Outliers Robustness in Multivariate Orthogonal Regression

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Abstract—This paper deals with the problem of multivariate affine regression in the presence of outliers in the data. The method discussed is based on weighted orthogonal least squares. The weights associated with the data satisfy a suitable optimality criterion and are computed by a two-step algorithm requiring a RANSAC step and a gradient-based optimization step. Issues related to the breakdown point of the method are discussed, and examples of application on various real multidimensional data sets are reported in the paper.

Index Terms—Computer vision, influential observations, orthogonal least squares, outliers, pattern recognition, regression analysis.

I. INTRODUCTION

THE purpose of regression analysis is to fit equations to observed data. Affine regression, in particular, deals with the problem of determining an affine relation among a set of noisy multidimensional data points (see [2]). This problem has of course a very long history, dating back to Gauss and the Least Squares (LS) method, and is still playing a key role in a number of engineering endeavors such as numerical modeling, quality control, computer vision, and statistical data analysis in general.

More recently, issues related to the sensitivity of a regression method with respect to inconsistent data (often referred to as outliers or gross error data) led to the introduction of the so called *robust regression methods*. Robust regression is concerned with developing estimators that are not strongly affected by outliers and are insensitive to the underlying noise distribution. The theory of multidimensional robust estimators was developed in the seventies and the basic robust estimators are classified as M-estimators, R-estimators, and L-estimators [7]. The widely used M-estimators, in particular, minimize the sum of a symmetric positive definite unimodal function $\rho(r_i)$ of the estimation residuals r_i [5].

This class of robust estimators, however, do not perform well with respect to the concept of *breakdown point*. The breakdown point of a regression method is defined as the smallest relative amount of outlier contamination that may force the value of the estimate outside an arbitrary range. For the simple LS estimator, the breakdown point is zero, meaning that one single outlier is sufficient to move the estimate outside any predefined bound. For the class of M-estimators, the breakdown point

is still zero [13], while generalized M-estimators (GM-estimators) have breakdown point no better than a value that decreases with the number of regression coefficients [11]. A robust estimator achieving breakdown point 0.5 (which is the highest possible value for breakdown) is the Least Median of Squares (LMedS) estimator [13], which minimizes the median of the squared residuals. Although LMedS is now widely used in applications, some problems and limitations of the method have been pointed out in the literature. In particular, the robustness of LMedS is contingent upon the existence of at least one subset of the data carrying the correct (i.e., error free) model; when noise corrupts all the data, as in the gaussian case, the quality of the initial model estimate degrades and could lead to incorrect decisions. This problem is also common to regression methods based on the RANSAC paradigm (see the survey [12] for a comparison between LMedS and RANSAC) which is discussed in some detail in the sequel. Also, the convergence rate of LMedS is critical for large data sets, as the algorithm examines all the possible combinations of pairs of observations and computes an estimator for each combination, which includes performing a computer sort.

Much less research attention has been devoted to robust orthogonal regression, which is the subject of this paper. In this area, the recent studies of [14] and [15] focus the attention on case deletion diagnostic and influence measures for the deletion of one observation at a time. In this paper, we examine the problem of multidimensional orthogonal regression and address the issue of robustness introducing the Optimal Weighted Orthogonal Least Squares (OWOLS) algorithm, which provides high breakdown point maintaining the gaussian efficiency of LS regression methods and yielding the optimal weights as a by-product of the regression procedure. The so-found optimal weights represent influence coefficients of the data points on the final estimation residual, and take into account simultaneous deletion of multiple observations. The proposed technique is then tested on various multidimensional real data sets found in the literature.

The paper is organized as follows. Section II contains preliminary results and a closed-form solution to the k -dimensional weighted orthogonal fitting problem. In Section III, the main result concerning the optimal robust estimator is presented, while examples of application of the proposed methodology to several real data sets are presented in Section IV.

