Scalable methods for solving games in Adversarial Machine Learning

Roi Naveiro
EURO 2022

Adversarial Machine Learning

- Study and guarantee **robustness** of ML-based decisions wrt adversarial data manipulation.
- Conflict adversary - learning system modeled as a **game**.
- Classical Decision Makers, Humans: **discrete** and **low dimensional** decision spaces.
- New Decision Makers, Algorithms: **continuous** and **high dimensional** decision spaces.

Scalable gradient-based methods for solving sequential games in the new paradigm

Motivation - Adversarial Regression

- R_J and R_D are two competing wine brands.
- R_D has a system to automatically measure wine quality training a regression over some quality indicators. (Response value: wine quality, Covariates: quality indicators).
- R_J, aware of the actual superiority of its competitor's wines, decides to **hack** R_D's system by manipulating the value of several quality indicators **at operation time**, to artificially decrease R_D's quality rates.

CUNEF UNIVERSIDAD

Motivation - Adversarial Regression

- R_D is **aware** of the possibility of being hacked and decides to train its regression in an **adversarial robust** manner.
- R_D models this **conflict** as a game between a *learner* (R_D) and a *data generator* (R_J). (Brückner and Scheffer, 2011).
- The *data generator* tries to fool the learner **modifying input data at application time**, inducing a change between the data distribution at training $[p(x, y)]$ and test $[\bar{p}(x, y)]$ times.

The Learner Problem

- Given a feature vector $\boldsymbol{x} \in \mathbb{R}^p$ and target $\boldsymbol{y} \in \mathbb{R}$, the learner's decision is to choose the weight vector of a linear model $\boldsymbol{f_w}(\boldsymbol{x}) = \boldsymbol{x}^\top \boldsymbol{w}$, minimizing **theoretical costs at application time**

$$\theta_l(w, \bar{p}, c_l) = \int c_l(x, y)(f_w(x) - y)^2 \, \mathrm{d}\bar{p}(x, y),$$

- To do so, the learner has a training matrix $\boldsymbol{X} \in \mathbb{R}^{n \times p}$ and a vector of target values $\boldsymbol{y} \in \mathbb{R}^n$ (a sample from distribution $\boldsymbol{p}(\boldsymbol{x}, \boldsymbol{y})$ at training time).

The Data Generator Problem

- The data generator aims at **changing features of test instances** to induce a transformation from $p(x, y)$ to $\bar{p}(x, y)$.

- $z(x, y)$ is the data generator's target value for instance x with real value y

- The data generator aims at **choosing the data transformation** that minimizes the theoretical costs given by

$$\theta_d(w, \bar{p}, c_d) = \int c_d(x, y)(f_w(x) - z(x, y))^2 \,\mathrm{d}\bar{p}(x, y) + \Omega_d(p, \bar{p})$$

Regularized Empirical Costs

- Theoretical costs defined above depend on the unknown distributions $\boldsymbol{p}$ and $\bar{\boldsymbol{p}}$.
- We focus on their regularized empirical counterparts, given by

$$\hat{\theta}_l(w, \bar{X}, c_l) = \sum_{i=1}^{n} c_{l,i}(f_w(\bar{x}_i) - y_i)^2 + \Omega_l(f_w),$$
$$\hat{\theta}_d(w, \bar{X}, c_d) = \sum_{i=1}^{n} c_{d,i}(f_w(\bar{x}_i) - z_i)^2 + \Omega_d(X, \bar{X}).$$

Resulting Stackelberg Game

- We assume the learner acts first, choosing a weight vector $\boldsymbol{w}$. Then the data generator, after observing $\boldsymbol{w}$, chooses his optimal data transformation.

$$\begin{aligned} \arg\min_{w} \quad & \widehat{\theta}_l(w, T(X, w, c_d), c_l) \\ \text{s.t.} \quad & T(X, w, c_d) = \arg\min_{X'} \widehat{\theta}_d(w, X', c_d) \end{aligned}$$

The general problem

Defender (D) makes decision $\boldsymbol{\alpha} \in \mathbb{R}^n$. Attacker (A), after observing $\boldsymbol{\alpha}$, makes decision $\beta \in \mathbb{R}^m$

$$
\begin{aligned}
\arg\max_{\alpha} \quad & u_D[\alpha, \beta^*(\alpha)] \\
\text{s.t.} \quad & \beta^*(\alpha) = \arg\max_{\beta} u_A(\alpha, \beta)
\end{aligned}
$$

- In AML, α and β usually **high dimensional** and **continuous**.

