Robust Estimation and GANs

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«Theoretical methods of Deep Learning»

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Problem statement

Huber's ε-contamination problem

- Given i.i.d. observations

$$X_1, \dots, X_n \sim (1-\varepsilon)P_\theta + \varepsilon Q$$

  the task is to estimate the model parameter θ for $\varepsilon \in [0, 1)$.
- Meaning: each observation has a $1-\varepsilon$ probabilty to be drawn from P_θ and the other ε probability to be drawn from the unknown contamination distribution Q.
- Example: normal mean estimation problem with $P_\theta = \mathcal{N}(\theta, I_p)$.
- Motivation: robust statistics and theoretical computer science needs to find both statistically optimal and computationally feasible procedures.

Previous results

Minimax rates of estimation

- It has been shown that the minimax rate $R(\varepsilon)$ of estimating θ under Huber's ε-contamination problem takes the form of

$$R(\varepsilon) \asymp \max\{R(0), \omega(\varepsilon, \Theta)\},$$

  where $\omega(\varepsilon, \Theta)$ is the modulus of continuity between the loss function and the TV distance with respect to the space $\theta \in \Theta$.
- For the normal mean estimation problem, the minimax rate with respect to the squared ℓ_2 loss scales like $\max\{\frac{p}{n}, \varepsilon^2\}$, and is achieved by Tukey's median:

$$\widehat{\theta} = \operatorname*{argsup}_{\eta \in \mathbb{R}^p} \inf_{\|u\|=1} \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}\left\{u^T (X_i - \eta) \geq 0\right\}$$

Proposed method, idea

Computation problems

- Despite the statistical optimality of Tukey's median, its computation is not tractable. In fact, even an approximate algorithm takes $O(\exp(Cp))$ in time.
- How to achieve minimax optimal robust estimation and develop good computational strategies?
- Authors proposed the method based on minimizers of variational lower bounds of the total variation distance between the empirical measure and the model distribution.
- Variational lower bounds are computed through neural network approximations.

f-divergence

Variational lower bound

- Given a strictly convex function f that satisfies $f(1) = 0$, the f-divergence between two probability distributions P and Q with densities p and q respectively is defined by

$$D_f(P\|Q) = \int f\left(\frac{p}{q}\right) dQ.$$

- Examples: $f(x) = x\log(x)$ and $f(x) = ReLU(x-1)$ gives KL divergence and TV distance respectively.
- Convex conjugate of f: $f^*(t) \stackrel{\text{def}}{=} \sup_{u\in\text{dom}_f}(ut - f(u))$.
- It's easy to prove for any function class $\mathcal{T}$:

$$D_f(P\|Q) \geq \sup_{T\in\mathcal{T}} [E_P T(X) - E_Q f^*(T(X))]$$

f-GAN

Robust Estimation with f-GAN

- With i.i.d. observations $X_1, \ldots, X_n \sim P$, this variational lower bound naturally leads to the following learning method:

$$\widehat{P} = \operatorname*{arginf}_{Q \in \mathcal{Q}} \sup_{T \in \mathcal{T}} \left[\frac{1}{n} \sum_{i=1}^{n} T(X_i) - E_Q f^*(T(X)) \right].$$

- The idea of f-GAN is to find a $\widehat{P}$ so that the best discriminator T in the class $\mathcal{T}$ cannot tell the difference between $\widehat{P}$ and the empirical distribution $\frac{1}{n}\sum_{i=1}^{n} \delta_{X_i}$.
- How to choose the function f that leads to robust learning procedures which are easy to optimize? How to specify the discriminator class to learn the parameter of interest with minimax rate under Huber's ε-contamination model?

TV-GAN

Robust Estimation with TV-GAN

- For $f(x) = ReLU(x-1)$ we have $f^*(t) = t\mathbb{I}(0 \le t \le 1)$.
- For discriminator $D(x) = T(x) \in [0,1]$ with Gaussian location family $\mathcal{Q} = \{\mathcal{N}(\eta, I_p) : \eta \in \mathbb{R}^p\}$ we obtain

$$\widehat{\theta} = \underset{\eta \in \mathbb{R}^p}{\operatorname{arginf}} \sup_{D \in \mathcal{D}} \left[\frac{1}{n} \sum_{i=1}^{n} D(X_i) - E_{N(\eta, I_p)} D(X) \right].$$

- Need to specify the class of discriminators $\mathcal{D}$ to solve the classification problem between $\mathcal{N}(\eta, I_p)$ and $\frac{1}{n}\sum_{i=1}^{n} \delta_{X_i}$.
- One of the simplest discriminator classes is the logistic regression:

$$\mathcal{D} = \left\{ D(x) = \operatorname{sigmoid}\left(w^T x + b\right) : w \in \mathbb{R}^p, b \in \mathbb{R} \right\}$$