II. WEIGHTED ORTHOGONAL LS REGRESSION

In this section, we present a closed-form solution to the problem of determining the k -dimensional affine set closest in the Orthogonal Least Squares (OLS) sense to a set of N

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TABLE I
WEISS TWO DIMENSIONAL
DATA

i	x_1	x_2	i	x_1	x_2	i	x_1	x_2
1	-0.9	1.3	10	-0.3	1.5	19	0.6	0.6
2	-0.9	1.4	11	-0.2	1.4	20	0.9	0.7
3	-0.8	1.4	12	-0.1	1.3	21	0.9	0.6
4	-0.8	1.3	13	0	1.2	22	0.7	0.5
5	-0.9	1.7	14	0.1	1.1	23	0.8	0.4
6	-0.9	1.8	15	0.2	1	24	0.9	0.3
7	-0.6	1.8	16	0.3	0.9	25	0.5	1.8
8	-0.5	1.7	17	0.4	0.8	26	0.6	1.2
9	-0.4	1.6	18	0.6	0.7	*	*	*

Fig. 1. Plot of Weiss data and OWOLS regression line.

points in $\mathbb{R}^n$. This result is related to the Total Least Squares (TLS) problem [4], [17] and it is also known in Computer Vision ([16] gives an alternative proof for the particular case of subspaces—affine sets through the origin—and unitary weights).

Let $X \in \mathbb{R}^{n \times N}$ be a matrix containing by columns the N observed data $x_i \in \mathbb{R}^n$, $i = 1, \dots, N$ and let a k -dimensional affine set be described by

$$\mathcal{F}_k = \{x \in \mathbb{R}^n: A^T x = b; A \in \mathcal{Q}^{n \times m}, b \in \mathbb{R}^m\} \quad (1)$$

where $m = n - k$, and $\mathcal{Q}^{n \times m}$ is the set of matrices in $\mathbb{R}^{n \times m}$ whose columns form an orthonormal set. From the definition, it follows for instance that in a n -dimensional space $\mathcal{F}_{n-1}$ represents a hyperplane, $\mathcal{F}_1$ represents a line and $\mathcal{F}_0$ represents a point.

If nonnegative weights $w_i \geq 0$ are associated to each data point, the weighted OLS (WOLS) problem is posed as

$$(A^*, b^*) = \arg \min_{A \in \mathcal{Q}^{n \times m}, b \in \mathbb{R}^m} f(A, b, X, w) \quad (2)$$

where

$$\begin{aligned} f(A, b, X, w) &= \sum_{i=1}^N w_i^2 \|A^T x_i - b\|^2 \\ &= \|(A^T X - bu^T)W\|_F^2 \end{aligned} \quad (3)$$

with $w = [w_1, w_2, \dots, w_N]^T$, $u \in \mathbb{R}^N = [1, 1, \dots, 1]^T$, $W = \text{diag}\{w\}$, and the subscript F indicates the Frobenius matrix

TABLE II
OPTIMAL WEIGHTS FOR THE WEISS DATA

i	$\bar{w}_i$	i	$\bar{w}_i$	i	$\bar{w}_i$
1	0.0097	10	1.0000	19	1.0000
2	0.0127	11	1.0000	20	0.0403
3	0.0173	12	1.0000	21	0.0721
4	0.0127	13	1.0000	22	1.0000
5	0.0392	14	1.0000	23	1.0000
6	0.0706	15	1.0000	24	1.0000
7	1.0000	16	1.0000	25	0.0051
8	1.0000	17	1.0000	26	0.0175
9	1.0000	18	0.7025	*	*