Gradient Methods

- Forget about analytical solutions!
- **Gradient methods** require computing $\mathbf{d}_\alpha \boldsymbol{u}_D$ (and moving $\boldsymbol{\alpha}$ in the direction of increasing gradient...)

$$
\begin{aligned}
\mathrm{d}_\alpha u_D &= \partial_\alpha u_D + \mathrm{d}_\alpha \beta^*(\alpha) \cdot \partial_\beta u_D \big|_{\beta^*(\alpha)} \\
&= \partial_\alpha u_D - \partial_\beta u_D \cdot \partial^2_{\alpha\beta} u_A \cdot \left[\partial^2_\beta u_A\right]^{-1} \big|_{\beta^*(\alpha)}
\end{aligned}
$$

- Inverting the Hessian has cubic complexity!
- We need a different strategy...

Backward Solution

- Under **certain conditions** (Bottou, 1998), we can approximate our problem by

$$\begin{aligned} \arg\max_{\alpha} \quad & u_D\left[\alpha, \beta(\alpha, T)\right] \\ \text{s.t.} \quad & \partial_t \beta(\alpha, t) = \partial_\beta u_A[\alpha, \beta(\alpha, t)] \\ & \beta(\alpha, 0) = 0. \end{aligned}$$

- Where $T \gg 1$.
- $\lim_{t\to\infty} \beta(\alpha, t) = \beta^*(\alpha)$.
- Let's try to solve this problem instead.

Backward Solution

- It can be proved that (Naveiro and Ríos, 2019)

$$\mathrm{d}_\alpha u_D[\alpha, \beta(\alpha, T)] = \partial_\alpha u_D[\alpha, \beta(\alpha, T)] - \int_0^T \lambda(t) \partial_\alpha \partial_\beta u_A[\alpha, \beta(\alpha, t)] \, \mathrm{d}t$$

- Provided that λ satisfies the **adjoint equation**

$$\mathrm{d}_t \lambda(t) = -\lambda(t) \ \partial_\beta^2 u_A[\alpha, \beta(\alpha, t)]$$

- With initial conditions $\lambda(T) = -\partial_\beta u_D(\alpha, \beta)$.

Backward Solution

Algorithm 1 Approximate total derivative of defender utility function with respect to her decision using the backward solution

procedure APPROXIMATE DERIVATIVE USING BACKWARD METHOD(α, T)

  $\beta_0(\alpha) = 0$

  for $t = 1, 2, \ldots, T$ **do**

    $\beta_t(\alpha) = \beta_{t-1}(\alpha) + \eta \partial_\beta u_A(\alpha, \beta)\Big|_{\beta_{t-1}}$

  end for

  $\lambda_T = -\partial_\beta u_D(\alpha, \beta)\Big|_{\beta_T}$

  $\mathrm{d}_\alpha u_D = \partial_\alpha u_D[\alpha, \beta_T(\alpha)]$

  for $t = T-1, T-2, \ldots, 0$ **do**

    $\mathrm{d}_\alpha u_D = \mathrm{d}_\alpha u_D - \eta \lambda_{t+1} \partial_\alpha \partial_\beta u_A(\alpha, \beta)\Big|_{\beta_{t+1}}$

    $\lambda_t = \lambda_{t+1} \left[I + \eta \partial_\beta^2 u_A(\alpha, \beta)\Big|_{\beta_{t+1}} \right]$

  end for

  return $\mathrm{d}_\alpha u_D$

end procedure

Backward Solution - Complexity Analysis

Time complexity

- If $\tau(n, m)$ is the time required to evaluate $u_D(\alpha, \beta)$ and $u_A(\alpha, \beta)$, computing their derivatives requires time $\mathcal{O}(\tau(n, m))$.
- First loop $\mathcal{O}(T\tau(n, m))$.
- Second loop needs computing Hessian Vector Products, by basic results of AD, they have same complexity as function evaluations!
- Thus, overall time complexity is $\mathcal{O}(T\tau(n, m))$.

Space complexity

- We need to store $\beta_t(\alpha)$ for all t.
- $\sigma(n, m)$ is the space requirement for storing each $\beta_t(\alpha)$.
- Overall space complexity $\mathcal{O}(T\sigma(n, m))$.

