Deep discriminative to kernel generative modeling

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Abstract. The fight between discriminative versus generative goes deep, in both the study of artificial and natural intelligence. In our view, both camps have complementary value, so, we sought to synergistic combine them. Here, we propose a methodology to convert deep discriminative networks to kernel generative networks. We leveraged the fact that deep models, including both random forests and deep networks, learn internal representations which are unions of polytopes with affine activation functions to conceptualize them both as generalized partitioning rules. From that perspective, we used foundational results on the relationship between histogram rules and kernel density estimators to obtain class conditional kernel density estimators from the deep models. We then studied the trade-offs we observed from implementing this strategy in low-dimensional settings, both theoretically and empirically, as a first step towards understanding. Theoretically, we show conditions under which our generative models are more efficient than the corresponding discriminative approaches. Empirically, when sample sizes are relatively high, the discriminative models tend to perform as well or better on discriminative metrics, such as classification rates and posterior calibration. However, when sample sizes are relatively low, the generative models outperform the discriminative ones even on discriminative metrics. Moreover, the generative ones can also sample from the distribution, obtain smoother posteriors, and extrapolate beyond the convex hull of the training data to handle OOD inputs more reasonably. Via human experiments we illustrate that our kernel generative networks (Kragen) behave more like humans than deep discriminative networks. We believe this approach may be an important step in unifying the thinking and approaches across the discriminative and generative divide.

1 Introduction

For biological agents, experience is not only important to excel in the relevant skills but also to learn where the agent should not be confident at all. From an evolutionary perspective, it is a mandatory property for the biological intelligence to ensure its survival. In short, any intelligent system should get more conscious about its limitations with more experience. However, most of the traditional machine learning models seem to defy this natural law of being intelligent. Although with more training data (experience) they get better at inferring on the samples lying within the convex hull of the training data [1–4], they yield highly confident predictions over the samples lying far away from the training data. Uniform confidence over the classes in the out-of-distribution (OOD) region is crucial for applications like autonomous driving and computer-assisted surgery, where any aberrant reading should be detected and taken care of immediately [1, 5]. An intelligent model capable of detecting OOD data can be a life-saver in these cases.

Intuitively, the easiest solution for OOD sample detection is to learn a function that gives higher scores for in-distribution data and lower scores for OOD data, and thereby re-scale the posterior from the original model accordingly [6]. However, any model that could learn how to detect OOD samples, would have its own problem of being overconfident for the corresponding OOD samples [7, 8]. Again, as mentioned in Hein et al. [1], re-scaling the posteriors cannot solve the OOD overconfidence problem in ReLU (rectified linear unit) networks. Many previous algorithms [1, 7, 9] tried different approaches by modifying the training loss function. Among them, Hein et al. [1] and Hendrycks et al. [7] tried to calibrate the network confidence over the OOD data by exhaustively training the network to be less confident on the OOD data. However, this process would require infinite OOD data for a satisfactory robustness

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against all possible OOD scenarios. Moreover, these huge OOD data would require a model with larger capacity. At the same time, one can adversarially manipulate an OOD sample to find another OOD sample where the model is overconfident [1, 10, 11]. Erdil et al. [12] proposed kernel density estimation techniques over the features learned at different layers of a deep network and combined the scores from all the layers using logistic regression. However, a single model having both good in-distribution performance and OOD robustness is highly desirable.

In this paper, we consider replacing the constant or affine functions learned over the polytopes in random forests and ReLU networks, respectively [1, 4, 13]. We propose two novel kernel density polytope techniques named Kernel Density Forest (KDF) and Kernel Density Network (KDN). They converge to the true training distribution in the limit when we have infinite training samples for random forests and ReLU networks with sufficient complexity, respectively. At the same time, the estimated likelihood from the kernel density polytopes decreases for samples far away from the training samples. By adding suitable bias to the kernel density estimate, we can achieve uniform posterior over the classes in the OOD region. It completely excludes the need for providing OOD examples to the model. We conduct several simulation studies that show both KDF and KDN are robust against OOD samples while maintain good performance in the in-distribution region.

2 Background

In this section, we formulate the problem we are going to address and provide necessary background information about the OOD overconfidence problem in random forests and deep networks.

