Approximating the Row-Wise Weighted Total Least Squares Linear Regression Solution

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ABSTRACT

Motivated by applications as a kernel of nonlinear regression algorithms, the row-wise weighted total least squares regression problem is examined to find a consistent and accurate estimator. Specifically, the estimator will have a time complexity linear in the number of observations and a space complexity constant in the same value, as the number of observations can be quite large in many modern applications, often many orders of magnitude larger than the number of input and output features. Further, to accommodate large data sets, an algorithm is sought to update an intermediate representation from each observation, allowing for parallelization of the necessary computation. Four related algorithms are proposed, based on approximating the noncentral second moment of the underlying data by a weighted mean, requiring only linear time in the number of observations. Experimental findings show the proposed algorithm to be competitive with existing methods intended to solve other variants of the Total Least Squares problem. Directions for continued iteration and further investigation are proposed.

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INTRODUCTION

Motivation

- Linear regression is useful in economics, scientific modeling, signal denoising, and, recently, machine learning.
- Neural Networks are usually trained with Stochastic Gradient Descent, but this is very slow.
- Extreme Learning Machines (ELMs) (Huang *et al*.) are a recent method of training neural networks very quickly, but it only works for Single-Layer Feed-Forward neural networks, a very restrictive class.
- Extensions to deep neural networks exist, such as Multi-Layer ELM and Deep ELM, but they ignore second-order information, allowing noise to build up over layers. A method of considering which directions are easier or harder to modify may help improve these methods.

Background

- Ordinary Least Squares (OLS) is one common method of linear regression, which minimizes the sum of the squared distances of the points from the regression in the y-direction only.
  - This is equivalent to assuming data is exact in the x-direction, but noisy in the y-direction, and the amount of noise is the same for each observation, but this is often an unreasonable assumption.
- Total Least Squares (TLS) accounts for errors in input variables by minimizing the sum of the squared distances of each point to the regression perpendicular to the regression.
  - This is equivalent to assuming isotropic noise distributions and the same amount of noise for each observation. Noisy often has internal correlations this doesn't account for, however.
- Generalized Total Least Squares (GTLS) allows the noise in the input and output variables to be correlated. This means the noise is assumed to be homoscedastic (the same), but not isotropic (uncorrelated) for all samples.
- Row-Wise Weighted Total Least Squares (RW-TLS) expands on this, allowing each sample to have a different noise distribution. This is called heteroskedasticity, and it provides a very general model, applicable to many situations.

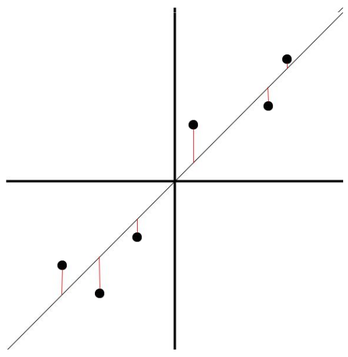


Figure 1. OLS Regression Error. OLS minimizes the sum of the squares of the red distances.

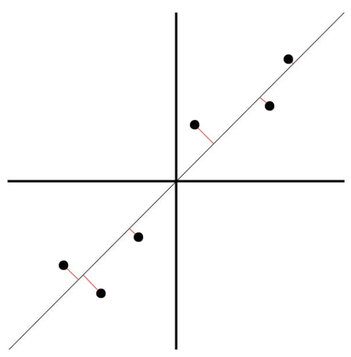


Figure 2. TLS Regression Error. TLS minimizes the sum of the squares of the red distances.

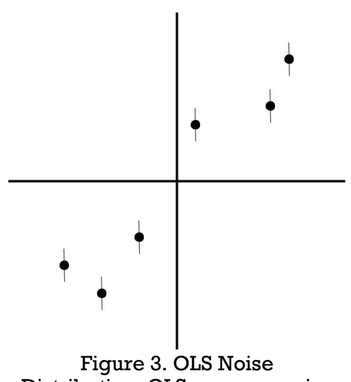


Figure 3. OLS Noise Distribution. OLS assumes noise exists only in the y direction, and that the variance is constant.

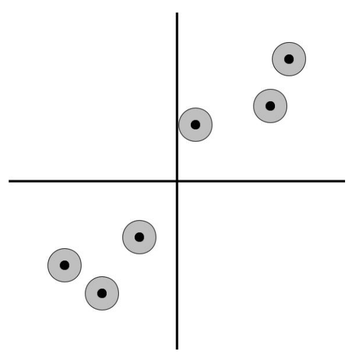


Figure 4. TLS Noise Distribution. TLS assumes noise is isotropic with constant variance across data points.