Forward Solution

- Under **certain conditions**, we can approximate our problem by

$$
\begin{aligned}
\arg\max_{\alpha} \quad & u_D\left[\alpha, \beta_T(\alpha)\right] \\
\text{s.t} \quad & \beta_t(\alpha) = \beta_{t-1}(\alpha) + \eta_t \partial_\beta u_A(\alpha, \beta)\Big|_{\beta_{t-1}} \qquad t = 1, \ldots, T \\
& \beta_0(\alpha) = 0.
\end{aligned}
$$

- Again, $T \gg 1$.
- $\lim_{t \to \infty} \beta_t(\alpha) = \beta^*(\alpha)$.

Forward Solution

- Using the chain rule

$$\mathrm{d}_\alpha u_D[\alpha, \beta_T(\alpha)] = \partial_\alpha u_D[\alpha, \beta_T(\alpha)] + \partial_{\beta_T} u_D[\alpha, \beta_T(\alpha)]\, \mathrm{d}_\alpha \beta_T(\alpha)$$

- To obtain $\mathrm{d}_\alpha \beta_T(\alpha)$ we can sequentially compute

$$\mathrm{d}_\alpha \beta_t(\alpha) = \mathrm{d}_\alpha \beta_{t-1}(\alpha) + \eta_{t-1} \left[\partial_\alpha \partial_\beta u_A(\alpha, \beta)\Big|_{\beta_{t-1}} + \partial_\beta^2 u_A(\alpha, \beta)\Big|_{\beta_{t-1}} \mathrm{d}_\alpha \beta_{t-1}(\alpha) \right]$$

- This induces a dynamical system in $\mathrm{d}_\alpha \beta_t(\alpha)$ that can be iterated in parallel to the dynamical system in $\beta_t(\alpha)$!

Forward Solution

Algorithm 2 Approximate total derivative of defender utility function with respect to her decision using the forward solution.

procedure APPROXIMATE DERIVATIVE USING FORWARD METHOD(α, T)
    $\beta_0(\alpha) = 0$
    $\mathrm{d}_\alpha \beta_0(\alpha) = 0$
    for $t = 1, 2, \ldots, T$ **do**
        $\beta_t(\alpha) = \beta_{t-1}(\alpha) + \eta \partial_\beta u_A(\alpha, \beta)\Big|_{\beta_{t-1}}$
        $\mathrm{d}_\alpha \beta_t(\alpha) = \mathrm{d}_\alpha \beta_{t-1}(\alpha) + \eta_{t-1} \left[\partial_\alpha \partial_\beta u_A(\alpha, \beta)\Big|_{\beta_{t-1}} + \partial_\beta^2 u_A(\alpha, \beta)\Big|_{\beta_{t-1}} \mathrm{d}_\alpha \beta_{t-1}(\alpha) \right]$
    end for
    $\mathrm{d}_\alpha u_D = \partial_\alpha u_D[\alpha, \beta_T(\alpha)] + \partial_{\beta_T} u_D[\alpha, \beta_T(\alpha)]\, \mathrm{d}_\alpha \beta_T(\alpha)$
    return $\mathrm{d}_\alpha u_D$
end procedure

