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

$$f(X_{\lambda_i}(\omega); \theta_f) = f(X_{\lambda_j}(\omega); \theta_f) \tag{1}$$

for any sample $\omega \in \Omega$ and any λ_i, λ_j pair of values of the nuisance parameter.

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

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

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 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 $\{\omega | f(X_{\lambda_i}(\omega); \theta_f) = y\}$ and $\{\omega' | f(X_{\lambda_j}(\omega'); \theta_f) = y\}$ do not need to be the same for the equality to hold. With this distinction, but as only Eqn. 2 is of direct interest in this work, we further simplify notations by denoting the pivotal quantity criterion as

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

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29th Conference on Neural Information Processing Systems (NIPS 2016), Barcelona, Spain.

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 model $r(\cdot; \theta_r) : \mathbb{R} \mapsto \Lambda$ of parameters θ_r and associated loss $\mathcal{L}_r(\theta_r)$. This model takes as input realizations of $f(X; \theta_f)$ and produces as output estimates $r(f(X; \theta_f)) = \hat{p}(\lambda | f(X; \theta_f))$ that $f(X; \theta_f)$ is generated from the nuisance value λ. 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. 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

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

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

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

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

[GL: Sketch the optimization algoritm]

4 Theoretical results

[GL: proof 1: if r optimal and r(f(x)) = 1/N then f is pivotal. [OK]] [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.