Voronoi Convolutional Neural Networks

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Abstract

In this technical report, we investigate extending convolutional neural networks to the setting where functions are not sampled in a grid pattern. We show that by treating the samples as the average of a function within a cell, we can find a natural equivalent of most layers used in CNN. We also present an algorithm for running inference for these models exactly using standard convex geometry algorithms.

1 Introduction

When dealing with real world problems, we usually model them by real functions with an \( n \)-dimensional continuous domain, for instance \( f : \mathbb{R}^2 \to \mathbb{R}^3 \) for RGB images. For this paper we use \( U \) to denote the domain of the function and \( \mathbb{T} \) to be the target space. However, continuous domains are not directly usable in computation. As a result, we usually approximate \( f : U \to \mathbb{T} \) with an approximate function \( f_U : U \to \mathbb{T} \) where \( U \) is a finite set and \( f_U \) is a discretization of \( f \).

Example 1 When \( U = [0, 1]^2 \) and \( \mathbb{T} = \mathbb{R} \), it is standard to set

\[
U = \{(i/w, j/h) : i, j \in \mathbb{R}, 0 \leq i < w, 0 \leq j < h\}.
\]

We can set \( f_U \) by a restriction map. In this instance, any function \( f : U \to \mathbb{T} \) can be approximated as a two dimensional array, which is a standard representation of gray scale images, for instance.

If \( f \) is compactly supported, then we can assume that \( U \subseteq [0,1]^s \) and \( \mathbb{T} \subseteq \mathbb{R}^t \). Using the standard grid discretization above, the function can be described in a \((s + 1)\)-dimensional tensor. However, one could ask: «could we replace grid discretizations with something more general?»

In this paper, we propose using piecewise constant approximation on a Voronoi [1] Ch. 7 partition of the domain for this purpose. We chose this approximation since it is the building block for a novel generalization of the standard convolutional neural network, which we call Voronoi Convolutional Neural Networks.
2 Partitioning

Let \( f : U \to \mathbb{R}^n \), and let \( S \subset U \). In this paper we use the notation
\[
|S| = \int_S dx,
\]
where \( |S| = \int_S dx \) is the volume of \( S \).

Let \( U = \{S_k\} \) be a partitioning of \( U \), the domain of \( f \), such that \( U = \bigcup S_k \) and \( S_i \cap S_j = \emptyset \) for all \( i \neq j \). Then define the piecewise constant approximation of \( f \) on \( U \), denoted by \( f_U \), by
\[
f_U(x) = \sum_{S \in U} f(S) \chi_S(x),
\]
where \( \chi_S(x) \) is the indicator function for the set \( S \) (\( \chi_S(x) = 1 \) if \( x \in S \), otherwise, it is 0). Note that \( f_U \) is constant on each set \( S \in U \). As such, for any \( S \in U \) and \( s \in S \) we have \( f_U(s) = f_U(S) \).

We would like to formulate the typical neural network operations on the space of functions of the form \( f_U : U \to \mathbb{R}^n \).

Example 2 Let \( U = [0,1]^2 \). The standard \( w \times h \) grid partitioning of \( U \) is given by \( U = \{S_{i,j} : 0 < i < w, 0 < j < h\} \) where
\[
S_{i,j} = \left\{(x,y) \in U : \frac{i}{w} \leq x < \frac{i+1}{w}, \frac{j}{h} \leq y < \frac{j+1}{h}\right\}.
\]
Then for any \( f : [0,1]^2 \to \mathbb{R}^n \), we can describe \( f_U \) as an \((w,h,n)\)-tensor.

Note that the approximations of \( f \) in examples 1 and 2 are defined by \((w,h,n)\)-tensors. However, in case of example 1 the entries of the tensor are the value of the underlying function, while in example 2 the entries are the average value of the function over the cell \( S_{i,j} \). In general, if \( U \) has \( k \) elements in it, any function \( f_U : U \to \mathbb{R}^n \) can be described as a \((k,n)\)-tensor.