2.1 Problem Formulation

Consider a supervised learning problem with independent and identically distributed training samples \( \{(x_i, y_i)\}_{i=1}^N \) such that \((X, Y) \sim P_{X \times Y}\), where \(X \sim P_{in}\) is a \(X \in \mathbb{R}^d\) valued input and \(Y = \{1, \cdots, K\}\) valued label. We consider the OOD-distributions \(P_{out}\) with their support spanning the whole feature space excluding the support of \(P_{in}\). In other words, \(P_{out} := \bigcup_j P_j\), where \(P_j\) is any distribution having no overlap with \(P_{in}\). Note that this notion of OOD is different from that of the traditional OOD learnability literature [15] where the OOD distribution may share support with the training distribution. Here the goal is to learn a model \(g: \mathbb{R}^d \times \{1, \cdots, K\} \rightarrow [0, 1]^K\) such that,

\[
g(x) = \begin{cases} P[Y = k | X = x], & \forall k \text{ if } x \sim P_{in} \\ P[Y = k], & \forall k \text{ if } x \sim P_{out} \end{cases}
\]

where \(P[Y = k | X = x]\) is the true posterior probability of class \(k\) given by,

\[
P[Y = k | X = x] = \frac{f_k(x)P[Y = k]}{\sum_{i=1}^K f_i(x)P[Y = i]}
\]

Here, \(f_i(x)\) is the true training class conditional density function of class \(i\). The class prediction \(\hat{y}\) for a test sample \(x\) is obtained by,

\[
\hat{y} = \arg \max (g(x))
\]

2.2 Overconfidence Problem in Random Forests

Random forests (RFs) split the feature space \(\mathbb{R}^d\) into a union of axis aligned polytopes \(Q_r\) such that \(\mathbb{R}^d = \bigcup_{r=1}^p Q_r\), and calculate a constant posterior over those polytopes by counting the number of training samples within each polytope. For instance, the posterior probability of class \(k\) w.r.t to the polytope \(Q_r\) is given by,

\[
P[Y = k | x \in Q_r] = \frac{N_{rk}}{N_r}
\]
where \( N_{rk} \) is the total number of samples with class label \( y \) in the polytope \( Q_r \) and \( N_r \) is the total number of samples in the same polytope. The polytopes lying at the boundary of the training data extend to the whole feature space and hence encompass all the OOD samples. Since the posterior probability for a class is constant across each of those outer polytopes, decision trees and random forests (ensemble of decision trees) tend to be overconfident when making predictions for the OOD inputs.

### 2.3 Overconfidence Problem in Deep Networks

Consider a deep network (DN) \( F : \mathbb{R}^d \to [0, 1]^K \) with \( L + 1 \) number of layers. If \( W^{(l)} \in \mathbb{R}^{u_l \times u_{l-1}} \) is the weight matrix and \( b^{(l)} \in \mathbb{R}^{u_l} \) is the bias vector of layer \( l \), then for \( x \in \mathbb{R}^d \) we can recursively define the pre- and post-activation output of each layer \( l \) \((l = 1, \ldots, L + 1)\) as,

\[
F^{(l)} = W^{(l)} G^{(l-1)}(x) + b^{(l)}
\]

and

\[
G^{(l)} = \sigma(F^{(l)}(x))
\]

respectively. Here, \( \sigma(t) = \max\{0, t\} \) is the ReLU activation function and \( G^{(0)}(x) = x \).

A trained deep network, at the penultimate layer \((l = L)\), induces a finite set of convex polytopes \( \{Q_{i}^{r}\}_{i=1}^{P} \) in the input space \( \mathbb{R}^d \) such that \( \bigcup_{i=1}^{P} Q_{i} = \mathbb{R}^d \). Every point \( x \) contained within a polytope \( Q_{i} \) activates the same unique subset of neurons in the network. Therefore, when restricted to \( Q_{i} \), the penultimate layer output \( F^{(L+1)}(.) \) reduces to an affine function:

\[
F^{(L+1)}(x) = V_{i}^{(L+1)} \cdot x + a_{i}^{(L+1)} \quad \forall x \in Q_{i}
\]

where \( V_{i}^{(L+1)} \) and \( a_{i}^{(L+1)} \) are unique to \( Q_{i} \). Hein et al. [1] provides explicit expressions for \( V_{i}^{(L+1)} \) and \( a_{i}^{(L+1)} \) in their work.

In summary, a deep network partitions the input space into a finite number of polytopes and learns a unique affine function over each polytope. Since the polytopes located at the training data (in-distribution) boundary extend to infinity, evaluating an affine function over such regions would amount to producing predictions with high confidence scores for inputs that are far away from the training data. This gives rise to the overconfidence problem of the deep networks when it comes to OOD inputs.

### 3 Kernel Density Polytopes

In this section, we describe how we fit Gaussian kernels over the polytopes learnt using RFs and DNs, respectively. This leads to the two main contributions of our work, KDFs and KDNs.

