Adversarial Training of Neural Networks against Systematic Uncertainty

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Abstract

1 Introduction

[GL: Distinction between statistical and systematic uncertainty.] [GL: Define nuisance parameters.] [GL: We want to build an accurate classifier whose output remains invariant with respect to systematic uncertainties.] [GL: Motivate the criterion (which may not be obvious for the ML crowd). See pivotal quantity motivation.]

2 Problem statement

Let assume a probability space $(\Omega, \mathcal{F}, P)$, where Ω is a sample space, $\mathcal{F}$ is a set of events and P is a probability measure. Let consider the multivariate random variables $X_\lambda : \Omega \mapsto \mathbb{R}^p$ and $Y : \Omega \mapsto \mathcal{Y}$, where X_λ depends on a nuisance parameter $\lambda \in \Lambda$ whose values define a parameterized family of its systematic uncertainties. That is, X_λ and Y induce together a joint probability distribution $p(X, Y|\lambda)$, where the conditional on λ denotes X_λ. For training, let further assume a finite set $\{x_i, y_i, \lambda_i\}_{i=1}^N$ of realizations $X_{\lambda_i}(\omega_i), Y(\omega_i)$, for $\omega_i \in \Omega$ and known values λ_i of the nuisance parameter. Our goal is to learn a function $f(\cdot; \theta_f) : \mathbb{R}^p \mapsto \mathcal{Y}$ of parameters θ_f (e.g., a neural network-based classifier if $\mathcal{Y}$ is a finite set of classes) and minimizing a loss $\mathcal{L}_f(\theta_f)$. In addition, we require that $f(X_\lambda; \theta_f)$ should be robust to the value of the nuisance parameter λ – which remains unknown at test time. More specifically, we aim at building f such that in the ideal case

$$f(X_\lambda(\omega); \theta_f) = f(X_{\lambda'}(\omega); \theta_f) \tag{1}$$

for all samples $\omega \in \Omega$ and all λ, λ' pairs of values of the nuisance parameter.

Since we do not have training tuples $(X_\lambda(\omega), X_{\lambda'}(\omega))$ (for the same unknown ω), we propose instead to solve the closely related problem of finding a predictive function f such that

$$P(\{\omega | f(X_\lambda(\omega); \theta_f) = y\}) = P(\{\omega' | f(X_{\lambda'}(\omega'); \theta_f) = y\}) \text{ for all } y \in \mathcal{Y}. \tag{2}$$

In words, we are looking for a predictive function f which is a pivotal quantity [1] with respect to the nuisance parameter. That is, such that the distribution of $f(X_\lambda; \theta_f)$ is invariant with respect to the value of λ. Note that a function f for which Eqn. 1 is true necessarily satisfies Eqn. 2. The converse is however in general not true, since the sets of samples $\{\omega | f(X_\lambda(\omega); \theta_f) = y\}$ and $\{\omega' | f(X_{\lambda'}(\omega'); \theta_f) = y\}$ do not need to be the same for the equality to hold. In order to simplify notations, and as only Eqn. 2 is of direct interest in this work, we denote from here on the pivotal quantity criterion as

$$p(f(X; \theta_f)|\lambda) = p(f(X; \theta_f)|\lambda') \text{ for all } \lambda, \lambda' \in \Lambda. \tag{3}$$

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3 Method

Adversarial training was first proposed by [2] as a way to build a generative model capable of producing samples from random noise $z \sim p_Z$. More specifically, the authors pit a generative model $g : \mathcal{Z} \mapsto \mathbb{R}^p$ against an adversary classifier $d : \mathbb{R}^p \mapsto \{0, 1\}$ whose antagonistic objective is to recognize real data X from generated data $g(Z)$. Both models g and d are trained simultaneously, in such a way that g learns to produce samples that are difficult to identify by d, while d incrementally adapts to changes in g. At the equilibrium, g models a distribution whose samples can be identified by d only by chance. That is, assuming enough capacity in d and g, the distribution $p_{g(Z)}$ eventually converges towards the real distribution p_X.

In this work, we repurpose adversarial training as a means to constraint the predictive model f in order to satisfy Eqn. 3. In particular, we pit f against an adversary classifier $r(\cdot; \theta_r) : \mathbb{R} \mapsto \Lambda$ of parameters θ_r and associated loss $\mathcal{L}_r(\theta_f, \theta_r)$. Assuming that Λ defines a finite family of nuisance values λ_l (for $l = 1, \ldots, |\Lambda|$), this classifier takes as input realizations of $f(X; \theta_f)$, for the current value θ_f of f parameters, and produces as output probability estimates $r(f(X; \theta_f); \theta_r)_l = \hat{p}(\lambda_l | f(X; \theta_f))$ that $f(X; \theta_f)$ is generated from the nuisance value λ_l. If $p(f(X; \theta_f)|\lambda)$ varies with λ, then the corresponding correlation can be captured by r. By contrast, if $p(f(X; \theta_f)|\lambda)$ is invariant with λ, as we require, then r should perform poorly and be close to random guessing. Training f such that it additionally minimizes the performance of r therefore acts as a regularization towards Eqn. 3.