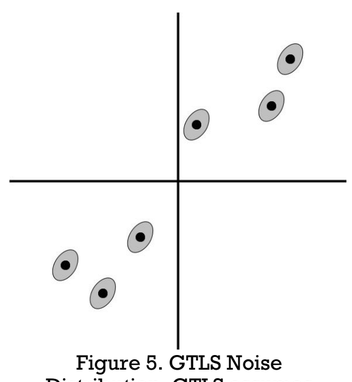


Figure 5. GTLS Noise Distribution. GTLS assumes noise follows the same distribution for each data point.

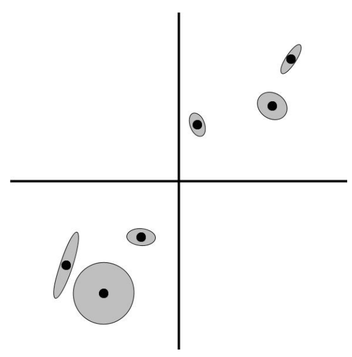


Figure 6. RW-TLS Noise Distribution. RW-TLS allows the noise distributions to vary arbitrarily between data points.

CRITERIA

- Time complexity: linear in number of observations, ideally parallelizable
  - The number of observations can be far greater than the number of features in many applications
- Statistical consistency: convergence to the underlying regression
- Experimental utility: data reconstruction and recovery of weight matrix

PROPOSED APPROACH

- The ideal solution could be recovered from the covariance matrix of the underlying data through eigen-decomposition.
- Each observation provides an estimate of this covariance matrix.
- Estimate the underlying covariance matrix as the mean of the estimates, weighted by their respective precision tensors.
- Alternatively, use a scalar, such as the inverse of the spectral radius, determinant, or trace of the noise covariance matrix as the weight

Algorithm 3 Precision Method

Require: $\{x_n\}_{n=1}^N \in \mathbb{R}^F$, $\{y_n\}_{n=1}^N \in \mathbb{R}^K$, $\{\Sigma_n^{(x)}\}_{n=1}^N \in \mathbb{R}^{F\times F}$, $\{\Sigma_n^{(y)}\}_{n=1}^N \in \mathbb{R}^{K\times K}$, $\{\Sigma_n^{(xy)}\}_{n=1}^N \in \mathbb{R}^{F\times K}$

$Z \leftarrow 0_{(F+K)\times(F+K)}$
$P \leftarrow 0_{(F+K)\times(F+K)\times(F+K)\times(F+K)}$
for $n \leftarrow 1..N$ **do**
  $c \leftarrow \begin{bmatrix} x_n \\ y_n \end{bmatrix}$
  $\Sigma \leftarrow \begin{bmatrix} \Sigma_n^{(x)} & \Sigma_n^{(xy)} \\ \Sigma_n^{(xy)\top} & \Sigma_n^{(y)} \end{bmatrix}$
  $M_{ij} \leftarrow c_i c_j + \Sigma_{ij}$
  $V_{ijkl} \leftarrow c_i c_k \Sigma_{jl} + c_i c_l \Sigma_{jk} + c_j c_k \Sigma_{il} + c_j c_l \Sigma_{ik} + \Sigma_{ik}\Sigma_{jl} + \Sigma_{il}\Sigma_{jk}$
  $Z_{ij} \leftarrow Z_{ij} + V_{ijkl}^{-1} M_{kl}$
  $P \leftarrow P + V^{-1}$
end for
$E_{ij} \leftarrow P_{ijkl}^{-1} Z_{kl}$
$Q, \Lambda \leftarrow \text{EIGEN}(E)$
return $(Q_{:F,:F}^\top)^{-1} Q_{:F,-K:}^\top$

Algorithm 4 Radius Method

Require: $\{x_n\}_{n=1}^N \in \mathbb{R}^F$, $\{y_n\}_{n=1}^N \in \mathbb{R}^K$, $\{\Sigma_n^{(x)}\}_{n=1}^N \in \mathbb{R}^{F\times F}$, $\{\Sigma_n^{(y)}\}_{n=1}^N \in \mathbb{R}^{K\times K}$, $\{\Sigma_n^{(xy)}\}_{n=1}^N \in \mathbb{R}^{F\times K}$