#### 3.1 Kernel Density Forests

Consider \( T \) number of decision trees in a random forest ensemble. Each tree \( t \) partitions the feature space into \( M_t \) polytopes resulting in a set of \( \{Q_{r,t}\}_{r=1}^{M_t} \). The intersection of these polytopes gives a new set of polytopes \( \{Q_{r}\}_{r=1}^{P} \) for the forest. We are interested in fitting a Gaussian kernel \( K_\nu(.) \) for each polytope \( Q_{r} \) for each class \( k \). Naturally, we would estimate the parameters \( \mu_{rk} \) and \( \Sigma_{rk} \) of \( K_\nu(.) \) from the samples with label \( k \) contained within \( Q_{r} \). However, in order to improve the estimates for these parameters, we also incorporate the samples from other polytopes \( Q_{s} \) based on the similarity between \( Q_{r} \) and \( Q_{s} \).

In order to measure this similarity, for any point \( x_{r} \in Q_{r} \) with label \( k \), we push every other sample point \( x_{s} \in Q_{s} \) with the same label down the trees. If the two points end up in the same leaf across all the trees, they belong to the same polytope, i.e. \( Q_{r} = Q_{s} \). The two points belong to different polytopes \( (Q_{r} \neq Q_{s}) \) if they only share a fraction or none of matching leaves. Hence, we weigh down
Algorithm 1: Fit a KDX model.

Require:
1. \( M \) \( \triangleright \) the parent learner (random forest or deep network model)
2. \( \mathcal{D}_n = (\mathbf{X}, y) \in \mathbb{R}^{N \times d} \times \{1, \ldots, K\}^N \) \( \triangleright \) training data

Ensure: \( g \) \( \triangleright \) a KDX model

1: function \( \text{KDX} \cdot \text{FIT}(M, \mathbf{X}, y) \)
2: \( \theta \leftarrow M \cdot \text{FIT}(\mathbf{X}, y) \) \( \triangleright \) train the parent learner
3: for \( k = 1, \ldots, K \) do
4: \( \mathbf{X}_k \leftarrow \) input samples with label \( k \) \( \triangleright \mathbf{X}_k \in \mathbb{R}^{N_k \times d} \)
5: \( \{Q_r\}_{r=1}^{m_k} \leftarrow \text{GETPOLYTOPES}(\mathbf{X}_k, \theta) \) \( \triangleright \) iterate over each polytope in class \( k \)
6: for \( r = 1, \ldots, m_k \) do
7: \( g_r \cdot N_{rk} \leftarrow \text{COMPUTEWEIGHTS}(Q_r, \mathbf{X}_k, \theta) \) \( \triangleright \mathbf{w}_{rk} \in [0, 1]^{N_k} \)
8: \( g_r \cdot \mu_{rk}, g_r \cdot \Sigma_{rk} \leftarrow \text{ESTIMATEPARAMETERS}(\mathbf{X}_k, \mathbf{w}_{rk}) \) \( \triangleright \) Estimate parameters using weighted MLE
9: end for
10: end for
11: return \( g \)
12: end function

the contribution from a neighboring polytope \( Q_s \) for estimating the kernel in the current polytope \( Q_r \) using the following weighting scheme:

\[
    w_{rs} = \begin{cases} 
        \frac{l_{rs}}{T}, & \text{if } Q_r \neq Q_s \\ 
        1, & \text{if } Q_r = Q_s 
    \end{cases}
\]

where \( l_{rs} \) is the total number trees \( x_r \) and \( x_s \) end up in the same leaf node. The higher the weight, the closer two polytopes are to each other in the feature space. With the weights defined above, we estimate the parameters of kernel \( K_r(\cdot) \) using weighted maximum likelihood estimator over the sample points for each label. By summing over the estimated kernels, we arrive at an estimate \( \hat{f}_k(x) \) for the class conditional density:

\[
    \hat{f}_k(x) = \frac{1}{N_k} \sum_{r=1}^{p} N_{rk} K_r(x)
\]

where \( N_{rk} \) is the total number of samples that end up in the current polytope \( Q_r \) and \( N_k = \sum_{r=1}^{p} N_{rk} \) is the total number of training samples with class \( k \).

3.2 Kernel Density Networks: Consider the deep network \( F \) described in section 2.3. We can obtain the set of polytopes \( \{Q_{rk}\}_{r=1}^{m_k} \) by grouping the samples having label \( k \) that activate the same subset of neurons in the network. Note that \( Q_{rk_1} \cap Q_{rk_2} = \emptyset, \forall r_1 \neq r_2 \). From Hein et al. [1] it follows that for each \( x \in Q_{rk} \), the pre-activation function \( F^{(l)}(x) \) of layer \( l \) reduces to the affine function \( V^{(l)}_{rk} x + a^{(l)}_{rk} \), for \( l = 1, \ldots, L \).