TABLE III
HAWKINS, BRADU AND KASS FOUR DIMENSIONAL DATA, AND OPTIMAL
WEIGHTS $\bar{w}_i$ FROM OWOLS REGRESSION

i	x_1	x_2	x_3	x_4	$\bar{w}_i$	i	x_1	x_2	x_3	x_4	$\bar{w}_i$
1	10.1	19.6	28.3	9.7	0.0061	39	2.1	0	1.2	-0.7	1.0000
2	9.5	20.5	28.9	10.1	0.0056	40	0.5	2	1.2	-0.5	1.0000
3	10.7	20.2	31	10.3	0.0055	41	3.4	1.6	2.9	-0.1	1.0000
4	9.9	21.5	31.7	9.5	0.0061	42	0.3	1	2.7	-0.7	1.0000
5	10.3	21.1	31.1	10	0.0057	43	0.1	3.3	0.9	0.6	0.7641
6	10.8	20.4	29.2	10	0.0059	44	1.8	0.5	3.2	-0.7	1.0000
7	10.5	20.9	29.1	10.8	0.0050	45	1.9	0.1	0.6	-0.5	1.0000
8	9.9	19.6	28.8	10.3	0.0054	46	1.8	0.5	3	-0.4	1.0000
9	9.7	20.7	31	9.6	0.0060	47	3	0.1	0.8	-0.9	0.4401
10	9.3	19.7	30.3	9.9	0.0054	48	3.1	1.6	3	0.1	1.0000
11	11	24	35	-0.2	1.0000	49	3.1	2.5	1.9	0.9	1.0000
12	12	23	37	-0.4	1.0000	50	2.1	2.8	2.9	-0.4	1.0000
13	12	26	34	0.7	1.0000	51	2.3	1.5	0.4	0.7	1.0000
14	11	34	34	0.1	1.0000	52	3.3	0.6	1.2	-0.5	0.8960
15	3.4	2.9	2.1	-0.4	0.9753	53	0.3	0.4	3.3	0.7	0.3011
16	3.1	2.2	0.3	0.6	1.0000	54	1.1	3	0.3	0.7	1.0000
17	0	1.6	0.2	-0.2	1.0000	55	0.5	2.4	0.9	0	1.0000
18	2.3	1.6	2	0	1.0000	56	1.8	3.2	0.9	0.1	1.0000
19	0.8	2.9	1.6	0.1	1.0000	57	1.8	0.7	0.7	0.7	1.0000
20	3.1	3.4	2.2	0.4	1.0000	58	2.4	3.4	1.5	-0.1	1.0000
21	2.6	2.2	1.9	0.9	1.0000	59	1.6	2.1	3	-0.3	1.0000
22	0.4	3.2	1.9	0.3	1.0000	60	0.3	1.5	3.3	-0.9	1.0000
23	2	2.3	0.8	-0.8	0.6553	61	0.4	3.4	3	-0.3	1.0000
24	1.3	2.3	0.5	0.7	1.0000	62	0.9	0.1	0.3	0.6	0.8883
25	1	0	0.4	-0.3	1.0000	63	1.1	2.7	0.2	-0.3	1.0000
26	0.9	3.3	2.5	-0.8	1.0000	64	2.8	3	2.9	-0.5	1.0000
27	3.3	2.5	2.9	-0.7	0.6761	65	2	0.7	2.7	0.6	0.9491
28	1.8	0.8	2	0.3	1.0000	66	0.2	1.8	0.8	-0.9	1.0000
29	1.2	0.9	0.8	0.3	1.0000	67	1.6	2	1.2	-0.7	1.0000
30	1.2	0.7	3.4	-0.3	1.0000	68	0.1	0	1.1	0.6	0.4791
31	3.1	1.4	1	0	1.0000	69	2	0.6	0.3	0.2	1.0000
32	0.5	2.4	0.3	-0.4	1.0000	70	1	2.2	2.9	0.7	0.5188
33	1.5	3.1	1.5	-0.6	1.0000	71	2.2	2.5	2.3	0.2	1.0000
34	0.4	0	0.7	-0.7	1.0000	72	0.6	2	1.5	-0.2	1.0000
35	3.1	2.4	3	0.3	1.0000	73	0.3	1.7	2.2	0.4	0.7570
36	1.1	2.2	2.7	-1	1.0000	74	0	2.2	1.6	-0.9	1.0000
37	0.1	3	2.6	-0.6	1.0000	75	0.3	0.4	2.6	0.2	0.8942
38	1.5	1.2	0.2	0.9	0.7477						

norm ($\|Y\|_F^2 = \text{Tr}(YY') = \text{Tr}(Y'Y)$, where $\text{Tr}(\cdot)$ is the trace operator). The following proposition characterizes the solution of the WOLS regression problem.

Proposition 1: The optimal solution (A^*, b^*) of (2) is given by

$$A^* = [a_1^*, a_2^*, \dots, a_m^*]; \quad b^* = \frac{1}{\nu} A^{*T} X W^2 u \quad (4)$$

where $a_1^*, a_2^*, \dots, a_m^*$ are the m unit norm eigenvectors associated with the first m smallest eigenvalues of the positive semidefinite matrix

$$H = X \left(W^2 = \frac{1}{\nu} W^2 u u^T W^2 \right) X^T \quad (5)$$

and $\nu = \sum_{i=1}^N w_i^2$. The value of the objective function at the optimum is given by

$$f^*(X, w) = f(A^*, b^*, X, w) = \sum_{i=1}^m \lambda_i \quad (6)$$

where λ_i are the eigenvalues of H arranged in increasing order.

