

---

# Verification of deep probabilistic models

---

**Krishnamurthy (Dj) Dvijotham**  
DeepMind  
London, UK  
dvij@cs.washington.edu

**Marta Garnelo**  
DeepMind  
London, UK  
garnelo@google.com

**Alhussein Fawzi**  
DeepMind  
London, UK  
afawzi@google.com

**Pushmeet Kohli**  
DeepMind  
London, UK  
pushmeet@google.com

## Abstract

Probabilistic models are a critical part of the modern deep learning toolbox - ranging from generative models (VAEs, GANs), sequence to sequence models used in machine translation and speech processing to models over functional spaces (conditional neural processes, neural processes). Given the size and complexity of these models, safely deploying them in applications requires the development of tools to analyze their behavior rigorously and provide some guarantees that these models are consistent with a list of desirable properties or *specifications*. For example, a machine translation model should produce semantically equivalent outputs for innocuous changes in the input to the model. A functional regression model that is learning a distribution over monotonic functions should predict a larger value at a larger input. Verification of these properties requires a new framework that goes beyond notions of verification studied in deterministic feedforward networks, since requiring worst-case guarantees in probabilistic models is likely to produce conservative or vacuous results. We propose a novel formulation of verification for deep probabilistic models that take in conditioning inputs and sample latent variables in the course of producing an output: We require that the output of the model satisfies a linear constraint *with high probability over the sampling of latent variables and for every choice of conditioning input to the model*. We show that rigorous lower bounds on the probability that the constraint is satisfied can be obtained efficiently. Experiments with neural processes show that several properties of interest while modeling functional spaces can be modeled within this framework (monotonicity, convexity) and verified efficiently using our algorithms.

## 1 Introduction

Several deep learning models are inherently probabilistic in nature. Common examples include generative models like variational autoencoders [Kingma and Welling, 2013, Sohn et al., 2015], functional regression models like neural processes [Garnelo et al., 2018a,b], models with attention mechanisms [Xu et al., 2015] and sequence to sequence models [Van Den Oord et al., 2016]. Given the widespread application of such models, it is of interest to develop tools that formally verify consistency of these models with specifications of interest (for example, a functional regression model should only produce functions within the class of functions of interest - monotonic, convex etc., or an attention model only attends to a relevant parts of the input). However, verification in a worst-case sense over inputs and probabilistic components is likely to lead to meaningless or trivial results. For example, models that have Gaussian latent variables can produce garbage outputs if the

latent variables take extreme large positive or negative values (which is possible, albeit unlikely). Thus, a different form of verification is necessary in such models. We propose the following notion here - for all conditioning inputs to the model within a given set of interest, with high probability over the sampling of latent variables, the output of the network satisfies a certain property. Formally, the contributions of this paper are:

- Formalizing a notion of verification that is applicable to deep probabilistic models and extending verification algorithms to apply to deep probabilistic models, like VAEs [Kingma and Welling, 2013], conditional VAEs [Sohn et al., 2015], conditional neural processes [Garnelo et al., 2018a] and neural processes [Garnelo et al., 2018b].
- Experimental results on neural processes [Garnelo et al., 2018b] showing that the verification algorithm can prove interesting properties about a learnt neural process model.

## 2 Verification of deep probabilistic models

We formulate the problem of verification of deep probabilistic models. We focus on a special architecture here (extension to more general models will be pursued in future work). Since verification is concerned with checking properties of ML models after they have been trained, we are primarily interested in the decoder of deep probabilistic models like conditional VAEs [Sohn et al., 2015] and (conditional) neural processes [Garnelo et al., 2018b,a]. A typical architecture for the decoder phase of these models is a neural network that receives as input both a conditioning input, denoted  $x$ , and a latent variable sampled from a distribution generated by the encoder, denoted  $z$ . In most architectures, it is common for the latent variable  $z$  to be sampled from a Gaussian distribution.

Thus, the output of the model is given by  $f(x, z)$ ,  $z \sim \mathcal{N}(0, I)$  where  $f$  is a decoder network.<sup>1</sup> We will assume that  $f$  is composed of layers of transformations of the form  $x_{k+1} = W_k h_k(x_k) + b_k$  where  $h_k$  is a component-wise nonlinearity (like ReLU/sigmoid/tanh) and  $(W_k, b_k)$  define a linear transformation. Note that this can capture convolutional networks as well, since a convolution is simply a specially structured linear transformation. We will use  $x$  to denote either single inputs or a stacked vector of several inputs. If  $x$  is a stacked vector, we assume that the network outputs a stacked vector of outputs corresponding to each input in  $x$ .