We are interested in fitting a Gaussian kernel \( K_r(\cdot) \) over the polytope \( Q_{rk} \). The simplest way of estimating the mean \( \mu_{rk} \) and bandwidth (covariance) matrix \( \Sigma_{rk} \) of \( K_r(\cdot) \) is to estimate them from the
Algorithm 2 Computing weights in KDF

Require:
(1) $Q_r$ $\triangleright$ a polytope in class $k$
(2) $X_k \in \mathbb{R}^{N_k \times d}$ $\triangleright$ input samples with class label $k$
(3) $\theta$ $\triangleright$ parent random forest model

Ensure: $w \in [0, 1]^{N_k}$ $\triangleright$ weights for each input sample in class $k$

1: function COMPUTEWEIGHTS($Q_r, X_k, \theta$)
2: $L \leftarrow$ PUSHDOWNTREES($X_k$) $\triangleright$ push the samples $X_k$ down the $T$ trees in total and store the leaf number they end up in $L \in \mathbb{R}^{N \times T}$
3: $l \leftarrow$ COUNTMATCHES($L$) $\triangleright$ count the number times the samples end up in the leaf as those for the samples in the current polytope and $l \in \mathbb{R}^{N_k}$
4: $w \leftarrow \frac{1}{T}$
5: return $w$
6: end function

$|Q_{rk}| = N_{rk}$ number of training samples within $Q_{rk}$. However, in order to improve the kernel parameter estimates we also incorporate samples that lie within a neighborhood of $Q_{rk}$. To this end, we employ a weighting function $w(\cdot)$ that assigns a weight of 1 for samples within $Q_{rk}$ and decreasing weights for input samples outside $Q_{rk}$ as they move away from it:

(3.3) $w(x) = \begin{cases} \exp(-d/h), & \text{if } \exp(-d/h) \geq T \\ 0, & \text{else} \end{cases}$

where

(3.4) $d = \sum_{l=1}^{L} \| F^{(l)}(x) - (V^{(l)}_{rk} x + a^{(l)}_{rk}) \|_2$

For a given sample $x$, (3.4) measures the difference between pre-activation output of each layer and the affine restriction of $Q_{rk}$ at that layer across the network. It is apparent that $d = 0$ for every $x \in Q_{rk}$ and $d$ gets higher as $x$ moves away from $Q_{rk}$. This measure is converted to a weight within $[0, 1]$ by (3.3). $T$ is a threshold used to set the extremely small weights to zero, and $h$ is a parameter that controls the neighborhood size.

Based on the weights above, we estimate the parameters of $K_r(\cdot)$ from the samples having label $k$ using the weighted maximum likelihood estimator.

By summing over the kernels learnt over each $Q_{rk}$, we arrive at the class conditional density estimate $\hat{f}_k(x)$:

(3.5) $\hat{f}_k(x) = \frac{1}{N_k} \sum_{r=1}^{m_k} N_{rk} K_r(x)$

where, $N_k = \sum_{r=1}^{m_k} N_{rk}$ is the total number of training samples in class $k$.

3.3 Inference So far we have the class conditional densities estimated in (3.2) and (3.5). Note that these density functions are estimated as summation of Gaussian kernels. Hence, the likelihoods out
Algorithm 3 Computing weights in KDN

Require:
1. \( Q_r \) \( \triangleright \) a polytope in class \( k \)
2. \( X_k \in \mathbb{R}^{N_k \times d} \) \( \triangleright \) input samples with class label \( k \)
3. \( \theta \) \( \triangleright \) parent deep network model with parameters \( \{W_l, b_l\}_{l=1}^{L+1} \)

Ensure: \( w \in [0, 1]^{N_k} \) \( \triangleright \) weights for each input sample in class \( k \)

1: function COMPUTEWEIGHTS(\( Q_r, X_k, \theta \))
2: \( \{W_l, b_l\}_{l=1}^{L+1} \leftarrow \theta \)
3: \( A_0 \leftarrow X_k^T \)
4: \( A_{0,ref} \leftarrow X_k^T \)
5: \( d = 0 \)
6: for \( l = 1, \ldots, L \) do
7: \( m_l \leftarrow \text{ReLU} \) activation pattern induced by any \( x \in Q_r \) in the layer \( l \) of \( \theta \)
8: \( Z_l \leftarrow W_l A_{l-1} + b_l \)
9: \( A_l \leftarrow \text{ReLU}(Z_l) \)
10: \( Z_{l,ref} \leftarrow W_l A_{l-1,ref} + b_l \)
11: \( A_{l,ref} \leftarrow \text{diag}(m_l) Z_{l,ref} \)
12: \( d \leftarrow d + d(A_l - A_{l,ref}) \) \( \triangleright d(M_{r \times c}) \in \mathbb{R}^c \) returns the L2-norms of the column vectors of \( M \)
13: end for
14: \( w \leftarrow e^{-d/h} \)
15: \( w \leftarrow \text{THRESHOLD}(w, T) \) \( \triangleright \) Set the weights less than \( T \) to zero
16: return \( w \)
17: end function