TV-GAN optimality

TV-GAN optimality for Huber's ε-contamination problem

Assume $\frac{p}{n} + \varepsilon^2 \leq c$ for some sufficiently small constant $c > 0$. With i.i.d. observations $X_1, \ldots, X_n \sim (1-\varepsilon)P_\theta + \varepsilon Q$, the estimator

$$\widehat{\theta} = \underset{\eta \in \mathbb{R}^p}{\operatorname{arginf}} \sup_{D \in \mathcal{D}} \left[\frac{1}{n} \sum_{i=1}^{n} D\left(X_i\right) - E_{N(\eta, I_p)} D(X) \right]$$

with logistic regression discriminators family $\mathcal{D}$ satisfies

$$\|\widehat{\theta} - \theta\|^2 \leq C \cdot \max\left\{\frac{p}{n}, \epsilon^2\right\}$$

with probability at least $1 - \exp\left(-C^{'}(p + n\varepsilon^2)\right)$ uniformly over all $\theta \in \mathbb{R}^p$ and all Q. The constants $C, C^{'} > 0$ are universal.

TV-GAN optimization

Algorithm `TV-GAN optimization`$(S, D_w, G_\eta, \gamma_d, \gamma_w, m, K, T)$:

input: $S = \{X_i\}_{i=1}^m \in \mathbb{R}^p$ - observation set; $D_w(x), G_\eta(z) = z + \eta$ - discriminator/generator networks.

for $t = 1, \ldots, T$ **do**

  for $k = 1, \ldots, K$ **do**

    Sample mini-batch $\{X_i\}_{i=1}^m$ from S;

    Sample $\{Z_i\}_{i=1}^m$ from $\mathcal{N}(0_p, I_p)$;

    $$g_w \leftarrow \nabla_w \left[\frac{1}{m} \sum_{i=1}^m D_w(X_i) - \frac{1}{m} \sum_{i=1}^m D_w(G_\eta(Z_i)) \right];$$

    $w \leftarrow w + \gamma_d g_w$;

  end

  Sample $\{Z_i\}_{i=1}^m$ from $\mathcal{N}(0_p, I_p)$;

  $$g_\eta \leftarrow \nabla_\eta \left[-\frac{1}{m} \sum_{i=1}^m D_w(G_\eta(Z_i)) \right], \ \eta \leftarrow \eta - \gamma_g g_\eta;$$

end

end

TV-GAN

Numerical optimization details

- Initialization of w: $w \sim \mathcal{N}(0, 0.05)$ independently on each element or Xavier. Initialization of b: zero.
- Initialization of η: coordinatewise median of S.
- Though TV-GAN can achieve the minimax rate, it may suffer from optimization difficulties especially when the distributions Q and $\mathcal{N}(\theta, I_p)$ are far away from each other.
- The main obstacle is, with optimization based on gradient, the discriminator may be stuck in a local maximum which will then pass wrong signals to the generator.

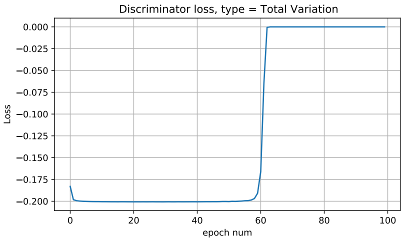
1D Example

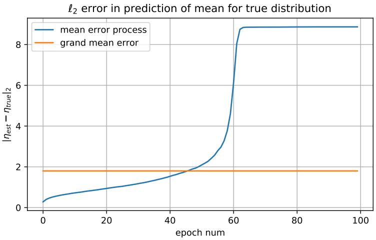
Example

- Let's consider the case with Gaussian contamination distribution.
- The first case $P = (1-\varepsilon)\mathcal{N}(1,1) + \varepsilon\mathcal{N}(10,1)$, when Q and $\mathcal{N}(\theta, I_p)$ are far away.
- The second case $P = (1-\varepsilon)\mathcal{N}(1,1) + \varepsilon\mathcal{N}(1.5,1)$, when Q and $\mathcal{N}(\theta, I_p)$ are close.
- The second case is hard, which is well predicted by the minimax theory of robust estimation.
- We will use 50000 examples of P with batch size $= 500$ for training.

TV-GAN optimization

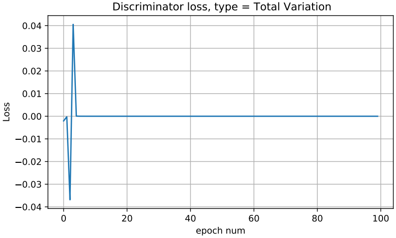
TV-GAN may suffer from optimization difficulties for $\eta_{cont} = 10$.
Figure: training of η estimation of TV-GAN for true initialization $\eta_0 = \eta_{true}$.
Orange curve - ℓ_2-error for grand mean $\eta_{est} = (1-\varepsilon)\eta_{true} + \varepsilon\eta_{cont}$.