Proof: See Appendix A.

The regression estimate found in (4) will be referred to as WOLS regressor, while in the case of unitary weights, we recover the standard OLS regression. In the following section, we consider the variation of the value (6) of the objective function at an optimal point, with respect to variations of the weights vector. This will lead to an “influence-adjustment” scheme where a set of suitably computed optimal weights provide information about the influence on the regression of each observation. Data corresponding to low weights are influential observations for the regression that can potentially be removed from the sample space.

III. OPTIMAL WEIGHTED OLS

The WOLS estimator introduced in the previous section is of course not a robust regressor, since it is based on LS minimization having zero breakdown point, as previously discussed. Consider now the following estimator (OWOLS)

$$(\bar{A}, \bar{b}) = \arg \min_{A \in \mathbb{Q}^{n \times m}, b \in \mathbb{R}^m} f(A, b, X, \bar{w}) \quad (7)$$

where

$$\bar{w} = \arg \min_{w \in \mathbb{R}^N} f^*(X, w) \quad (8)$$

subject to:

$$\sum_{i=1}^N w_i \geq N - N_o, \quad (9)$$

$$w_i \in [0, 1]; \quad \forall i. \quad (10)$$

In (9), N_o is an estimated upper bound on the number of outliers present in the data. Clearly, OWOLS is still a weighted OLS estimator, where the weights $\bar{w}$ are computed so to satisfy the optimality condition (8) under the constraints (9), (10). A vector w satisfying (9), (10) will be called in the sequel a *feasible* weight vector. The usual definition of breakdown point [1] is based on the variation of the regression coefficients vector returned by the regression estimator; this is no longer practical in our general case, as a matrix A and a vector b are returned by the OWOLS estimator. Let us introduce the following measure of robustness—denoted in the sequel as *residual breakdown point*—defined in terms of the final regression residual $\bar{f}(X)$, which is the value of the objective function in (7) at the optimum

$$\bar{f}(X) = f(\bar{A}, \bar{b}, X, \bar{w}). \quad (11)$$

Let $Z \in \mathbb{R}^{n \times N}$ be any sample of N observations, and let $\bar{f}(Z)$ be the value of the final regression residual when a regression estimator $\mathcal{T}$ is applied to Z . Consider now all possible corrupted

Fig. 2. Residual plot of the OLS estimator on the Hawkins, Bradu and Kass data. $A^T = [0.9567, 0.0106, -0.2895, -0.0265]$, $b = 1.0000$. Final estimation error $f^* = 67.63$.

Fig. 3. Residual plot of the OWOLS estimator on the Hawkins, Bradu and Kass data. $A^T = [-0.2360, -0.0609, 0.1128, 0.9633]$, $b = -0.3852$. Final estimation error $\bar{f} = 13.08$.

samples $\tilde{Z}$ obtained upon replacing any p of the original observations by arbitrary values. The residual breakpoint $\epsilon(\mathcal{T}, Z)$ is defined as

$$\epsilon(\mathcal{T}, Z) = \min \left\{ \frac{p}{N} : \sup_{\tilde{Z}} |\bar{f}(Z) - \bar{f}(\tilde{Z})| = \infty \right\}. \quad (12)$$

Proposition 2: For $N_o < 0.5N$, the residual breakdown point of the OWOLS regression estimator is $\epsilon = N_o/N$.

Proof: We show that for any $p < N_o$, $|\bar{f}(Z) - \bar{f}(\tilde{Z})|$ is bounded for any choice of $\tilde{Z}$. Let $\bar{w}$ be the global minimum solution of (8), then

$$\bar{f}(Z) = f^*(Z, \bar{w}) \leq f^*(Z, w), \quad \forall \text{ feasible } w. \quad (13)$$

If one defines $f_{\text{sup}} = \sup f^*(Z, w)$ over all feasible w , then

$$f^*(Z, w) \leq f_{\text{sup}}, \quad \forall \text{ feasible } w. \quad (14)$$

For any corrupted sample $\tilde{Z}$, let $\tilde{w}$ be a vector of weights having zero at the p locations of the corrupted observations and one elsewhere, then $\tilde{w}$ is feasible and

$$f^*(Z, \tilde{w}) = f^*(\tilde{Z}, \tilde{w}) \geq \bar{f}(\tilde{Z}). \quad (15)$$