of these functions decrease for sample points far away from the training samples. We can exploit this phenomenon to detect OOD samples. To be specific, we add the a bias to the class conditional density \( \hat{f}_k \):

\[
\tilde{f}_k(x) = \hat{f}_k(x) + \delta
\]

where the bias is given by

\[
\delta = \frac{\min \{ \min \{ \{ \hat{f}_k(x_i) \}_{i=1}^{N_k} \}_{k=1}^{K} \} }{CN}
\]

where \( C \) is a constant. Intuitively, the point in the training sample which yields minimum likelihood out of \( \hat{f}_k \) lies in the training data boundary. By multiplying it with a suitable constant, we can make \( \tilde{f}_k \) in (3.6) dominant compared to the bias in the in-distribution region whereas the bias term would dominate in the OOD region. Note that in (3.7), \( \delta \to 0 \) as the total training points, \( N \to \infty \). Now the inference step is common to both KDF and KDN. During inference, the class posterior probability (confidence) \( \hat{P}[Y = k | X = x] \) of class \( k \) for a test point \( x \) is estimated using the Bayes rule as follows:

\[
\hat{P}[Y = k | X = x] = \frac{\tilde{f}_k(x) \hat{P}[Y = k]}{\sum_{i=1}^{K} \tilde{f}_i(x) \hat{P}[Y = i]}
\]

where \( \hat{P}[Y = k] \) is the prior probability of class \( k \) estimated from the training data.
4 Theory

Theorem 1. Given the polytope size $h_r \to 0$, the number of samples within each polytope $N_{rk} \to \infty$ and $N_{rk}$ grows slowly compared to the total sample size $N_k \to 0$, kernel density polytope is an unbiased estimator of the true class conditional in-distribution density function $f_k(x)$.

Proof. Consider a point $x \in Q_s$. The class conditional density estimate for $x$ can be written as-

$$
\hat{f}_k(x) = \frac{1}{N_k} \sum_{r=1}^{p} N_{rk} K_r(x)
= \frac{1}{N_k} \sum_{r=1}^{p} N_{rk} \sum_{i=1}^{N_k} \mathbb{1}_{\{x_i \in Q_r\}} K_r(x)
= \frac{1}{N_k} \sum_{i=1}^{N_k} \mathbb{1}_{\{x_i \in Q_s\}} K_s(x) + \frac{1}{N_k} \sum_{r=1, r \neq s}^{p} \sum_{i=1}^{N_k} \mathbb{1}_{\{x_i \in Q_r\}} K_r(x)
= \frac{N_{sk} K_s(x)}{N_k} + \sum_{r=1, r \neq s}^{p} \frac{N_{rk} K_r(x)}{N_k}
$$

Now the polytope sample counts $N_{sk}, N_{rk}$ can be considered as binomially distributed as $N_{sk} \sim B(N_k, P_s), N_{rk} \sim B(N_k, P_r)$. By using mean value theorem, $P_r = h_r f_k(\zeta_r)$, where $\zeta_r \in Q_r$. Now,

$$
\mathbb{E}[\hat{f}_k(x)] = \frac{N_k P_r \mathbb{E}[K_s(x)]}{N_k} + \frac{\text{Cov}(N_{sk}, K_s(x))}{N_k}
+ \sum_{r=1, r \neq s}^{p} \frac{N_k P_r \mathbb{E}[K_r(x)]}{N_k} + \sum_{r=1, r \neq s}^{p} \frac{\text{Cov}(N_{rk}, K_r(x))}{N_k}
\Rightarrow h_s f_k(\zeta_s) \mathbb{E}[K_s(x)] + \frac{\text{Cov}(N_{sk}, K_s(x))}{N_k}
+ \sum_{r=1, r \neq s}^{p} h_r f(\zeta_r) \mathbb{E}[K_r(x)] + \sum_{r=1, r \neq s}^{p} \frac{\text{Cov}(N_{rk}, K_r(x))}{N_k}
$$

Consider, a forest with infinitely deep trees, i.e., $h_s, h_r \to 0$. For this case, $w_{rs} = 0$ whenever $Q_r \neq Q_s$. Therefore, as $h_s, h_r \to 0$, $f_k(\zeta_s) \to f_k(x)$ and $K_r(x) \to 0$ (as $x \notin Q_r$). Again, as $N_k \to \infty$ and $h_s \to 0$, the kernel bandwidth goes to zero and its center converges to $x$. Moreover, as the kernel bandwidth reduces, $K_s(\cdot)$ decays faster and the kernel resembles a uniform distribution over the polytope $Q_s$. As the area under the kernel is 1, $\mathbb{E}(K_s(x)) \to \frac{1}{h_s}$. Again, as $N_k \to \infty$ and $\frac{N_{sk}}{N_k} \to 0$, all the covariance terms go to 0. Therefore, $\mathbb{E}[\hat{f}_k(x)]$ becomes an asymptotically unbiased estimator of $f_k(x)$.