As for generative adversarial networks, we propose to train f and r simultaneously, which we carry out by considering the value function

$$E(\theta_f, \theta_r) = \mathcal{L}_f(\theta_f) - \mathcal{L}_r(\theta_f, \theta_r) \tag{4}$$

that we optimize by finding the saddle point $(\hat{\theta}_f, \hat{\theta}_r)$ such that

$$\hat{\theta}_f = \arg\min_{\theta_f} E(\theta_f, \hat{\theta}_r), \tag{5}$$

$$\hat{\theta}_r = \arg\max_{\theta_r} E(\hat{\theta}_f, \theta_r). \tag{6}$$

The adversarial training procedure to obtain $(\hat{\theta}_f, \hat{\theta}_r)$ is formally presented in Algorithm 1 in the case of f being a classifier and of the cross-entropy loss for both $\mathcal{L}_f$ and $\mathcal{L}_r$. The algorithm consists in using stochastic gradient descent alternatively to optimize Eqn. 5 and 6.

Algorithm 1 Adversarial training of a classifier f against an adversary r.
Inputs: training data $\{x_i, y_i, \lambda_i\}_{i=1}^N$
Outputs: $\hat{\theta}_f, \hat{\theta}_r$
Hyper-parameters: Number T of training iterations, Number K of gradient steps to update r.

for $t = 1$ to T **do**
  for $k = 1$ to K **do** ▷ Update r
    Sample minibatch $\{x_m, \lambda_m\}_{m=1}^M$ of size M;
    With θ_f fixed, update r by ascending its stochastic gradient $\nabla_{\theta_r} E(\theta_f, \theta_r) :=$

$$\nabla_{\theta_r} \sum_{m=1}^{M} \left[\sum_{\lambda_l \in \Lambda} 1(\lambda_m = \lambda_l) \log r(f(x_m; \theta_f); \theta_r)_l \right];$$

  end for
  Sample minibatch $\{x_m, y_m, \lambda_m\}_{m=1}^M$ of size M; ▷ Update f
  With θ_r fixed, update f by descending its stochastic gradient $\nabla_{\theta_f} E(\theta_f, \theta_r) :=$

$$\nabla_{\theta_f} \sum_{m=1}^{M} \left[- \sum_{y_c \in \mathcal{Y}} 1(y_m = y_c) \log f(x_m; \theta_f)_c + \sum_{\lambda_l \in \Lambda} 1(\lambda_m = \lambda_l) \log r(f(x_m; \theta_f); \theta_r)_l \right];$$

end for

4 Theoretical results

In this section, we show that in the setting of Algorithm 1, the procedure converges to a classifier f which is a pivotal quantity in the sense of Eqn. 3. Results below are derived in a non-parametric setting, by assuming that both f and r have enough capacity. To simplify the presentation, we also assume the uniform prior $p(\lambda) = \frac{1}{|\Lambda|}$ for all $\lambda \in \Lambda$, e.g. by having the same number of training samples for each modality λ of the nuisance parameter.

Proposition 1. *Let θ_f be fixed and $\hat{\theta}_r = \arg\max_{\theta_r} E(\theta_f, \theta_r)$. If $r(f(X;\theta_f);\hat{\theta}_r)_l = \frac{1}{|\Lambda|}$ for all λ_l, then f is a pivotal quantity.*

Proof. Let us first recall that the cross-entropy for distributions p and q is minimized when $p = q$. For $\mathcal{L}_r$ defined as the cross-entropy between the true conditional distribution of the nuisance $p_{\lambda|f(X;\theta_f)}$ and the approximate conditional distribution of the nuisance $p_{r(f(X;\theta_f);\theta_r)|f(X)}$, the optimal parameters $\hat{\theta}_r = \arg\max_{\theta_r} E(\theta_f, \theta_r) = \arg\min_{\theta_r} L_r(\theta_f, \theta_r)$ are therefore such that $p_{\lambda|f(X;\theta_f)} = p_{r(f(X;\theta_f);\hat{\theta}_r)|f(X)}$.

In other words, for all $\lambda_l \in \Lambda$, we have $r(f(X;\theta_f);\hat{\theta}_r)_l = p(\lambda_l|f(X;\theta_f))$. By assumption, $r(f(X;\theta_f);\hat{\theta}_r)_l = \frac{1}{|\Lambda|}$, and therefore $p(\lambda_l|f(X;\theta_f)) = \frac{1}{|\Lambda|}$. Using the Bayes' rule, we write

$$\begin{aligned} p(f(X;\theta_f)|\lambda_l) &= \frac{p(\lambda_l|f(X;\theta_f))p(f(X;\theta_f))}{p(\lambda_l)} \\ &= \frac{\frac{1}{|\Lambda|}p(f(X;\theta_f))}{\frac{1}{|\Lambda|}} \\ &= p(f(X;\theta_f)), \end{aligned}$$

which holds for all $\lambda_l \in \Lambda$ and implies that f is a pivotal quantity. □

Proposition 2. *[GL: proof 2: if Lf can be minimized under the pivotal constraint, then at the saddle point r is such that r(f(x)) = 1/N. [OK]]*

5 Experiments

6 Related work

[GL: Similar to domain adaptation, but with infinitely many domains, as parameterized by λ, also related to transfer learning.]

7 Conclusions

Acknowledgments

References

[1] M. H. Degroot and M. J. Schervish, *Probability and statistics*. 4 ed., 2010.

[2] I. Goodfellow, J. Pouget-Abadie, M. Mirza, B. Xu, D. Warde-Farley, S. Ozair, A. Courville, and Y. Bengio, "Generative adversarial nets," in *Advances in Neural Information Processing Systems*, pp. 2672–2680, 2014.