Amongst possible partitioning schemes, we are particularly interested in Voronoi partitioning, as 1) it is a strict superset of grid partitioning, and 2) it simplifies the discretization of convolution by decomposing a domain into convex polytopes.

Remark 3 We chose piecewise constant approximation, since it makes the math work later in this paper. However, other class of functions can work here as well. For instance, if the partitions are all polyhedra, one can use generalized barycentric coordinates to get a continuous approximation of the underlying function.

3 Convolutions

Let \( U = \mathbb{R}^a \), and consider two functions \( f : U \to \mathbb{R}^m \), and \( \kappa : U \to \mathbb{R}^{m \times n} \) (i.e. \( \kappa(x) \) is an \( m \times n \) matrix). Recall the definition of convolution \( f \) and \( \kappa \), denoted
by $\kappa \circledast f : \mathbb{U} \to \mathbb{R}^n$:

$$(\kappa \circledast f)[x] = \int_{\mathbb{U}} \kappa(x - \tau) \cdot f(\tau) \, d\tau. \quad (1)$$

Consider three partitions $\mathcal{U}, \mathcal{V}$, and $\mathcal{W}$ of $\mathbb{U}$. Let us now assume that $f = f_U$ (i.e. $f$ is constant on each $U \in \mathcal{U}$) and $\kappa = \kappa_V$. We wish to compute the approximation of $(\kappa \circledast f)$ on $\mathcal{W}$. In particular, for $W \in \mathcal{W}$:

$$(\kappa \circledast f)(W) = \frac{1}{|W|} \int_W (\kappa \circledast f)[w] \, dw
\quad = \frac{1}{|W|} \int_W \int_U \kappa(w - u) \cdot f(u) \, du \, dw
\quad = \frac{1}{|W|} \int_W \sum_{U \in \mathcal{U}} \int_U \kappa(w - u) \cdot f(U) \, du \, dw
\quad = \frac{1}{|W|} \sum_{U \in \mathcal{U}} \left( \int_W \int_U \kappa(w - u) \, dw \right) \cdot f(U)
\quad = \frac{1}{|W|} \sum_{U \in \mathcal{U}} K_{U,W} \cdot f(U)$$

where in the expression above:

$$K_{U,W} = \int_W \int_U \kappa(w - u) \, du \, dw
\quad = \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \kappa(x - u) \chi_U(u) \chi_W(w) \, du \, dw.$$

Recall, as before, $\chi_S$ is the indicator function for set $S$. Also, note that $K_{U,W}$ is an $m \times n$ matrix and $f(U)$ is an $m$-dimensional vector.

4 Volume computation

We can find numerical approximation for $K_{U,W}$ in general case. However, when $U, V$, and $W$ are all convex polytopes, then we can compute $K_{U,W}$ using convex geometry algorithms. First note that we can rewrite $K_{U,W}$ (for all sets $U$ and $V$) as

$$K_{U,W} = \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \kappa(x - u) \chi_U(u) \chi_W(w) \, du \, dw
\quad = \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \kappa(x) \chi_U(u) \chi_W(x + u) \, du \, dx
\quad = \int_{\mathbb{R}^n} \kappa(x) \left( \int_{\mathbb{R}^n} \chi_U(u) \chi_W(x - u) \, du \right) \, dx
\quad = \int_{\mathbb{R}^n} \kappa(x) \left( \int_{\mathbb{R}^n} \chi_U(x - W) \chi_W(u) \, du \right) \, dx.$$
\[
= \int_{\mathbb{R}^a} \kappa(x) |U \cap (W - x)| \, dx.
\]

Where $| \cdot |$ indicates the volume of a partition. In particular note that

\[
K_{U,W} = \int_{\mathbb{R}^a} \kappa(x) |U \cap (W - x)| \, dx \\
= \sum_V \int_V \kappa(V) |U \cap (W - x)| \, dx \\
= \sum_V \kappa(V) \int_{\mathbb{R}^a} \int_{\mathbb{R}^a} \chi_V(x) \chi_U(y) \chi_W(x + y) \, dx \, dy \\
= \sum_V \kappa(V) K_{V,U,W}^V
\]

