Robust Linear Regression by Subquantile Minimization

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April 23, 2023

Presentation Overview

Huber Contamination Model

Problem

The Huber Contamination Model is the following:

$$\hat{P} = (1 - \varepsilon)P + \varepsilon Q \text{ where } \varepsilon \in (0, 0.5)$$

where P and Q represent the general linear models

$$\boldsymbol{y}_P = \mathbf{P}\boldsymbol{\beta}_P + \epsilon_P$$

$$\boldsymbol{y}_Q = \mathbf{Q}\boldsymbol{\beta}_Q + \epsilon_Q$$

$\boldsymbol{\beta}_P$ and $\boldsymbol{\beta}_\mathbf{Q}$ are oracle regressors and ϵ_P and ϵ_Q represent 0-centered gaussian noise.

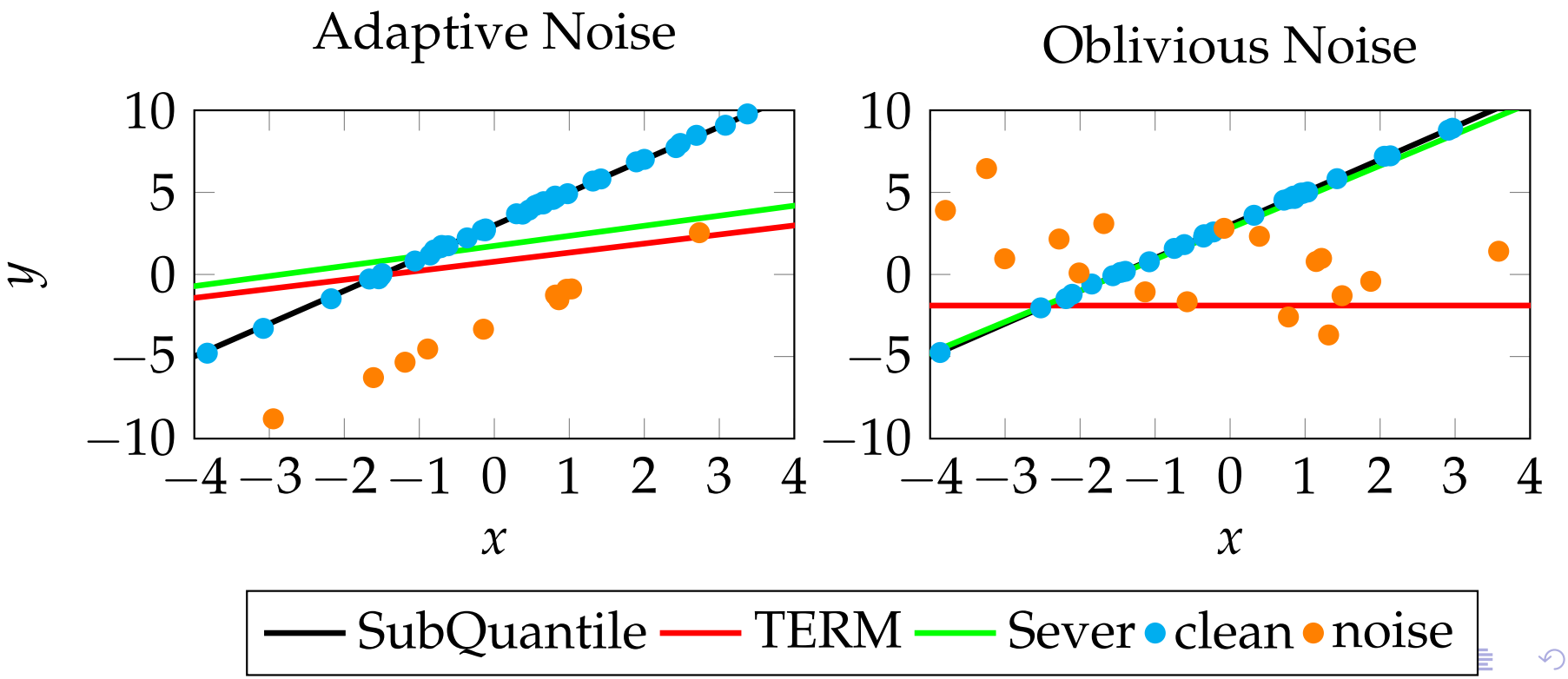
Our goal is to learn a model that learns a good distribution of P from $\hat{P}$

Motivation

Definition

Oblivious Noise is noise generated independent of the target distribution

Adaptive Noise is noise which is generated with knowledge of the target distribution.



Theorem

The expected optimal parameters of the corrupted model $\hat{P}$

$$\mathbb{E}\left[\boldsymbol{X}^{\dagger}\boldsymbol{y}\right] = (1-\varepsilon)\boldsymbol{\beta}_P + \varepsilon\boldsymbol{\beta}_Q$$

where $\boldsymbol{X}^{\dagger} \triangleq \left(\boldsymbol{X}^{\top}\boldsymbol{X}\right)^{-1}\boldsymbol{X}^{\top}$, i.e. the Moore-Penrose Inverse.

