18: Effects of the uncertainty size $\rho$ on RMSE for NW-BuresW when $N = 30$.

Figure 19: Effects of the uncertainty size $\rho$ on RMSE for NW-LogDet when $N = 20$.  

23
Figure 20: Effects of the uncertainty size $\rho$ on RMSE for NW-BuresW when $N = 20$.

Figure 21: Effects of the uncertainty size $\rho$ on RMSE for NW-LogDet when $N = 10$.

Figure 22: Effects of the uncertainty size $\rho$ on RMSE for NW-BuresW when $N = 10$. 

24
Further results for the effects of the nearest neighbor size $N$. We illustrate further empirical results for different uncertainty size $\rho$ in all 8 datasets (e.g., similar to Figure 4 where $\rho = 0.1$ in the KIN dataset).

- For $\rho = 10$, we illustrate results for NW-LogDet and NW-BuresW in Figure 23 and Figure 24 respectively.

- For $\rho = 1$, we illustrate results for NW-LogDet and NW-BuresW in Figure 25 and Figure 26 respectively.

- For $\rho = 0.1$, we illustrate results for NW-LogDet and NW-BuresW in Figure 27 and Figure 28 respectively.

- For $\rho = 0.01$, we illustrate results for NW-LogDet and NW-BuresW in Figure 29 and Figure 30 respectively.

![Figure 23: Effects of the nearest neighbor size $N$ on RMSE for NW-LogDet when $\rho = 10$.](image)

![Figure 24: Effects of the nearest neighbor size $N$ on RMSE for NW-BuresW when $\rho = 10$.](image)
Figure 25: Effects of the nearest neighbor size $N$ on RMSE for NW-LogDet when $\rho = 1$.

Figure 26: Effects of the nearest neighbor size $N$ on RMSE for NW-BuresW when $\rho = 1$.

Figure 27: Effects of the nearest neighbor size $N$ on RMSE for NW-LogDet when $\rho = 0.1$. 
Figure 28: Effects of the nearest neighbor size $N$ on RMSE for NW-BuresW when $\rho = 0.1$.

Figure 29: Effects of the nearest neighbor size $N$ on RMSE for NW-LogDet when $\rho = 0.01$.

Figure 30: Effects of the nearest neighbor size $N$ on RMSE for NW-BuresW when $\rho = 0.01$. 
Further results for varying shifting w.r.t. $\kappa$. We first illustrate corresponding results for NW-BuresW in Figure 31, similar as results in Figure 5 for NW-LogDet.

We next illustrate further empirical results for different uncertainty size $\rho$ and different perturbation $\tau$ in the KIN dataset (e.g., similar to Figure 5 and Figure 31 where $\rho = 0.1$ for the left plots and $\tau = 0.2N$ for the right plots).

- For NW-LogDet, we illustrate results on effects of perturbation intensity $\kappa$ for different perturbation proportion $\tau$ in Figure 32 and Figure 33 respectively.

- For NW-BuresW, we illustrate results on effects of perturbation intensity $\kappa$ for different perturbation proportion $\tau$ in Figure 34 and Figure 35 respectively.

Figure 31: Effects of perturbation intensity $\kappa$ for NW-BuresW estimate. Left plot: different perturbation $\tau$, right plot: different uncertainty size $\rho$.

Figure 32: Effects of perturbation intensity $\kappa$ for NW-LogDet estimate for different perturbation proportion $\tau$. 

28
Figure 33: Effects of perturbation intensity $\kappa$ for NW-LogDet estimate for different uncertainty size $\rho$.

Figure 34: Effects of perturbation intensity $\kappa$ for NW-BuresW estimate for different perturbation proportion $\tau$.

Figure 35: Effects of perturbation intensity $\kappa$ for NW-BuresW estimate for different uncertainty size $\rho$.
Further results for effects of $N$ on computational time. We illustrate further effects of $N$ on computational time in all 8 datasets (e.g., similar to Figure 6 for the KIN dataset).

- For NW-LogDet, we illustrate further effects of $N$ on computational time in all 8 datasets in Figure 36.
- For NW-BuresW, we illustrate further effects of $N$ on computational time in all 8 datasets in Figure 37.

![Figure 36: Effects of $N$ on computational time for NW-LogDet.](image)

![Figure 37: Effects of $N$ on computational time for NW-BuresW.](image)