Forward Solution - Complexity Analysis

Time complexity

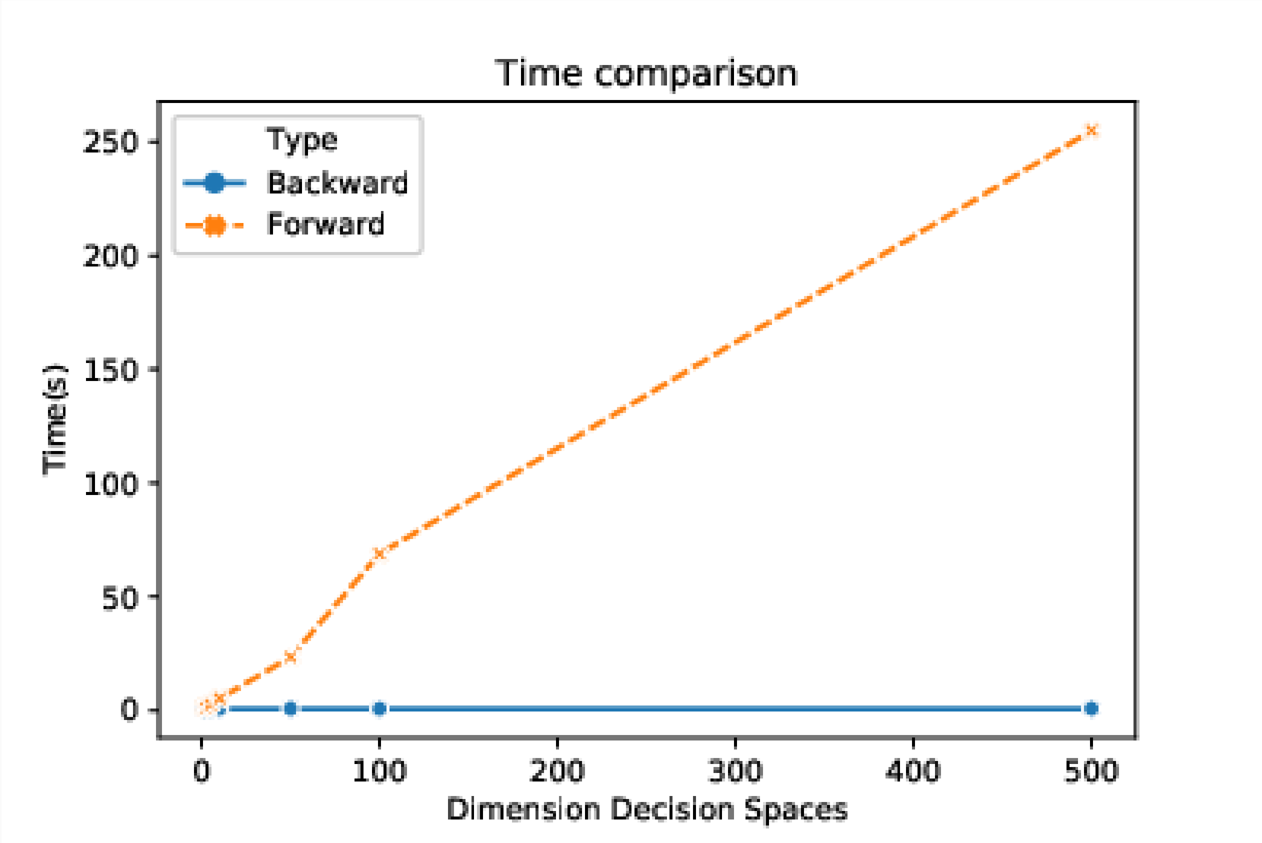
- Computing $\partial_\beta^2 u_A(\alpha, \beta)$ requires time $\mathcal{O}(m\tau(m,n))$ as it requires computing m Hessian vector products.
- Computing $\partial_\alpha \partial_\beta u_A(\alpha, \beta)$ requires computing n Hessian vector products and thus time $\mathcal{O}(n\tau(m,n))$.
- If we compute the derivative in the other way, first we derive with respect to β and then with respect to α, the time complexity is $\mathcal{O}(m\tau(m,n))$.
- Thus, computing $\partial_\alpha \partial_\beta u_A(\alpha, \beta)$ requires $\mathcal{O}(\mathbf{min}(n,m)\tau(m,n))$.
- Overall, $\mathcal{O}(\mathbf{max}[\mathbf{min}(n,m), m]T\tau(m,n)) = \mathcal{O}(mT\tau(m,n))$.

Space complexity

- The values $\beta_t(\alpha)$ are overwritten at each iteration.
- Overall space complexity is $\mathcal{O}(\sigma(m,n))$.

Conceptual Example

- Attacker's utility is $u_A(\alpha, \beta) = -\sum_{i=1}^{n} 3(\beta_i - \alpha_i)^2$ and the defender's one is $u_D(\alpha, \beta) = -\sum_{i=1}^{n} (7\alpha_i + \beta_i^2)$.
- $\mathcal{O}(T\tau(m, n))$ vs $\mathcal{O}(mT\tau(m, n))$.



