Learning to Pivot with Adversarial Networks

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Systematic uncertainties – the known unknowns in science

- In science, the data generation process is often not uniquely specified or known exactly, hence to the presence of systematic uncertainties.
- Data generation processes are rather formulated as a family of data generation processes parametrized by nuisance parameters.
- One of the challenges of applying machine learning to scientific problems is the need to incorporate systematics.

Problem statement

- Let us assume a family of data generation processes $p(X, Y, Z)$ where
  - X are the data,
  - Y are the target labels,
  - Z are the nuisance parameters specifying systematic uncertainties.
- We want to learn a regression function $f : \mathcal{X} \mapsto \mathcal{S}$ of parameters θ_f.
- We want inference based on $f(X; \theta_f)$ to be robust to the value $z \in \mathcal{Z}$ of the nuisance parameter – *which remains unknown at test time*.
  - We want a classifier that does not change with systematic variations, even though the data might.

Pivot

- We define robustness as requiring the distribution of $f(X;\theta_f)$ conditional on Z (and possibly Y) to be invariant with the nuisance parameter Z. That is, such that

  $$p(f(X;\theta_f) = s|z) = p(f(X;\theta_f) = s|z')$$

  for all $z, z' \in \mathcal{Z}$ and all values $s \in \mathcal{S}$ of $f(X;\theta_f)$. If f satisfies this criterion, then f is known as a pivotal quantity.

- Alternatively, this amounts to find f such that $f(X;\theta_f)$ and Z are independent random variables.

Adversarial Networks

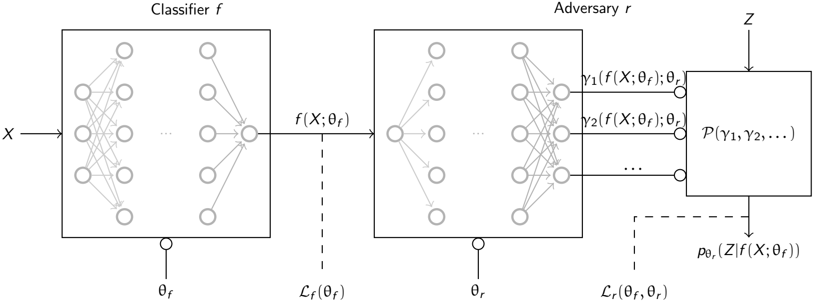
- Let consider a classifier f built as usual, minimizing the cross-entropy

$$\mathcal{L}_f(\theta_f) = \mathbb{E}_{x \sim X}\mathbb{E}_{y \sim Y|x}[-\log p_{\theta_f}(y|x)].$$

- We pit f against an adversary network r producing as output a function $p_{\theta_r}(z|f(X;\theta_f) = s)$ modeling the posterior probability density of the nuisance parameter conditional on $f(X;\theta_f) = s$. We set r to minimize the cross entropy

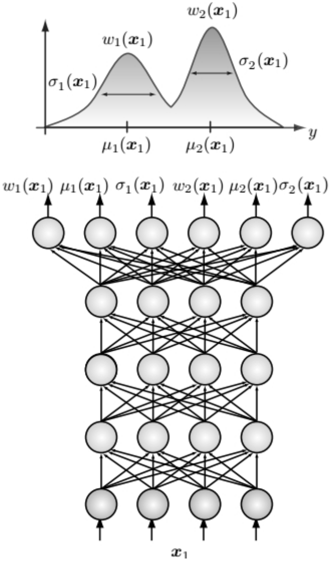
$$\mathcal{L}_r(\theta_f, \theta_r) = \mathbb{E}_{s \sim f(X;\theta_f)}\mathbb{E}_{z \sim Z|s}[-\log p_{\theta_r}(z|s)].$$

  - If the adversary can predict the nuisance parameter from the classifier's output, then it means that some information about the nuisance parameter is carried out through it: the classifier is dependent on the systematics.