5 Experiments

In this section, we illustrate how KDFs and KDNs perform better than their respective parent models on simulation datasets. We also demonstrate how our algorithms’ posterior estimates better correspond to those of human intelligence.

5.1 Simulations

We construct five types of binary class simulations:
Figure 1: Simulation distributions and posterior estimates by different algorithms. Binary simulation data are generated within the region bounded by \([-1, 1] \times [-1, 1]\), then posteriors are estimated within the \([-2, 2] \times [-2, 2]\) region. Kernel Density Forests (KDFs) and Kernel Density Networks (KDNs) yield better estimates when compared to their respective parent models—random forests (RFs) and ReLU deep networks (DNs). They achieve particularly good posteriors in the out-of-distribution (OOD) region, while RFs and DNs yield overconfident posteriors.
• **Gaussian XOR** is a two-class classification problem with equal class priors. Conditioned on being in class 0, a sample is drawn from a mixture of two Gaussians with means $\pm [0.5, -0.5]^T$ and standard deviations of 0.25. Conditioned on being in class 1, a sample is drawn from a mixture of two Gaussians with means $\pm [0.5, -0.5]^T$ and standard deviations of 0.25.

• **Spiral** is a two-class classification problem with the following data distributions: let $K$ be the number of classes and $S \sim$ multinomial$(\frac{1}{K}, \ldots, \frac{1}{K}, n)$. Conditioned on $S$, each feature vector is parameterized by two variables, the radius $r$ and an angle $\theta$. For each sample, $r$ is sampled uniformly in $[0, 1]$. Conditioned on a particular class, the angles are evenly spaced between $\frac{4\pi(k-1)t_K}{K}$ and $\frac{4\pi(k)t_K}{K}$, where $t_K$ controls the number of turns in the spiral. To inject noise along the spirals, we add Gaussian noises to the evenly spaced angles $\theta' : \theta = \theta' + N(0, 0.09)$. The observed feature vector is then $(r \cos(\theta), r \sin(\theta))$. 

Figure 2: Binary classifications on simulation data. Each line shows median results from 45 repetitions and the shadowed regions represent the 25 and 75-th quantiles.
of a hidden layer with 10 posteriors (regions, demonstrating their overconfidence problems. Meanwhile, both KDFs and KDNs yield uniform posteriors. It is apparent that RFs and DNs yield highly confident predictions outside the in-distribution random forest has 500 nodes in each layer and is trained using the Adam optimizer at a learning rate of 3 × 10⁻⁴. Figure 1 illustrates the posteriors learned using these four models along with the true posteriors. It is apparent that RFs and DNs yield highly confident predictions outside the in-distribution regions, demonstrating their overconfidence problems. Meanwhile, both KDFs and KDNs yield uniform posteriors over the classes outside [−1, 1] × [−1, 1], which is consistent with human intelligence as described in Section 5.3. Furthermore, KDFs and KDNs also improve the posteriors within the in-distribution regions, showing no compromise while overcoming the overconfident problems in their parent models.

Figure 2 reports the algorithms’ in-distribution performance and confidence scores in both in-distribution and OOD regions. In terms of generalization error, both KDFs and KDNs achieve similar or even better performance compared to that of their respective parent models. Furthermore, our proposed models always achieve posteriors closer to the true posteriors compared to those of RFs and DNs, as illustrated in the Hellinger distance curves (Figure 2, second column). The mean maximum

| Simulation | AUROC | FPR@95 | AUROC | FPR@95 | AUROC | FPR@95 | AUROC | FPR@95 |
|------------|-------|--------|-------|--------|-------|--------|-------|--------|
| RF         | 0.89(±0.03) | 0.32(±0.09) | 0.98(±0.00) | 0.22(±0.08) | 0.90(±0.00) | 0.14(±0.01) | 0.93(±0.05) | 0.09(±0.01) |
| KDF        | 0.98(±0.01) | 0.32(±0.28) | 0.91(±0.00) | 0.22(±0.08) | 0.90(±0.00) | 0.14(±0.01) | 0.93(±0.05) | 0.09(±0.01) |
| DN         | 0.89(±0.03) | 0.22(±0.08) | 0.98(±0.00) | 0.14(±0.01) | 0.90(±0.00) | 0.12(±0.01) | 0.93(±0.05) | 0.09(±0.01) |
| KDN        | 0.99(±0.00) | 0.32(±0.38) | 0.90(±0.00) | 0.14(±0.01) | 0.90(±0.00) | 0.12(±0.01) | 0.93(±0.05) | 0.09(±0.01) |

Table 1: Performance metrics on the out-of-distribution (OOD) region: area under the receiver operating characteristic (AU-ROC) and false negative rates at 95% recall (FPR@95).