Application - Adversarial Regression

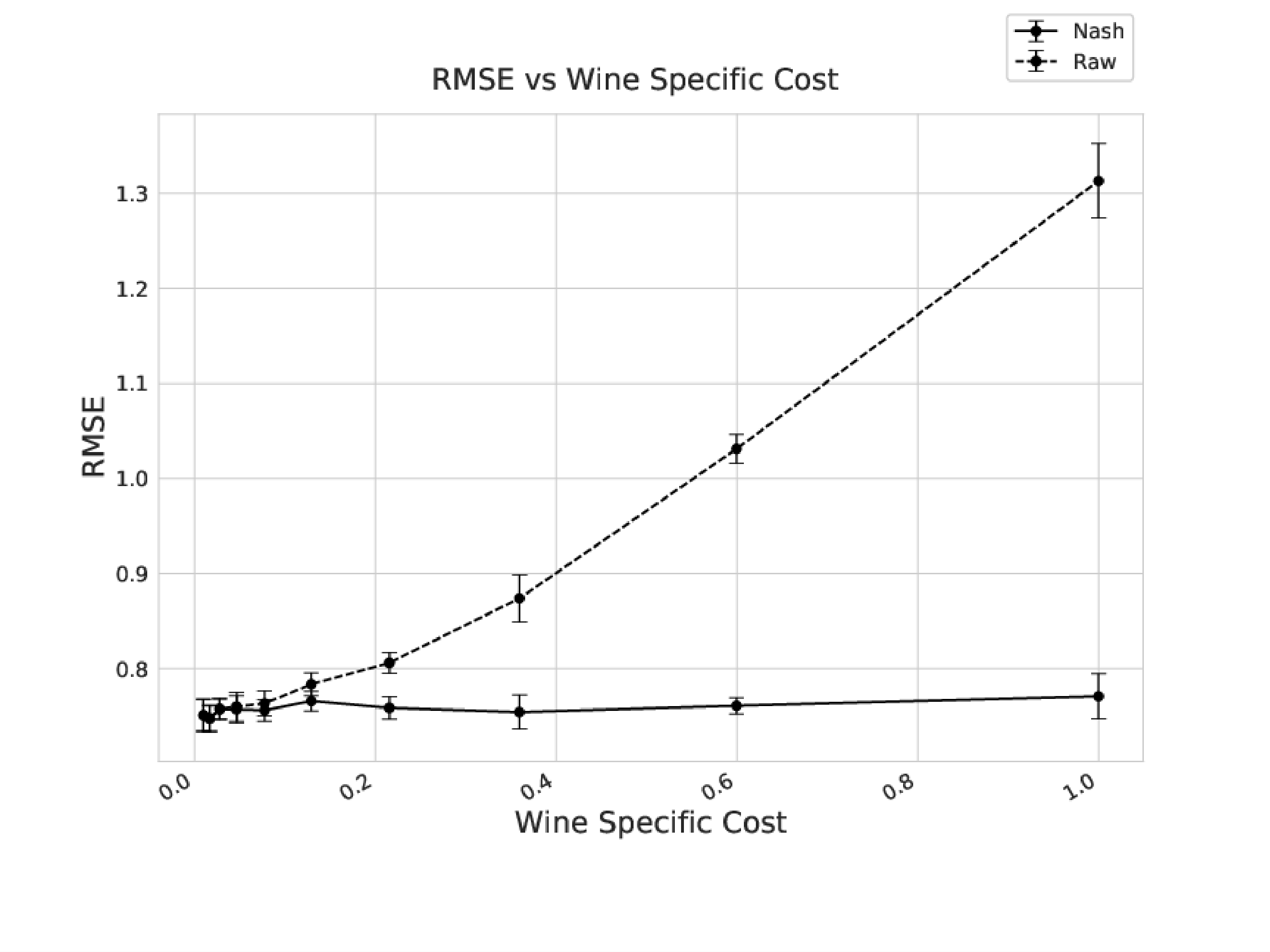
- We compare ridge regression versus *adversarial robust regression* in the wine problem.
- For ridge regression, we compute the weights in the usual way, and test them in data attacked using those weights.
- For *adversarial robust regression* we compute the weights solving

$$\begin{aligned} \arg\min_{w} \quad & \widehat{\theta}_l(w, T(X, w, c_d), c_l) \\ \text{s.t.} \quad & T(X, w, c_d) = \arg\min_{X'} \widehat{\theta}_d(w, X', c_d) \end{aligned}$$

and test them in data attacked using those weights.

- Note the dimension of the attacker's decision space is huge! He needs to modify $\boldsymbol{k = 3263}$ data points each with $\boldsymbol{n = 11}$ components!

Adversarial Regression



Conclusions and future work

- New algorithmic method able to solve **huge Stackelberg Games** (dimension of decision sets of the order of 10^4).
- Could be implemented in any **Automatic Differentiation** library (Pytorch, tensorflow...).
- Novel derivation of the backward solution formulating the Stackelberg game as a PDE-constrained optimization problem.
- Application to games with uncertain outcomes.
- Application to Bayesian Stackelberg Games and ARA.
- Several attackers?

Thank you!!

roi.naveiro@icmat.es

www.github.com/roinaveiro/GM_SG

www.roinaveiro.github.io