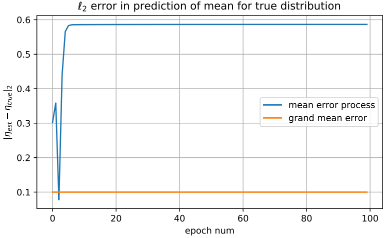




TV-GAN optimization

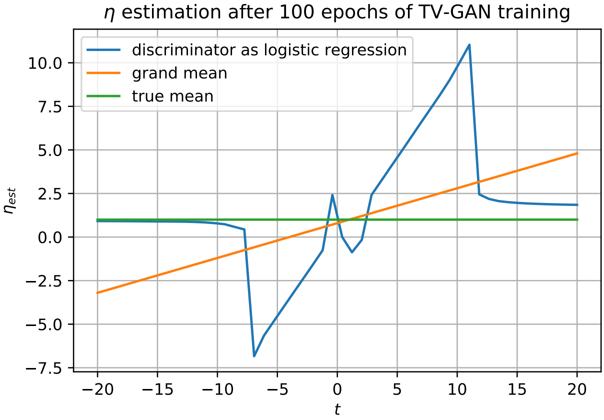
TV-GAN may suffer from optimization difficulties for $\eta_{cont} = 1.5$.
Figure: training of η estimation of TV-GAN for true initialization $\eta_0 = \eta_{true}$.
Orange curve - ℓ_2-error for grand mean $\eta_{est} = (1 - \varepsilon)\eta_{true} + \varepsilon\eta_{cont}$.





TV-GAN optimization

What about very large η_{cont}?
Figure: estimation of η after training TV-GAN for different $\eta_{cont} = t$ with 100 epochs. Orange curve - $\eta_{est}(t) = (1 - \varepsilon)\eta_{true} + \varepsilon t$.



JS-GAN

Robust Estimation with JS-GAN

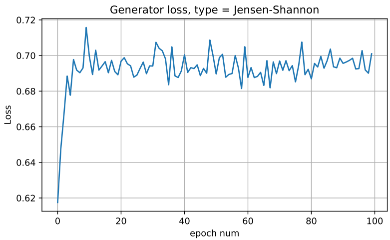
- For $f(x) = x\log(x) - (x+1)\log\left(\frac{x+1}{2}\right)$ we have $f^*(t) = -\log(1-t)$.
- For discriminator $D(x) = T(x) \in [0,1]$ with Gaussian location family $\mathcal{Q} = \{\mathcal{N}(\eta, I_p) : \eta \in \mathbb{R}^p\}$ we obtain

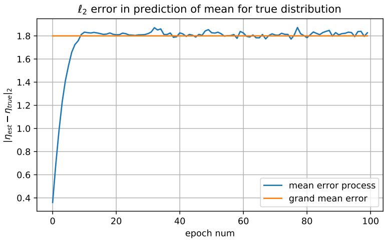
$$\widehat{\theta} = \operatorname*{arginf}_{\eta\in\mathbb{R}^p} \sup_{D\in\mathcal{D}} \left[\frac{1}{n}\sum_{i=1}^{n} \log\left(D\left(X_i\right)\right) + E_{N(\eta,I_p)} \log\left(1 - D(X)\right)\right].$$

- Need to specify the class of discriminators $\mathcal{D}$ to solve the classification problem between $\mathcal{N}(\eta, I_p)$ and $\frac{1}{n}\sum_{i=1}^{n}\delta_{X_i}$.
- We will see numerically that logistic regression in that case doesn't lead to robust estimation, but hidden layer built into the neural nets works well.

JS-GAN with logistic regression

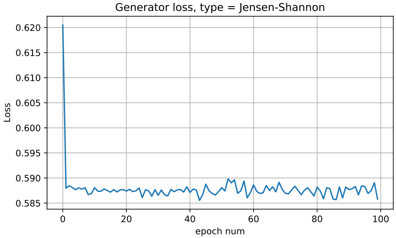
Training JS-GAN with logistic regression as discriminator for $\eta_{cont} = 10$ with Adam and $\gamma_d = 0.2, \gamma_g = 0.02$.
Left figure - loss for generator, right figure - ℓ_2-error in prediction of η_{true}.
Orange curve - ℓ_2-error for grand mean $\eta_{est} = (1 - \varepsilon)\eta_{true} + \varepsilon\eta_{cont}$.