- **Circle** is a two-class classification problem with equal class priors. Conditioned on being in class 0, a sample is drawn from a circle centered at (0, 0) with a radius of 0.75. Conditioned on being in class 1, a sample is drawn from a circle centered at (0, 0) with a radius of 1, which is cut off by the region bounds. To inject noise along the circles, we add Gaussian noises to the circle radii \( r' = r + \mathcal{N}(0, 0.01) \).
- **Sinewave** is a two-class classification problem based on sine waves. Conditioned on being in class 0, a sample is drawn from the distribution \( y = \cos(\pi x) \). Conditioned on being in class 1, a sample is drawn from the distribution \( y = \sin(\pi x) \). We inject Gaussian noises to the sine wave heights \( y' = y + \mathcal{N}(0, 0.01) \).
- **Polynomial** is a two-class classification problem with the following data distributions: \( y = x^3 \). Conditioned on being in class 0, a sample is drawn from the distribution \( y = x^3 \). Conditioned on being in class 1, a sample is drawn from the distribution \( y = x^3 \). Gaussian noises are added to variables \( y' = y + \mathcal{N}(0, 0.01) \).

As in Figure 1, all data samples (10,000 per simulation) are bounded within the [−1, 1] × [−1, 1] region and equally divided into two classes (5,000 per class). We evaluate model performance of RFs, KDFs, DNs, and KDNs using in-distribution generalization errors, in-distribution Hellinger distances between true and estimate class posteriors, area under the receiver operating characteristic (AUROC), false positive rate at 95 recall (FPR@95), and mean maximum confidence scores for both in-distribution and OOD regions [1]. We consider the annual region between [−1, 1] × [−1, 1] and [−5, 5] × [−5, 5] as the OOD region for the purpose of computing the relevant evaluation metrics.

### 5.2 Machine Experiments

Five types of simulation data (Section 5.1) are sampled within [−1, 1] × [−1, 1] to fit KDFs and KDNs along with their respective parent models: RFs and DNs. Each parent random forest has 500 trees, and each tree is split until class purity. Each parent deep network has four hidden layers with 10 nodes in each layer and is trained using the Adam optimizer at a learning rate of 3 × 10⁻⁴. Figure 1 illustrates the posteriors learned using these four models along with the true posteriors. It is apparent that RFs and DNs yield highly confident predictions outside the in-distribution regions, demonstrating their overconfidence problems. Meanwhile, both KDFs and KDNs yield uniform posteriors over the classes outside [−1, 1] × [−1, 1], which is consistent with human intelligence as described in Section 5.3. Furthermore, KDFs and KDNs also improve the posteriors within the in-distribution regions, showing no compromise while overcoming the overconfident problems in their parent models.

Figure 2 reports the algorithms’ in-distribution performance and confidence scores in both in-distribution and OOD regions. In terms of generalization error, both KDFs and KDNs achieve similar or even better performance compared to that of their respective parent models. Furthermore, our proposed models always achieve posteriors closer to the true posteriors compared to those of RFs and DNs, as illustrated in the Hellinger distance curves (Figure 2, second column). The mean maximum
confidence scores for both KDFs and KDNs become comparable with those of their parent models only at large sample sizes for the in-distribution region (Figure 2, third column), which are more reasonable. More interestingly, for KDFs and KDNs, the mean maximum confidence scores in the OOD regions always stay around 0.5. In stark contrast to that, RFs and DNs maintain very high scores (close to 1) in the OOD regions, which correspond to their overconfident posteriors (Figure 1).

Again, in Table 1, we show the OOD performance of KDFs and KDNs along with their parent models. RFs perform better than DNs in detecting OOD inputs, which is also evident in the human experiments (Section 5.3). However, both KDFs and KDNs are significantly better than RFs and DNs in terms of AUROC and FPR@95 for OOD detection. The two overconfident parent models result in a much higher number of false positives.