From (14) and (15), it follows that

$$\begin{aligned} |\bar{f}(Z) - \bar{f}(\tilde{Z})| &\leq |\bar{f}(Z)| + |\bar{f}(\tilde{Z})| \leq |\bar{f}(Z)| \\ &\quad + |f^*(Z, \tilde{w})| \leq |\bar{f}(Z)| + f_{\text{sup}} \end{aligned} \quad (16)$$

TABLE IV
AIRCRAFT DATA AND OPTIMAL WEIGHTS $\bar{w}_i$ FROM THE OWOLS ESTIMATOR

i	x_1	x_2	x_3	x_4	x_5	$\bar{w}_i$
1	6.3	1.7	8176	4500	2.76	1.0000
2	6.0	1.9	6699	3120	4.76	1.0000
3	5.9	1.5	9663	6300	8.75	1.0000
4	3.0	1.2	12837	9800	7.78	1.0000
5	5.0	1.8	10205	4900	6.18	1.0000
6	6.3	2.0	14890	6500	9.50	0.9403
7	5.6	1.6	13836	8920	5.14	0.8037
8	3.6	1.2	11628	14500	4.76	1.0000
9	2.0	1.4	15225	14800	16.70	1.0000
10	2.9	2.3	18691	10900	27.68	1.0000
11	2.2	1.9	19350	16000	26.64	1.0000
12	3.9	2.6	20638	16000	13.71	1.0000
13	4.5	2.0	12843	7800	12.31	1.0000
14	4.3	9.7	13384	17900	15.73	0.0040
15	4.0	2.9	13307	10500	13.59	0.1697
16	3.2	4.3	29855	24500	51.90	1.0000
17	4.3	4.3	29277	30000	20.78	1.0000
18	2.4	2.6	24651	24500	29.82	1.0000
19	2.8	3.7	28539	34000	32.78	1.0000
20	3.9	3.3	8085	8160	10.12	0.0476
21	2.8	3.9	30328	35800	27.84	1.0000
22	1.6	4.1	46172	37000	107.10	0.0346
23	3.4	2.5	17836	19600	11.19	1.0000

Fig. 4. Residual plots of the OLS estimator on the aircraft data.

Fig. 5. Residual plots of the OWOLS estimator on the aircraft data.

therefore $|\bar{f}(Z) - \bar{f}(\tilde{Z})|$ is bounded for any corrupted sample $\tilde{Z}$.

Proposition 2 indicates that if a global solution of (8) is found, the resulting OWOLS estimate has a residual breakdown point as high as 0.5. The requirement $N_o < 0.5N$ is needed because no robust regression method can work if more than half of the

data is corrupted by outliers, see for instance [13]. Notice also that each weight w_i is constrained in the interval $[0, 1]$, and that the constraint (9) implies that no more than N_o observations can be assigned a zero weight, that is no more than N_o observations may be removed from the sample space. A method for the numerical solution of (8) is discussed in the next section.

A. Computing the Optimal Weights

Determining the optimal weight vector w requires the numerical solution of the nonlinear optimization problem (8). The proposed procedure is divided into two steps.

Step 1: Use the RANSAC paradigm on the data to obtain a crude estimate of the number of influential observations N_o , and an initial feasible vector of weights w_0 .

Step 2: Use a gradient based optimization algorithm to solve (8) for the optimal weights, starting for the given initial feasible point w_0 .

Step 1: RANSAC (Random Sample Consensus) is a well known smoothing procedure [3] which uses as small an initial data set as feasible to instantiate a model, and enlarges this set with consistent data when possible. In the problem at hand, the minimum number of observations needed to determine a k -dimensional affine set is given by $n_p = k + 1$, and the RANSAC procedure is applied as follows.

- Randomly select a subset $X^{(1)}$ of n_p observations from X and use $X^{(1)}$ to instantiate a model.
- Determine the subset $X^{(2)}$ (the *consensus set*) of data that are within a δ -error tolerance from the instantiated model.
- Repeat the above steps N_s times and exit with the consensus set of greatest cardinality, $X^{(*)}$.
- Determine a new model based on the data in $X^{(*)}$ and rank the observations with respect to their residuals r_i from this model. A threshold on the residuals is used to estimate the number of outliers N_o .
- An initial feasible weight vector w_0 is determined as $w_{0,i} = \alpha e^{-r_i/\beta}$, where α, β are real parameters that are numerically determined such that the resulting w_0 is feasible, that is

$$\sum_{i=1}^N w_{0,i} \geq N - N_o; \quad w_{0,i} \in [0; 1].$$

The unspecified parameters used in the above procedure, namely the tolerance δ used to determine whether a point is compatible with a model and the number N_s of random subsets to try, are problem dependent and clear indications on how to choose them are reported in [3].