This theorem motivates our reasoning for optimizing over the Subquantile. We want a method to reduce ε.

Statistical Preliminaries of the Subquantile

1. The quantile is given as the following:

$$\mathcal{Q}_p = \inf \{x \in \mathbb{R} : p \leq F(x)\}$$

2. Let ℓ be the loss functions. We can now define risk as:

$$\mathcal{U} = \mathbb{E}\left[\ell(f(\boldsymbol{x}; \boldsymbol{\theta}), y)\right]$$

3. The p-Quantile of the Empirical Risk is given by:

$$\mathbb{L}_p = \frac{1}{p}\int_0^p \mathcal{Q}_q(\mathcal{U})dq = \mathbb{E}\left[\mathcal{U}|\mathcal{U} \leq \mathcal{Q}_p(\mathcal{U})\right] = \max_{t\in\mathbb{R}}\left\{t - \frac{1}{p}\mathbb{E}\left[(t-\mathcal{U})^+\right]\right\}$$

4. For the least squares regression case:

$$\mathbb{L}_p = \max_{t\in\mathbb{R}}\left\{t - \frac{1}{np}\sum_{i=1}^{n}\left(t - \left(\boldsymbol{\theta}^\top \boldsymbol{x}_i - y_i\right)\right)^+\right\}$$

Subquantile Optimization Problem

We are know able to define the optimization problem we will solve:

$$\boldsymbol{\theta}_{SM} = \underset{\boldsymbol{\theta}\in\mathbb{R}^d}{\operatorname{argmin}} \max_{t\in\mathbb{R}} \left\{ t - \frac{1}{np} \sum_{i=1}^{n} \left(t - \left(\boldsymbol{\theta}^\top \boldsymbol{x}_i - y_i \right) \right)^+ \right\}$$

The objective function is:

$$g(t_{(k)}, \boldsymbol{\theta}_{(k)}) = t_k - \frac{1}{np} \sum_{i=1}^{n} \left(t - (\boldsymbol{x}_i \boldsymbol{\theta} - y_i) \right)^+ \tag{1}$$

Algorithm:

$$t_{(k+1)} = \underset{t\in\mathbb{R}}{\operatorname{argmax}}\, g(t, \boldsymbol{\theta}_{(k)})$$

$$\boldsymbol{\theta}_{(k+1)} = \boldsymbol{\theta}_{(k)} - \alpha \nabla_{\boldsymbol{\theta}} g(t_{(k+1)}, \boldsymbol{\theta}_k)$$

Lemma

$$\nabla_{\boldsymbol{\theta}} g(t, \boldsymbol{\theta}_{(k)}) = \frac{1}{np} \sum_{i=1}^{np} 2\boldsymbol{x}_i \left(\boldsymbol{\theta}_{(k)}^{\top} \boldsymbol{x}_i - y_i \right)$$

where $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^{np}$ *represent the np points in the dataset with the lowest loss.*

Lemma

$$\underset{t_{k+1} \in \mathbb{R}}{\operatorname{argmax}}\, g(t, \boldsymbol{\theta}_{(k)}) = y_{np}$$

where y_{np} *represents the npth highest loss in the dataset.*

Here we are able to see the true nature of Subquantile Optimization. Each iteration we are optimizing over the points within the lowest np errors.

Optimization

Definition

$(t^*, \boldsymbol{\theta}^*)$ is a **Local Nash Equilibrium** of g if there exists $\delta > 0$ such that for any $t, \boldsymbol{\theta}$ satisfying $\|t - t^*\| \leq \delta$ and $\|\boldsymbol{\theta} - \boldsymbol{\theta}^*\| \leq \delta$

Lemma

Any Local Nash Equlibrium satisfies $\nabla_{\boldsymbol{\theta}} g(t_{(k)}, \boldsymbol{\theta}_{(k)}) = \mathbf{0}$ *and* $\nabla_t g(t_{(k)}, \boldsymbol{\theta}_{(k)}) = 0$

We first give intuition on what it means to be at a Local Nash Equilibrium. It means we have a $\boldsymbol{\theta}$ that gives minimizes ERM over the points within the lowest np errors.