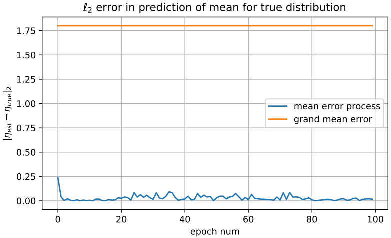




JS-GAN with 1 hidden layer NN

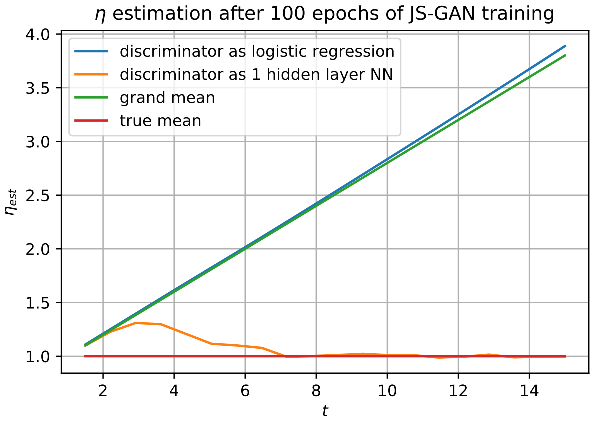
Training JS-GAN with 1 hidden layer NN (20 neurons) as discriminator for $\eta_{cont} = 10$ with Adam and $\gamma_d = 0.2, \gamma_g = 0.02$. Left figure - loss for generator, right figure - ℓ_2-error in prediction of η_{true}.
Orange curve - ℓ_2-error for grand mean $\eta_{est} = (1 - \varepsilon)\eta_{true} + \varepsilon\eta_{cont}$.





JS-GAN comparison

JS-GAN using discriminators without hidden layers always gives an estimator close to $0.2 + 0.8t$, , while the JS-GAN using discriminators with one hidden layer leads to robust estimation.



1 hidden layer NNs with bounded weights

Let's consider the following class of discriminators:

$$\mathcal{D} = \left\{ D(x) = \text{sigmoid}\left(\sum_{j \geq 1} w_j \sigma\left(u_j^T x + b_j\right) \right) : \sum_{j \geq 1} |w_j| \leq \varkappa, u_j \in \mathbb{R}^p, b_j \in \mathbb{R} \right\}$$

While the dimension of the input layer is p, the dimension of the hidden layer can be arbitrary, as long as the weights have a bounded ℓ_1 norm.

JS-GAN optimality

JS-GAN optimality for Huber's ε-contamination problem

Assume $\frac{p}{n} + \varepsilon^2 \le c$ for some sufficiently small constant $c > 0$ and set $\varkappa = O\left(\sqrt{\frac{p}{n}} + \varepsilon\right)$. With i.i.d. observations $X_1, \ldots, X_n \sim (1-\varepsilon)P_\theta + \varepsilon Q$, the estimator

$$\widehat{\theta} = \operatorname*{arginf}_{\eta \in \mathbb{R}^p} \sup_{D \in \mathcal{D}} \left[\frac{1}{n} \sum_{i=1}^{n} \log D\left(X_i\right) + E_{N(\eta, I_p)} \left(1 - \log D(X)\right) \right]$$

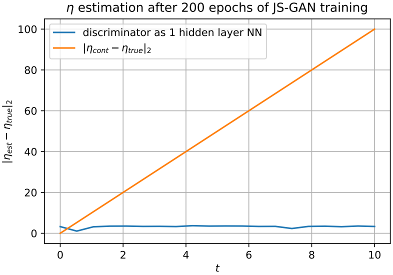
with 1 hidden layer NNs discriminators family $\mathcal{D}$ satisfies

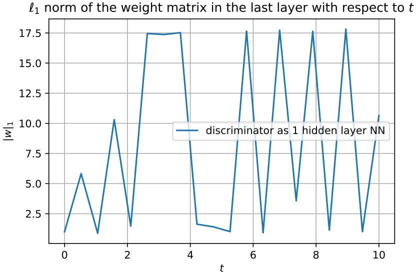
$$\|\widehat{\theta} - \theta\|^2 \le C \cdot \max\left\{\frac{p}{n}, \epsilon^2\right\}$$

with probability at least $1 - \exp\left(-C^{'}(p + n\varepsilon^2)\right)$ uniformly over all $\theta \in \mathbb{R}^p$ and all Q. The constants $C, C^{'} > 0$ are universal.

JS-GAN in big dimensionality

JS-GAN using discriminators with one hidden layer leads to robust estimation even in big dimensionality $p = 100$.





Conclusion

- Initialization in GANs plays significant role for the result.
- Needs for stopping criteria.
- Theory is very hard: Rademacher complexity, Dudley's integral entropy bound, VC-dimension for sigmoids.

Contribution

- Study the paper and technical proofs.
- Work with authors code and fix some mistakes.
- Source code and plots for the project can be found here `https://github.com/Daniil-Selikhanovych/f-gan`

Acknowledgment

I thank Maxim Panov for useful discussions and problem formulation!

References

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Thank you for attention!