Classifier f
Adversary r
Z
X
$f(X;\theta_f)$
$\gamma_1(f(X;\theta_f);\theta_r)$
$\gamma_2(f(X;\theta_f);\theta_r)$
$\dots$
$\mathcal{P}(\gamma_1, \gamma_2, \dots)$
$p_{\theta_r}(Z|f(X;\theta_f))$
θ_f
$\mathcal{L}_f(\theta_f)$
θ_r
$\mathcal{L}_r(\theta_f, \theta_r)$

Z can be either categorical or continuous

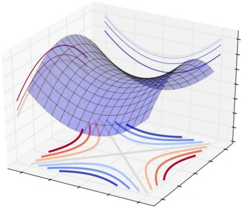
- If Z is categorical, then the posterior can be modeled with a standard (probabilistic) classifier.
- If Z is continuous, then the posterior can be modeled with a *mixture density network*.
- No constraint on the prior $p(Z)$.



Mixture density network

Adversarial training

What if the classifier forces the adversary to perform worse by simultaneously maximizing $\mathcal{L}_r$? It should reduce its dependence on the nuisance parameter, shouldn't it?



Formally, let us consider the value function

$$E(\theta_f, \theta_r) = \mathcal{L}_f(\theta_f) - \mathcal{L}_r(\theta_f, \theta_r)$$

that we optimize by finding the minimax solution

$$\hat{\theta}_f, \hat{\theta}_r = \arg \min_{\theta_f} \max_{\theta_r} E(\theta_f, \theta_r).$$

Theoretical motivation

Proposition. *If there exists a minimax solution* $(\hat{\theta}_f, \hat{\theta}_r)$ *such that* $E(\hat{\theta}_f, \hat{\theta}_r) = H(Y|X) - H(Z)$*, then* $f(\cdot; \hat{\theta}_f)$ *is both an optimal classifier and a pivotal quantity.*

Proof (sketch):

$$
\begin{aligned}
&\min_{\theta_f} \max_{\theta_r} \mathcal{L}_f(\theta_f) - \mathcal{L}_r(\theta_f, \theta_r) \\
=&\min_{\theta_f} \mathcal{L}_f(\theta_f) - \mathbb{E}_{s \sim f(X;\theta_f)}[H(Z|f(X;\theta_f) = s)] \\
=&\min_{\theta_f} \mathcal{L}_f(\theta_f) - H(Z|f(X;\theta_f)) \\
\geq& H(Y|X) - H(Z)
\end{aligned}
$$

where the equality holds when

- f is an optimal classifier (in which case $\mathcal{L}_f(\theta_f) = H(Y|X)$);
- $f(X;\theta_f)$ and Z are independent random variables (in which case $H(Z|f(X;\theta_f)) = H(Z)$).

Alternating stochastic gradient descent

for $t = 1$ to T **do**

  for $k = 1$ to K **do** ▷ Update r

    Sample minibatch $\{x_m, z_m, s_m = f(x_m; \theta_f)\}_{m=1}^{M}$ of size M;

    With θ_f fixed, update r by ascending its stochastic gradient $\nabla_{\theta_r} E(\theta_f, \theta_r) :=$

$$\nabla_{\theta_r} \sum_{m=1}^{M} \log p_{\theta_r}(z_m | s_m);$$

  end for

  Sample minibatch $\{x_m, y_m, z_m, s_m = f(x_m; \theta_f)\}_{m=1}^{M}$ of size M; ▷ Update f

  With θ_r fixed, update f by descending its stochastic gradient $\nabla_{\theta_f} E(\theta_f, \theta_r) :=$

$$\nabla_{\theta_f} \sum_{m=1}^{M} \left[-\log p_{\theta_f}(y_m | x_m) + \log p_{\theta_r}(z_m | s_m) \right],$$

  where $p_{\theta_f}(y_m | x_m)$ denotes $\mathbf{1}(y_m = 0)(1 - s_m) + \mathbf{1}(y_m = 1) s_m$;

end for

Accuracy versus robustness trade-off

- The assumption of existence of a classifier that is both optimal and pivotal may not hold.