Step 2: Once the initial feasible weight vector w_0 is given, any gradient based optimization method for non linear problems under linear constraints may be used to solve (8). In particular, closed form expressions for the gradient of the objective function $f^*(X, w)$ with respect to the weights are here derived as follows. Recalling (6), we have that

$$f^*(X, w) = \sum_{i=1}^m \lambda_i(H);$$

$$H = X \left(W^2 - \frac{1}{\nu} W^2 w w^T W^2 \right) X^T$$

therefore

$$\frac{\partial f^*}{\partial w_j} = \sum_{i=1}^m \frac{\partial \lambda_i(H)}{\partial w_j}.$$

Using a standard formula for eigenvalues derivatives [8] we have that

$$\frac{\partial \lambda_i(H)}{\partial w_j} = h_i^T \frac{\partial H}{\partial w_j} h_i \quad (17)$$

where h_i is the unit norm eigenvector associated with λ_i . The matrix derivative in (17) has the following expression

$$\frac{\partial H}{\partial w_j} = 2w_j \left(x_j x_j^T + \frac{1}{\nu^2} (Xw^2)(Xw^2)^T - \frac{1}{\nu} (q_j + q_j^T) \right)$$

where $q_j = Xw^2 x_j^T$, and $w^2 = [w_1^2, w_2^2, \dots, w_N^2]^T$.

IV. EXAMPLES

In this section, we describe the application of the presented procedure to the analysis of several real data sets encountered in the literature. We start with a two-dimensional (2-D) line-fitting example presented in [9] and [18]; the data are listed in Table I and displayed in Fig. 1.

Assuming an *a priori* fraction of outlier contamination equal to $\gamma = 30\%$, the *a priori* probability that a randomly selected data point is an inlier is equal to $\eta = 1 - \gamma = 0.7$. The estimated number N_s of subsets trials ensuring with probability $z = 0.95$ that at least one of the selected subsets is an in-model set is approximately $N_s = 3\eta^{-n_p} \simeq 6$ (see [3]). The N_s RANSAC trials yielded a best consensus set of cardinality 16. Data from the consensus set are then used to instantiate a new model, from which the estimate $N_o = 10$ and the initial weight vector w_0 are obtained. The numerical solution of (8) with starting point w_0 yielded the optimal weight vector $\bar{w}$ listed in Table II. The optimal regression parameters are $A^T = [-0.7046, -0.7096]$, $b = -0.8531$, and the regression line is shown in Fig. 1.

In this 2-D setting, the problem may of course seem to be “overkilled,” as the outlying points can easily be spotted by plotting the data. This is no longer true for data sets in spaces of dimension higher than three. It should be emphasized that in the multidimensional case, even the analysis of the scatter (or residual) plot does not help in general in discovering regression outliers that are leverage points (points with very high effect on the estimator, capable of tilting the estimate, see [13]).

We next analyze the data generated by Hawkins *et al.* [6] for illustrating the merits of a robust technique. This artificial data set offers the advantage that at least the position of the bad points is known, which avoids some of the controversies that are inherent in the analysis of real data. The Hawkins, Bradu and Kass data set (Table III) consists of 75 observations in four dimension. The first ten observations are bad leverage points while the remaining observations are good data. The problem is in this case to fit a hyperplane (affine set of dimension $k = n - 1$) to the observed data. In Fig. 2, we plot the regression residuals from the model obtained from the standard OLS estimator: the leverage point data are masked and do not show up from the residual plot.

Application of the RANSAC procedure (Step 1) to these data yields an estimated number of outliers $N_o = 14$ and an initial weights vector w_0 . Solving (8) (Step 2) eventually gives the optimal weight vector $\bar{w}$ listed in Table III. From the analysis of the optimal weights, the first ten observations are immediately pinpointed as the outliers in the data. The residual plot of the OWOLS estimator is shown in Fig. 3.