**Verification problem:** The verification problem, parameterized by a vector of coefficients  $c$  and scalar  $d, \epsilon$ , is defined as follows: Check that the predictor (decoder) function  $f$  satisfies the following:

$$\mathbb{P}(c^T f(x, z) + d \geq 0) \leq \epsilon \quad \forall x \in \mathcal{X} \quad (1)$$

where  $\mathcal{X}$  is a set of inputs of interest and  $\mathbb{P}$  refers to the probability measure induced by the random variable  $z$ . Thus, we require that the output  $y$  of the network satisfies the constraint  $c^T y + d \leq 0$  with probability at least  $1 - \epsilon$  for each input  $x \in \mathcal{X}$ .

In this paper, we will primarily work with neural processes that perform functional regression, where  $f$  predicts the value of an unknown function at a target point given a set of context points and corresponding function values. In this setting, it is of interest to verify that the outputs of the model satisfy properties of interest that are known to be satisfied for the class of functions being modeled: *Boundedness*: In several domains, the functions of interest ought to be bounded above (or below) by a fixed number  $a$  - for example, if the class of functions are cumulative distribution functions, they must be bounded between 0 and 1. This can be modeled as:

$$\mathbb{P}(f(x, z) - a \geq 0) \leq \epsilon \quad \forall x \in \mathcal{X}$$

or,  $f(x, z) \leq a$  with high probability.

*Monotonicity*: Monotonicity is another property of interest (that has to be true for CDFs):

$$\mathbb{P}(f(x_1, z) - f(x_2, z) \geq 0) \leq \epsilon \quad \forall (x_1, x_2) \in \mathcal{X}, x_1 \leq x_2$$

<sup>1</sup>Note here that the assumption  $z$  is sampled from a standard normal distribution is not restrictive, since if  $z \sim \mathcal{N}(\mu, \Sigma)$  we can always reparameterize  $z = \Sigma^{1/2} \tilde{z} + \mu$  where  $\tilde{z} \sim \mathcal{N}(0, I)$ . This framework can also extend to models with stochasticity entering at intermediate layers and to models with multiplicative interactions - such extensions will be pursued in an extended version of this paper.

or that  $f(x_1, z) \leq f(x_2, z)$  with high probability. Denoting  $x = (x_1, x_2)$  (the stacked vector of inputs) and choosing  $c = (1, -1)$ , this can again be modeled in our framework.

*Midpoint-Convexity:*

$$\mathbb{P}\left(\frac{f(x_1, z) + f(x_2, z)}{2} - f\left(\frac{x_1 + x_2}{2}, z\right) \geq 0\right) \leq \epsilon \quad \forall (x_1, x_2) \in \mathcal{X}$$

or that  $\frac{f(x_1, z) + f(x_2, z)}{2} \leq f\left(\frac{x_1 + x_2}{2}, z\right)$  with high probability (midpoint convexity is equivalent to convexity for continuous and bounded functions [Boyd and Vandenberghe, 2004]). Denoting  $x = (x_1, x_2, \frac{x_1 + x_2}{2})$  (the stacked vector of inputs) and choosing  $c = (\frac{1}{2}, \frac{1}{2}, -1)$ , this can again be modeled in our framework. This can be particularly useful in the context of Bayesian optimization [Frazier, 2018], where the posterior over functions produced by a model should be easy to optimize to find the next target point to acquire new information.

### 3 Verification algorithm

Ensuring that (1) is satisfied is challenging for two reasons: The space of inputs  $\mathcal{X}$  can be large and checking that the constraint holds is challenging (it has been shown to be NP-hard to check even approximately in [Weng et al., 2018]), in the worst case requiring a brute force enumeration approach using SMT [Katz et al., 2017] or mixed integer programming solvers [Bunel et al., 2017], which have not yet been scaled to realistically sized modern deep learning systems. However, for probabilistic models, an additional source of difficulty is that computing the probability  $\mathbb{P}(c^T f(x, z) + d \geq 0)$ , even for a fixed  $x$ , involves solving an intractable probabilistic inference problem. While this can be estimated via Monte-Carlo sampling, since in the context of verification we are interested in rigorous guarantees, estimates do not suffice. We develop an approach to overcome these challenges.

Consider the optimization problem  $\max_{x \in \mathcal{X}} c^T f(x, z) + d$ . Exploiting the fact that  $f$  is composed of multiple layers of simple transformations, we can write this as

$$\begin{aligned} & \max_{x_0, x_1, \dots, x_K} c^T x_K + d \\ \text{Subject to } & x_{k+1} = W_k h_k(x_k) + b_k, \quad k = 1, \dots, K-1 \\ & x_1 = W_0 x_0 + \tilde{W}_0 z + b_0, x_0 \in \mathcal{X} \end{aligned}$$

where  $(W_0, \tilde{W}_0, b_0)$  define the first linear layer that takes both the conditioning input  $x$  and the latent variable  $z$ .