- However, the value function E can be rewritten as

$$E_\lambda(\theta_f, \theta_r) = \mathcal{L}_f(\theta_f) - \lambda \mathcal{L}_r(\theta_f, \theta_r)$$

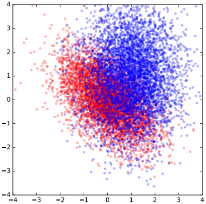
  where λ is a hyper-parameter controlling the trade-off between the performance of f and its independence with respect to the nuisance parameter.

  - Setting λ to a large value enforces f to be pivotal.
  - Setting λ close to 0 constraints f to be optimal.

Toy example

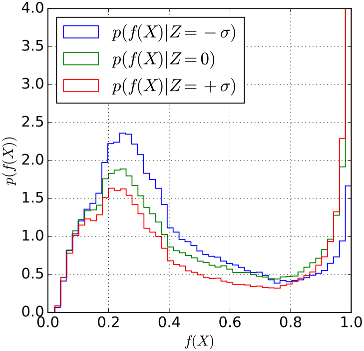
- Binary classification of 2D data drawn from multivariate gaussians with equal priors, such that

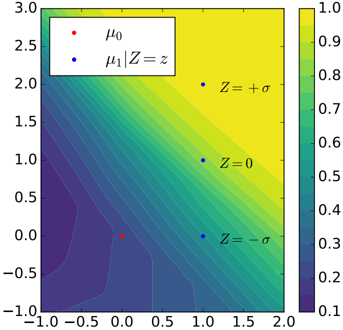
$$x \sim \mathcal{N}\left((0,0), \begin{bmatrix} 1 & -0.5 \\ -0.5 & 1 \end{bmatrix}\right) \qquad \text{when } Y = 0,$$
$$x \sim \mathcal{N}\left((1,1+Z), \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right) \qquad \text{when } Y = 1.$$



- The continuous nuisance parameter Z represents in this case our uncertainty about the exact location of the mean of the second gaussian. We assume a gaussian prior $z \sim \mathcal{N}(0,1)$.
- We assume training data $\{x_i, y_i, z_i\}_{i=1}^N \sim p(X, Y, Z)$.

Standard training without the adversary r

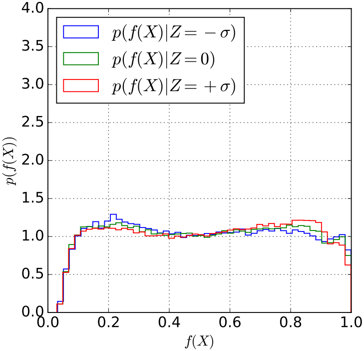


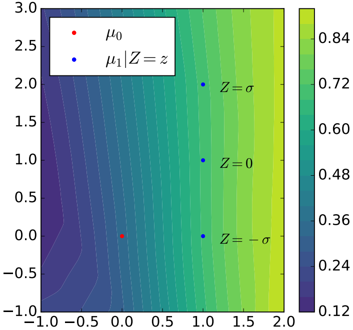


(Left) The conditional probability distributions of $f(X;\theta_f)|Z=z$ changes with z.

(Right) The decision surface strongly depends on X_2.