As a final example, we analyze a real data set of $N = 23$ five-dimensional observations relating the aspect ratio, lift-to-drag ratio, weight (in pounds), maximal thrust and cost (units of \$100 000) of 23 single-engine aircraft built over the years 1947–1979. The data are taken from [13] and listed in Table IV. Again in this case, we look for the $(n - 1)$ -dimensional affine set that explains the data. The application of the OWOLS regression yields the optimal weights reported in Table IV, and the regression parameters $A^T = [0.3474, -0.9375, 0.0001, 0.0000, 0.0221]$, $b = 1.4022$. In Figs. 4 and 5, the residual plots of the OLS regression and the OWOLS regression are compared. From the plot in Fig. 5, we may conclude that, according to the OWOLS procedure, the observations 14, 20, and 22 may be considered as outliers, and a better fit is obtained by giving to these observations an appropriately low weight, see Table IV.

V. CONCLUSIONS

In this paper, we discussed the problem of affine orthogonal regression on multidimensional data contaminated by outliers. The proposed solution is based on a two-step procedure. The first step uses the RANSAC paradigm to determine a feasible set of initial weights and an estimate of outlier contamination. In the second step, a gradient based minimization is used to determine the optimal weights and compute the regression parameters. When the minimization step converges to the global optimum, the corresponding regression estimate is guaranteed to have up to 0.5 residual breakpoint. The optimal weights provide a global measure of the influence of the observations on the final estimation residual. We remark however that the convergence to the global optimum cannot in general be guaranteed, and that the robustness of the estimator strongly relies on the step one RANSAC phase. Tests performed on various real data sets confirmed the efficiency and reliability of the proposed method for data sets of medium/moderate size.

APPENDIX

PROOF OF PROPOSITION 1

We here present a Proof of Proposition 1 based on Lagrange multipliers. Let us rewrite (2), with the unit norm constraints on the columns of A

$$\begin{aligned} \min_{A,b} f(A,b,X,w) \\ &= \sum_{i=1}^N w_i^2 \|A^T x_i - b\|^2 \\ &= \|(A^T X - bu')W\|_F^2 \quad (18) \\ \text{subject to: } &a_i^T a_i = 1, \quad i = 1, \dots, m. \quad (19) \end{aligned}$$

Letting $\Lambda = \text{diag} \{\lambda_1, \lambda_2, \dots, \lambda_m\}$ be a diagonal matrix having the Lagrange multipliers on the diagonal, the Lagrangian function for problem (18), (19) may be easily written as

$$\mathcal{L} = f(A, b, X, w) - \text{Tr} [(A^T A - I)\Lambda]. \quad (20)$$

Substituting for f , the lagrangian can be rewritten as

$$\begin{aligned} \mathcal{L} &= \text{Tr} [(A^T X - bu^T)W^2(X^T A - ub^T) - A^T A\Lambda + \Lambda] \\ &= \text{Tr} (A^T XW^2X^T A - 2A^T XW^2ub^T + \nu bb^T \\ &\quad - A^T A\Lambda + \Lambda). \end{aligned}$$

The necessary conditions for optimality require that the gradient of the lagrangian be zero (see for instance [10]), therefore

$$\nabla_A \mathcal{L} = 2A^T XW^2X^T - 2bu^T W^2X^T - 2\Lambda A^T = 0 \quad (21)$$

$$\nabla_b \mathcal{L} = -2A^T XW^2u + 2\nu b = 0. \quad (22)$$

From (22) follows

$$b = \frac{1}{\nu} A^T XW^2u \quad (23)$$

that substituted in (21) yields

$$A^T X \left(W^2 - \frac{1}{\nu} W^2 u u^T W^2 \right) X^T - \Lambda A^T = 0. \quad (24)$$

Defining H as in (5), one gets

$$HA - A\Lambda = 0 \quad (25)$$

which says that the columns of A must be m eigenvectors of the symmetric matrix H , associated with some eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_m$, in order to satisfy the necessary conditions for optimality. Moreover, being H symmetric, the eigenvectors of H form an orthogonal set, and can always be scaled to have euclidean norm one, so to satisfy (19).