General Theory

Lemma

Let $\hat{\boldsymbol{\nu}}$ be the losses of all the data ordered in ascending order. Then it follows:

$$\arg\max_{t\in\mathbb{R}} g(t,\boldsymbol{\theta}) = \hat{\boldsymbol{\nu}}_{np} \tag{2}$$

Therefore, in each maximizing step we take the element with the npth largest loss as $t_{(k+1)}$. With this choice of t_{k+1} it then follows:

Lemma

The derivative with respect to θ at the kth iteration step is:

$$\nabla_{\boldsymbol{\theta}} g(t_{(k+1)}, \boldsymbol{\theta}_{(k)}) = \frac{1}{np}\sum_{i=1}^{np} 2\boldsymbol{x}_i^T(\boldsymbol{x}_i\boldsymbol{\theta}_{(k)} - y_i)$$

where $\boldsymbol{x_1}, \ldots, \boldsymbol{x}_{np}$ represent the np points with the lowest squared error.

Optimization

Subquantile Optimization continuously optimizes over the np data points with the lowest squared error. In other words, we are trying to minimize the min-loss over the p-quantile. This gives a nice characterization of the optimization problem.

Theorem

The Subquantile min-max optimization problem is equivalent to the following min-min optimization problem:

$$\boldsymbol{\theta}_{SM} = \arg\min_{\boldsymbol{\theta} \in \mathbb{R}^d} \min_{S \in \Pi(X)} \|S\boldsymbol{\theta} - y_S\|_2^2$$

where Π *represents the* $\binom{n}{np}$ *matrices of* np *rows of* X

Proof.

If we let the np elements with error less than $t_{(k+1)}$ be rows of the matrix S, we see we have the same optimization problem. □

The reasoning for this characterization of this optimization algorithm is now it is easier to show convergence.

Prior Works

- [1] Sever computes the gradient of losses in each iteration. This incurs a $\mathcal{O}(dn^2)$ time complexity per iteration. Furthermore, points thrown out in early iterations are not resampled.
- [2] CRR runs in order complexity $\mathcal{O}(d^3 + nd)$. The theoretical guarantees of CRR are given only in the case of Oblivious Noise.
- [6] TERM utilizes a tilted empirical risk and empirically takes maximally $2\times$ the number of iterations a standard ERM algorithm would take to converge.
- Our work computes a np partition of the loss in each iteration. This incurs only a $\mathcal{O}(n)$ time complexity per iteration. Subquantile Minimization is novel in that it resamples points that may not have been in previous Subquantiles.

Drug Discovery

Objectives	Test RMSE (`Drug Discovery`)			
	$\epsilon = 0.1$	$\epsilon = 0.2$	$\epsilon = 0.3$	$\epsilon = 0.4$
ERM	$1.303_{(0.0665)}$	$1.790_{(0.0849)}$	$2.198_{(0.0645)}$	$2.623_{(0.1010)}$
CRR [2]	$1.079_{(0.0899)}$	$1.125_{(0.0832)}$	$1.385_{(0.1372)}$	$1.725_{(0.1136)}$
STIR [4]	$1.087_{(0.1256)}$	$1.167_{(0.0750)}$	$1.403_{(0.0987)}$	$1.668_{(0.1142)}$
Robust Risk [3]	$1.176_{(0.1110)}$	$1.336_{(0.1882)}$	$1.437_{(0.1723)}$	$1.800_{(0.0820)}$
SMART [5]	$1.094_{(0.1065)}$	$1.323_{(0.0758)}$	$1.578_{(0.0799)}$	$1.984_{(0.2020)}$
TERM [6]	$\mathbf{1.029_{(0.0707)}}$	$1.126_{(0.0776)}$	$1.191_{(0.1091)}$	$1.201_{(0.1409)}$
SEVER [1]	$1.043_{(0.0970)}$	$\mathbf{1.067_{(0.0457)}}$	$\mathbf{1.071_{(0.0807)}}$	$\mathbf{1.138_{(0.1162)}}$
Huber [7]	$1.412_{(0.0474)}$	$1.501_{(0.2918)}$	$2.231_{(0.9054)}$	$2.247_{(1.0399)}$
RANSAC [8]	$1.238_{(0.0529)}$	$1.643_{(0.1331)}$	$2.092_{(0.1935)}$	$2.679_{(0.1365)}$
SubQuantile($p = 1 - \epsilon$)	$\mathbf{0.966_{(0.1119)}}$	$\mathbf{1.002_{(0.1025)}}$	$\mathbf{1.010_{(0.0630)}}$	$\mathbf{1.082_{(0.1066)}}$
Genie ERM	$0.960_{(0.0845)}$	$0.982_{(0.0842)}$	$1.006_{(0.0879)}$	$1.030_{(0.0578)}$

Table: `Drug Discovery` Dataset. Empirical Risk over P with oblivious noise

Further Work

1. In the ridge regression case, experimentally, Subquantile Minimization converges in very few iterations to the optimal solution. Theoretically upper bound the number of iterations it will take given β_P, β_Q, and ϵ.
2. Applications of Subquantile Minimization in other Machine Learning domains such as robust classification in datasets such as CIFAR-10.
3. Proof of convergence for a stochatic Subquantile Minimization Algorithm.

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The End

Questions? Comments?