$Z \leftarrow 0_{(F+K)\times(F+K)}$
$w \leftarrow 0$
for $n \leftarrow 1..N$ **do**
  $c \leftarrow \begin{bmatrix} x_n \\ y_n \end{bmatrix}$
  $\Sigma \leftarrow \begin{bmatrix} \Sigma_n^{(x)} & \Sigma_n^{(xy)} \\ \Sigma_n^{(xy)\top} & \Sigma_n^{(y)} \end{bmatrix}$
  $M_{ij} \leftarrow c_i c_j + \Sigma_{ij}$
  $v = \rho(\Sigma)$
  $Z \leftarrow Z + V_{-1}^{-1} M_{A1}$
  $w \leftarrow w + v$
end for
$E_{ij} \leftarrow \frac{1}{w} Z$
$Q, \Lambda \leftarrow \text{EIGEN}(E)$
return $(Q_{:F,:F}^\top)^{-1} Q_{:F,-K:}^\top$

Algorithm 5 Determinant Method

Require: $\{x_n\}_{n=1}^N \in \mathbb{R}^F$, $\{y_n\}_{n=1}^N \in \mathbb{R}^K$, $\{\Sigma_n^{(x)}\}_{n=1}^N \in \mathbb{R}^{F\times F}$, $\{\Sigma_n^{(y)}\}_{n=1}^N \in \mathbb{R}^{K\times K}$, $\{\Sigma_n^{(xy)}\}_{n=1}^N \in \mathbb{R}^{F\times K}$

$Z \leftarrow 0_{(F+K)\times(F+K)}$
$w \leftarrow 0$
for $n \leftarrow 1..N$ **do**
  $c \leftarrow \begin{bmatrix} x_n \\ y_n \end{bmatrix}$
  $\Sigma \leftarrow \begin{bmatrix} \Sigma_n^{(x)} & \Sigma_n^{(xy)} \\ \Sigma_n^{(xy)\top} & \Sigma_n^{(y)} \end{bmatrix}$
  $M_{ij} \leftarrow c_i c_j + \Sigma_{ij}$
  $v = \det(\Sigma)$
  $Z \leftarrow Z + V_{-1}^{-1} M_{A1}$
  $w \leftarrow w + v$
end for
$E_{ij} \leftarrow \frac{1}{w} Z$
$Q, \Lambda \leftarrow \text{EIGEN}(E)$
return $(Q_{:F,:F}^\top)^{-1} Q_{:F,-K:}^\top$

Algorithm 6 Trace Method

Require: $\{x_n\}_{n=1}^N \in \mathbb{R}^F$, $\{y_n\}_{n=1}^N \in \mathbb{R}^K$, $\{\Sigma_n^{(x)}\}_{n=1}^N \in \mathbb{R}^{F\times F}$, $\{\Sigma_n^{(y)}\}_{n=1}^N \in \mathbb{R}^{K\times K}$, $\{\Sigma_n^{(xy)}\}_{n=1}^N \in \mathbb{R}^{F\times K}$

$Z \leftarrow 0_{(F+K)\times(F+K)}$
$w \leftarrow 0$
for $n \leftarrow 1..N$ **do**
  $c \leftarrow \begin{bmatrix} x_n \\ y_n \end{bmatrix}$
  $\Sigma \leftarrow \begin{bmatrix} \Sigma_n^{(x)} & \Sigma_n^{(xy)} \\ \Sigma_n^{(xy)\top} & \Sigma_n^{(y)} \end{bmatrix}$
  $M_{ij} \leftarrow c_i c_j + \Sigma_{ij}$
  $v = \text{Tr}(\Sigma)$
  $Z \leftarrow Z + V_{-1}^{-1} M_{A1}$
  $w \leftarrow w + v$
end for
$E_{ij} \leftarrow \frac{1}{w} Z$
$Q, \Lambda \leftarrow \text{EIGEN}(E)$
return $(Q_{:F,:F}^\top)^{-1} Q_{:F,-K:}^\top$

METHODOLOGY

- 100 datasets were generated with 5 input features and 3 output features, following a normal distribution, with each of 100, 1,000, 10,000, and 100,000 samples.
- Isotropic, homoscedastic, and heteroskedastic noise was added to each dataset.
- TLS, GTLS, and each algorithm were used to fit each dataset.
- The mean and standard error of the weight recovery error and data reconstruction error were reported