Evaluating now the objective (18) at the points that satisfy (23), (25), and (19), one gets

$$\begin{aligned} f(A, b, X, w) &= \text{Tr} \left(A^T XW^2X^T A - \frac{1}{\nu} A^T XW^2 u u^T W^2 X^T A \right) \\ &= \text{Tr} \left[A^T X \left(W^2 - \frac{1}{\nu} W^2 u u^T W^2 \right) X^T A \right] \\ &= \text{Tr}(A^T H A) = (\text{by (25)}) \\ &\quad \text{Tr}(A^T A \Lambda) = (\text{as } a_i^T a_i = 1, \quad i = 1, \dots, m) \\ &= \sum_{i=1}^m \lambda_i. \end{aligned} \quad (26)$$

The objective function f is then equal to the sum of the m selected eigenvalues of H , which is clearly minimized if the first m smallest eigenvalues of H are selected. The optimal matrix

A of the affine set must therefore contain by columns the m orthonormal eigenvectors of H associated to the first m smallest eigenvalues of H . The b parameter is then computed according to (23).

REFERENCES

- [1] D. L. Donoho and P. J. Huber, "The notion of breakdown point," in *A Festschrift for Erich Lehmann*, P. Bickel, K. Doksum, and J. L. Hodges, Eds. Belmont, CA: Wadsworth, 1983.
- [2] N. R. Draper and H. Smith, *Applied Regression Analysis*. New York: Wiley, 1966.
- [3] M. A. Fischler and R. C. Bolles, "Random sample consensus: A paradigm for model fitting with applications to image analysis and automated cartography," *Commun. ACM*, vol. 24, no. 6, pp. 381–395, 1981.
- [4] G. H. Golub and C. F. Van Loan, "An analysis of the total least squares problem," *SIAM J. Numer. Anal.*, vol. 17, no. 6, pp. 883–893, 1980.
- [5] F. R. Hampel, E. M. Ronchetti, and P. J. Rousseeuw, *Robust Statistics: The Approach Based on Influence Functions*. New York: Wiley, 1986.
- [6] D. M. Hawkins, D. Bradu, and G. V. Kass, "Location of several outliers in multiple regression data using elemental sets," *Technometrics*, vol. 26, pp. 197–208, 1984.
- [7] P. J. Huber, *Robust Statistics*. New York: Wiley, 1981.
- [8] J. Juang, P. Ghaemmaghami, and K. B. Lim, "Eigenvalue and eigenvector derivatives of a nondefective matrix," *J. Guidance*, vol. 12, no. 4, pp. 480–486, 1989.
- [9] B. Kamgar-Parsi, B. Kamgar-Parsi, and N. S. Netanyahu, "A nonparametric method for fitting a straight line to a noisy image," *IEEE Trans. Pattern Anal. Mach. Intell.*, vol. 11, no. 9, pp. 998–1001, 1989.
- [10] D. G. Luenberger, *Linear and Nonlinear Programming*. Reading, MA: Addison-Wesley, 1984, ch. 10.
- [11] R. A. Maronna, O. Bustos, and V. Yohai, "Bias and efficiency robustness of general M-estimators for regression with random carriers," in *Smoother Techniques for Curve Estimation*, T. Gasser and M. Rosenblatt, Eds. New York: Springer, 1993.
- [12] P. Meer, D. Mintz, A. Rosenfeld, and D. Yoon Kim, "Robust regression methods for computer vision: a review," *Int. J. Comput. Vis.*, vol. 6, no. 1, pp. 59–70, 1991.
- [13] P. J. Rousseeuw and A. M. Leroy, *Robust Regression and Outlier Detection*. New York: Wiley, 1987.
- [14] L. S. Shapiro and J. M. Brady, "Rejecting outliers and estimating errors in an orthogonal regression framework," *Philos. Trans. R. Soc. London A, Math. Phys., Sci.*, vol. 350, pp. 407–439, 1995.
- [15] P. H. S. Torr and D. W. Murray, "The development and comparison of robust methods for estimating the fundamental matrix," *Int. J. Comput. Vis.*, vol. 24, no. 3, pp. 271–300, 1997.
- [16] S. Ullman and R. Basri, "Recognition by linear combinations of models," *IEEE Trans. Pattern. Anal. Mach. Intell.*, vol. 13, no. 10, pp. 992–1006, 1991.
- [17] S. Van Huffel and J. Vandewalle, *The Total Least Squares Problem: Computational Aspects and Analysis*. Philadelphia, PA: SIAM, 1991.
- [18] I. Weiss, "Line fitting in a noisy image," *IEEE Trans. Pattern Anal. Mach. Intell.*, vol. 11, no. 3, pp. 325–329, 1989.

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