We first condition on the event  $z \in [\alpha, \beta]$  and assume that  $\mathcal{X} = [l_0, u_0]$  is a set defined by interval constraints on the input  $x$ . Given these, we can infer bounds for all the intermediate layers using the techniques described in [Dvijotham et al., 2018, Weng et al., 2018] to obtain  $l_k \leq x_k \leq u_k$ <sup>2</sup>. Since  $x_K = W_{K-1} h_{K-1}(x_{K-1}) + b_{K-1}$ , we can further simplify the problem to

$$\begin{aligned} & \max_{x_0, x_1, \dots, x_{K-1}} c^T (W_{K-1} h_{K-1}(x_{K-1}) + b_{K-1}) + d \\ \text{Subject to } & x_{k+1} = W_k h_k(x_k) + b_k, \quad k = 1, \dots, K-2 \\ & x_1 = W_0 x_0 + \tilde{W}_0 z + b_0 \\ & l_k \leq x_k \leq u_k, \quad k = 0, \dots, K-1 \\ & \alpha \leq z \leq \beta \end{aligned}$$

Taking the Lagrangian dual of this problem and rearranging terms using a construction similar to Dvijotham et al. [2018], we obtain

$$G(\lambda, z) = d + \nu_0^T z + \sum_{k=0}^{K-1} \max_{l_k \leq x_k \leq u_k} \nu_k^T h_k(x_k) - \lambda_{k-1}^T x_k + \lambda_k^T b_k \quad (2)$$

where  $\nu_k = W_k^T \lambda_k$  and  $\lambda_{K-1} = c$ ,  $\lambda_{-1} = 0$  and  $\lambda = \{\lambda_k\}_{k=0}^{K-2} \in \mathbb{R}^p$  ( $p$  is the sum of sizes of the intermediate layers). While the bounds on  $z$  do not appear explicitly,  $G$  depends on them via  $l_k, u_k$

---

<sup>2</sup>Note that  $l_k, u_k$  depend on  $\alpha, \beta$ .

Since the  $h_k$  are component-wise nonlinearities, the maximization can be solved independently for each dimension of  $x_k$  (typically in closed-form for most common activation functions, as described in [Dvijotham et al., 2018]) and thus the dual function can be computed easily. By weak duality [Boyd and Vandenberghe, 2004], we have  $c^T f(x, z) + d \leq G(\lambda, z) \quad \forall x \in \mathcal{X}, \lambda \in \mathbb{R}^p, z \in [\alpha, \beta]$ . Thus,

$$\mathbb{P}(c^T f(x, z) + d \geq 0 | z \in [\alpha, \beta]) \leq \mathbb{P}(G(\lambda, z) \geq 0 | z \in [\alpha, \beta])$$

Denote the events  $c^T f(x, z) + d \geq 0, z \in [\alpha, \beta]$  and  $G(\lambda, z) \geq 0$  as  $A, B, C$  respectively. We then have

$$P(A) = P(A|B)P(B) + P(A|\neg B)P(\neg B) \leq P(C|B)P(B) + P(\neg B) \leq P(C) + P(\neg B)$$

Thus,  $\mathbb{P}(c^T f(x, z) + d \geq 0) \leq \mathbb{P}(G(\lambda, z) \geq 0) + \mathbb{P}(z \notin [\alpha, \beta])$ . Define  $g(\lambda) = G(\lambda, z) - \nu_0^T z$  so that

$$\mathbb{P}(G(\lambda, z) \geq 0) = \mathbb{P}(\nu_0^T z \geq -g(\lambda)) = \mathbb{P}\left(\omega \geq -\frac{g(\lambda)}{\|\nu_0\|}\right) = \frac{1}{2}\text{erfc}\left(-\frac{g(\lambda)}{\sqrt{2}\|\nu_0\|}\right)$$

where  $\omega$  is a standard normal random variable and  $\text{erfc}$  is the Gaussian complementary error function.

**Theorem 1.** *The probability of violating the specification (1) can be bounded as:*

$$\mathbb{P}(c^T f(x, z) + d \geq 0) \leq \frac{1}{2}\text{erfc}\left(-\frac{g(\lambda)}{\sqrt{2}\|\nu_0\|}\right) + \mathbb{P}(z \notin [\alpha, \beta]) \quad (3)$$

for any choice of  $\lambda, \alpha, \beta$  with  $\alpha \leq \beta$ .

We note that since the RHS of (3) is differentiable wrt  $\lambda, \alpha, \beta$ , it can be optimized using gradient descent to find the tightest possible bound. By parameterizing  $\beta = \alpha + \eta^2$ , this can be done by solving an unconstrained optimization problem over  $\alpha, \eta, \lambda$  using gradient descent. Although nonconvex, in practice we find that this optimization can be solved efficiently.