5.3 Human Experiments To assess our assumptions about OOD confidence of natural intelligence, we also conducted experiments with human subjects. Two types of simulations are used for the experiments: Gaussian XOR and Spiral (Section 5.1). We recruited 150 participants from the Amazon Mechanical Turks platform. The participants were provided with basic instructions and the structural information regarding the experiments. They were subsequently asked to start the experiments where each individual was exposed to 100 trials of randomly chosen Gaussian XOR and Spiral simulations. Each simulation visualizes 100 randomly distributed points parameterized to aforementioned simulations confined within the \([-1, 1] \times [-1, 1]\) region. The participants were asked to provide a single estimate of confidence per each trial for a randomly distributed test point over the range of \([-3, 3] \times [-3, 3]\). Of 150 participants, 24 subjects were excluded from the analyses for failing to meet the following two criteria: 1. pass at least 4 out of 5 catch trials designed to challenge attention 2. do not miss more than 1\% of the data.

We analyzed the enumerated posterior estimates at all test points and their corresponding 2-dimensional coordinates. Figure 3 shows the estimated posteriors along a line at 82° through the origin at (0, 0). We can see human subjects give uniform posterior over the classes, i.e. 0.5 as we move farther away from the data convex hull specified by \([-1, 1] \times [-1, 1]\). In contrast, random forest and deep net models show significantly more confident posteriors in OOD regions than in-distribution.
regions. The results further confirm that, in terms of OOD detection, our algorithms built on kernel density polytopes resemble natural intelligence, avoiding the overconfidence of RFs and DNs.

6 Discussion In this paper, we have introduced a simple concept—replace the constant or affine function in each polytope of an ML model with a Gaussian kernel, which is locally fitted over the data within the corresponding and the neighboring polytopes. This leads to a lower class conditional likelihood for sample points far away from the convex hull of the training data compared to that for the sample points within in-distribution region. Adding a suitable bias to all the class conditional likelihoods makes this bias dominate in the OOD region yet negligible in the in-distribution region. Such a method results in the uniform posteriors over the classes in the OOD region without using OOD data for training. Experiments with human subjects show that this property correspond with human intelligence. Thus, KDFs and KDNs could be used to further explore how natural intelligence evaluate OOD information with existing knowledge.

Our proposed methods can have useful applications in learning scenarios like lifelong [14] and OOD learning [15], where the detection of OOD data can enable better transfer of knowledge between tasks. Moreover, the kernel density polytopes could be extended to many other algorithms, including convolutional neural networks. In other words, we can take the output from a certain layer in convolutional networks and fit a kernel density convolutional neural network (KDCNN) model that can achieve similar properties on image data. This could motivate future works on a KDCNN model that is robust to OOD data and adversarial attacks.

In conclusion, kernel density polytopes enable OOD detection without sacrificing any in-distribution performance. Models augmented with such a method could achieve better overall performance than the original and produce posteriors that resemble human decisions. In the meantime, our code, including the package and the experiments in this manuscript, is available from https://github.com/neurodata/kdg.

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Appendix A. Pseudocode.

Algorithm 4  Fit a KDX model.

Require:
(1)  $M$ \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \; \;
Algorithm 6 Computing weights in KDN

Require:
(1) $Q_{r}$ ▷ a polytope in class $k$
(2) $X_{k} \in \mathbb{R}^{d \times n_k}$ ▷ input samples with class label $k$
(4) $\theta$ ▷ parent neural network model with parameters $\{W_{l}, b_{l}\}_{l=1}^{L+1}$

Ensure: $w \in [0, 1]^{n_k}$ ▷ weights for each input sample in class $k$

1: function $\text{COMPUTE\_WEIGHTS}(Q_{r}, X_{k}, \theta)$
2: $\{W_{l}, b_{l}\}_{l=1}^{L+1} \leftarrow \theta$
3: $A_{0} \leftarrow X_{k}$
4: $A_{0,\text{ref}} \leftarrow X_{k}$
5: $d = 0$ ▷ $d \in \mathbb{R}^{n_k}$
6: for $l = 1, \ldots, L$ do
7: \hspace{1em} $m_{l} \leftarrow \text{ReLU}$ activation pattern induced by any $x \in Q_{r}$ in the layer $l$ of $\theta$
8: \hspace{1em} $Z_{l} \leftarrow W_{l}A_{l-1} + b_{l}$
9: \hspace{1em} $A_{l} \leftarrow \text{ReLU}(Z_{l})$
10: \hspace{1em} $Z_{l,\text{ref}} \leftarrow W_{l}A_{l-1,\text{ref}} + b_{l}$
11: \hspace{1em} $A_{l,\text{ref}} \leftarrow \text{diag}(m_{l})Z_{l,\text{ref}}$
12: \hspace{1em} $d \leftarrow d + d(A_{l} - A_{l,\text{ref}})$ ▷ $d(M_{r \times c}) \in \mathbb{R}^{c}$ returns the L2-norms of the column vectors of $M$
13: end for
14: $w \leftarrow e^{-d/h}$
15: $w \leftarrow \text{THRESHOLD}(w, T)$ ▷ Set the weights less than $T$ to zero
16: return $w$
17: end function