Algorithm 1 TLS Algorithm

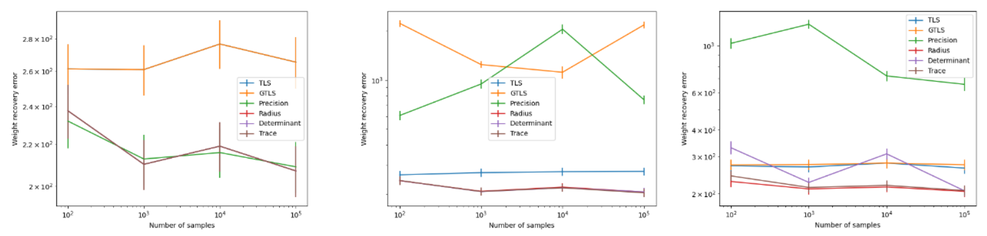
Require: $X \in \mathbb{R}^{N\times F}$, $Y \in \mathbb{R}^{N\times K}$

$C \leftarrow \begin{bmatrix} X \\ Y \end{bmatrix}$
$U, \Sigma, V^\top \leftarrow \text{SVD}(C)$
return $(V_{:F,:F}^\top)^{-1} V_{:F,-K:}^\top$

Algorithm 2 GTLS Algorithm

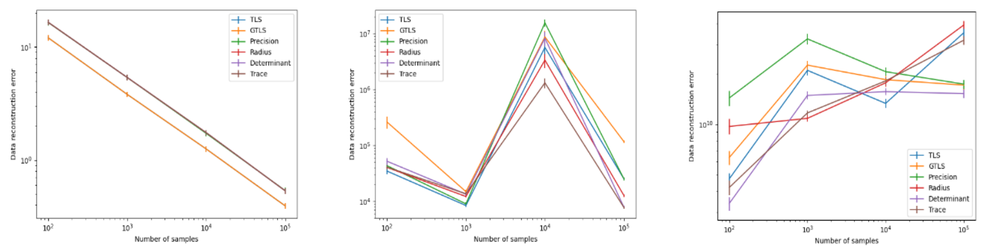
Require: $X \in \mathbb{R}^{N\times F}$, $Y \in \mathbb{R}^{N\times K}$, $\Sigma_X \in \mathbb{R}^{F\times F}$, $\Sigma_Y \in \mathbb{R}^{K\times K}$

$C \leftarrow \begin{bmatrix} X\Sigma_X^{-\frac{1}{2}} \\ Y\Sigma_Y^{-\frac{1}{2}} \end{bmatrix}$
$U, \Sigma, V^\top \leftarrow \text{SVD}(C)$
return $\Sigma_X^{-\frac{1}{2}} (V_{:F,:F}^\top)^{-1} V_{:F,-K:}^\top \Sigma_Y^{\frac{1}{2}}$



(a) Isotropic noise (b) Homoskedastic noise (c) Heteroskedastic noise

Figure 1: Weight recovery error by algorithm and number of samples for (a) isotropic, (b) homoskedastic, and (c) heteroskedastic noise conditions. Error bars represent standard errors of the reported means, across 100 trials.



(a) Isotropic noise (b) Homoskedastic noise (c) Heteroskedastic noise

Figure 2: Data reconstruction error by algorithm and number of samples for (a) isotropic, (b) homoskedastic, and (c) heteroskedastic noise conditions. Error bars represent standard errors of the reported means, across 100 trials.

DISCUSSION

- Experimental results are promising for the proposed algorithms.
- Routes for further improvement exist. For instance:
- The mapping from *E* to the estimated weight matrix is highly nonlinear. Accounting for this nonlinearity may allow for a more statistically efficient estimator.
- Other weights on the influence of each *M* matrix on the estimate of the covariance matrix of the underlying data may yield further improvements in accuracy or computational efficiency.

CONCLUSION

An effective and efficient algorithm for the Row-Wise Weighted Total Least Squares linear regression problem would have applications in various fields, such as economics, image processing, statistical modelling, and machine learning. Approximating the covariance matrix of the underlying data appears to provide an effective basis for such a solution. The proposed algorithms perform comparably with existing methods, and variants of the initial algorithm improve on the experimental accuracy of the algorithm, outperforming existing methods on the sample datasets. Routes exist to further improve on the proposed algorithms. Additional routes exist which may further improve the accuracy and efficiency of the proposed algorithm.

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