## 4 Experiments

A neural process [Garnelo et al., 2018b] may be viewed as a neural approximation of a gaussian process that learns a posterior distribution over functions. The NP is trained on functions that are cumulative distribution functions (CDFs) of beta distributions with varying parameters - at the end of training, we expect that the neural process has learned a posterior distribution that, with high probability, produces samples that look like a CDF. The decoder we use is a fully connected network with a 3 hidden layer of 64 units each and relu activations.

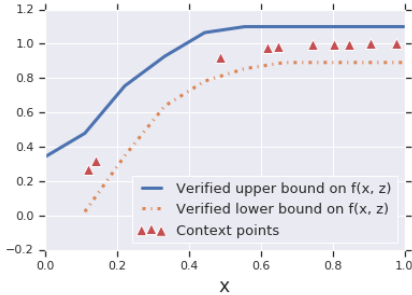


Figure 1: Verification of NP predictions

we consider intervals of width .02, ie  $x \in \mathcal{X} = [\delta, \delta + .02]$  and plot the value of  $a$  as a function of  $\delta$ . Similarly, we find the largest lower bound  $b$  such that  $f(x, z) \geq b$  with probability at least  $1 - \epsilon$ . The upper bound is plotted as a solid blue line, and the lower bound as a dashed yellow line. The results show that the values of  $a, b$  increase with  $\delta$ , and generally conform with the properties of a CDF, thus showing that our verification algorithm is indeed able to prove properties we expect to be true of the model.

## 5 Conclusions

We presented a novel verification formulation and algorithm for verification of deep probabilistic models. In future work, we will study more complex models (CVAEs, GANs), specifications (for example, verifying disentangled representations) and integration of verification into training.

## References

- Stephen Boyd and Lieven Vandenberghe. *Convex optimization*. Cambridge university press, 2004.
- Rudy Bunel, Ilker Turkaslan, Philip HS Torr, Pushmeet Kohli, and M Pawan Kumar. Piecewise linear neural network verification: A comparative study. *arXiv preprint arXiv:1711.00455*, 2017.
- Krishnamuthy Dvijotham, Robert Stanforth, Sven Gowal, Timothy Mann, and Pushmeet Kohli. Towards scalable verification of neural networks: A dual approach. In *Conference on Uncertainty in Artificial Intelligence*, 2018.
- Peter I Frazier. A tutorial on bayesian optimization. *arXiv preprint arXiv:1807.02811*, 2018.
- Marta Garnelo, Dan Rosenbaum, Chris J Maddison, Tiago Ramalho, David Saxton, Murray Shanahan, Yee Whye Teh, Danilo J Rezende, and SM Eslami. Conditional neural processes. *arXiv preprint arXiv:1807.01613*, 2018a.
- Marta Garnelo, Jonathan Schwarz, Dan Rosenbaum, Fabio Viola, Danilo J Rezende, SM Eslami, and Yee Whye Teh. Neural processes. *arXiv preprint arXiv:1807.01622*, 2018b.
- Guy Katz, Clark Barrett, David L Dill, Kyle Julian, and Mykel J Kochenderfer. Reluplex: An efficient smt solver for verifying deep neural networks. In *International Conference on Computer Aided Verification*, pages 97–117. Springer, 2017.
- Diederik P Kingma and Max Welling. Auto-encoding variational bayes. *arXiv preprint arXiv:1312.6114*, 2013.
- Kihyuk Sohn, Honglak Lee, and Xinchen Yan. Learning structured output representation using deep conditional generative models. In *Advances in Neural Information Processing Systems*, pages 3483–3491, 2015.
- Aaron Van Den Oord, Sander Dieleman, Heiga Zen, Karen Simonyan, Oriol Vinyals, Alex Graves, Nal Kalchbrenner, Andrew Senior, and Koray Kavukcuoglu. Wavenet: A generative model for raw audio. *arXiv preprint arXiv:1609.03499*, 2016.
- Tsui-Wei Weng, Huan Zhang, Hongge Chen, Zhao Song, Cho-Jui Hsieh, Duane Boning, Inderjit S Dhillon, and Luca Daniel. Towards fast computation of certified robustness for relu networks. *arXiv preprint arXiv:1804.09699*, 2018.
- Kelvin Xu, Jimmy Ba, Ryan Kiros, Kyunghyun Cho, Aaron Courville, Ruslan Salakhudinov, Rich Zemel, and Yoshua Bengio. Show, attend and tell: Neural image caption generation with visual attention. In *International conference on machine learning*, pages 2048–2057, 2015.