Reshaping f with adversarial training

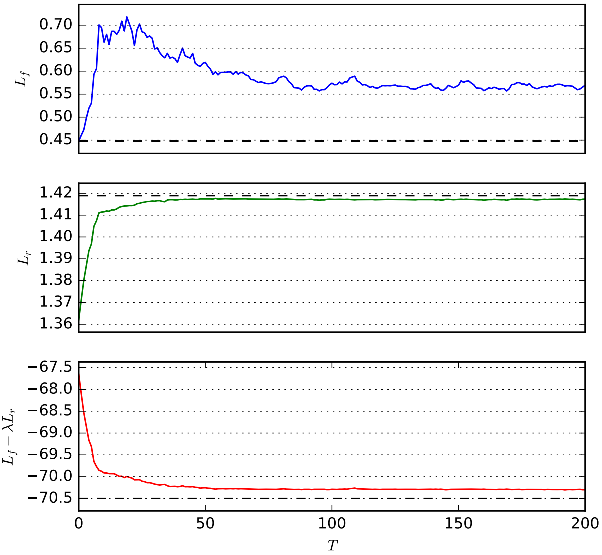




(Left) The conditional probability distributions of $f(X;\theta_f)|Z=z$ are now (almost) invariant with z!

(Right) The decision surface is now independent of X_2.

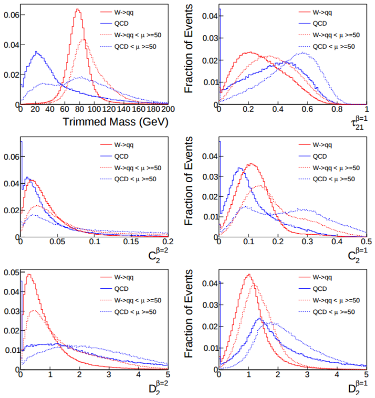
Dynamics of adversarial training



High energy physics example

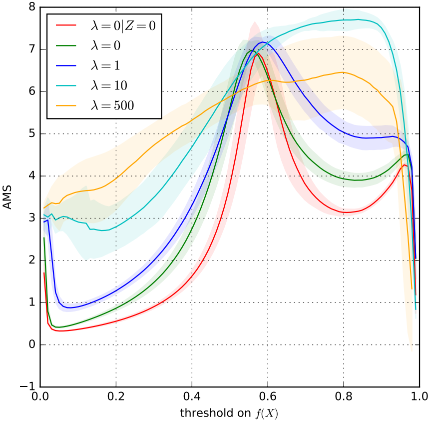
- Discriminate between QCD jets ($Y = 0$) and W-jets ($Y = 1$) from high-level features (data from Baldi et al, arXiv:1603.09349).

- Taking some liberty, we consider an extreme categorical nuisance parameter where
  - $Z = 0$ corresponds to events without pileup,
  - $Z = 1$ corresponds to events with pileup, for which there are an average of 50 independent pileup interactions overlaid.



Maximizing significance by tuning λ

- Since we do not expect to find a classifier f that is both optimal and pivotal, we optimize the accuracy-independence trade-off by tuning λ with respect to a higher level objective.
- Cut and count analysis: A natural higher-level context is a hypothesis test of a null with no signal events against an alternate hypothesis that is a mixture of signal and background events.
  - Background = 1000 weighted QCD jets, Signal = 100 weighted boosted W's.
  - Without systematics, optimizing $\mathcal{L}_f$ indirectly optimizes the power of a classical hypothesis test.
  - With systematics, we need to balance classification performance against robustness to the nuisance parameter.
  - To this end, we use the Approximate Median Significance (AMS) as higher-level objective.
  - Note that since we are performing a hypothesis test of the null, we only wish to impose the pivotal property on background events.



$\lambda = 0|Z = 0$: standard training from $p(X, Y, Z = 0)$.

$\lambda = 0$: standard training from $p(X, Y, Z)$.

$\lambda = 10$: trading accuracy for robustness wrt pileup results in a net benefit in terms of maximum statistical significance.

Summary

- We proposed a principled approach based on adversarial networks for building a model whose output can be constrained to be independent of a chosen nuisance parameter (or any random variable).
- The method supports both categorical and continuous nuisance parameters.
- Control is offered to tune the accuracy versus robustness trade-off in order to maximize a higher-level objective.

- We are looking for opportunities of (real) physics use cases! Come talk to us if interested!