Now assume $U$, $V$ and $W$ to be convex polytopes. Then we can define a convex polytope in $\mathbb{R}^{2a}$ so that $K_{U,W}^V$ is the volume of the given polytope. In particular, assume that each set is defined as the intersection of halfspaces:

\[
U = \bigcap_i H_i, \quad V = \bigcap_j H_j', \quad W = \bigcap_k H_k''.
\] (2)

Then we can rewrite

\[
K_{U,W}^V = \int_{\mathbb{R}^a} \int_{\mathbb{R}^a} \chi_V(x) \chi_U(y) \chi_W(x + y) \, dx \, dy \\
= \int_{\mathbb{R}^a} \int_{\mathbb{R}^a} \left( \prod_i \chi_{H_i}(x) \right) \left( \prod_j \chi_{H_j'}(y) \right) \left( \prod_k \chi_{H_k''}(x + y) \right) \, dx \, dy.
\]

Note that each term in the product is the composition of a Heaviside function with a linear function, hence the whole product is the indicator function of a convex polytope in $\mathbb{R}^{2a}$, and as such we can compute its volume using standard convex polytope algorithms.

## 5 Voronoi Convolutional Network

Let $P = \{ p_n \in U \}$ be a set of points. Then the Voronoi cell $U_p$ is defined as

\[
U_p = \{ x \in \mathbb{R}^a : d(x, p) \leq d(x, q) \forall q \in P \}.
\]

Note that the Voronoi cells $U_p$ form a partitioning:

\[
U_P = \{ U_p : p \in P \}.
\]

Furthermore, it is well known that each Voronoi cell is a convex polytope, and there are libraries that given a set of points, will compute the Voronoi cells as a convex polytope. We used `scipy.spatial` library for our computation.
We can now define our Voronoi Convolutional Networks. Each layer of such a network is given by a Voronoi partitioning of \( U \), denoted by \( \mathcal{U} \), and a function \( f : \mathcal{U} \to \mathbb{R}^m \). Note that a layer \( (\mathcal{U}, f) \) are encoded by set of \( k \) points in \( U \) and a tensor of shape \( k \times m \) for the function \( f \). We define few transition layers, similar to the ones used in CNNs.

- **Convolutions:** Given a set of convex spaces \( \mathcal{V} = \{V_1, \ldots, V_e\} \), we define \( \mathcal{V} \)-convolution as a matrix valued function \( \kappa : \mathcal{V} \to \mathbb{R}^{m \times n} \). Given a layer in VCNN \( (\mathcal{U}, f) \), a convolution \( \kappa \), and a partitioning \( \mathcal{W} \), we get a new layer \( (\mathcal{W}, f \odot \kappa) \) by

\[
(f \odot \kappa)(W) = \sum_{U, V} K_{U, W} \kappa(V) \cdot f(U).
\]

Given an activation function \( \sigma : \mathbb{R} \to \mathbb{R} \) as well, we get the new layer \( (\mathcal{W}, \sigma \circ (f \odot \kappa)) \).

- **(Average) Pooling:** Given a layer in VCNN \( (\mathcal{U}, f) \) and a partitioning \( \mathcal{W} \), then the pooling of \( f \) to \( \mathcal{W} \) is \( (\mathcal{W}, g) \) where

\[
g(W) = \sum_{V} \left| V \cap W \right| f(V).
\]

- **Mixup / \((1 \times 1)\)-convolution:** The equivalent to the \( 1 \times 1 \) convolution in 2D-CNNs, is just applying a matrix \( M \) to \( f \). In particular, for layer \( (\mathcal{V}, f) \), applying the MixUp we get \( (\mathcal{V}, M \circ f) \).

- **Concat:** We can concatenate two layers if they are both defined on the same domain. That is given \( (\mathcal{V}, f) \) and \( (\mathcal{V}, g) \), we define the concatenation of these two layers to be \( (\mathcal{V}, f \oplus g) \).

We define a VCNN as a network that is built as a stack of the layers above. Notice that a VCNN is differentiable if the transition layers are differentiable. As such, we can apply back propagation to train a network for solving particular problems.

The following two examples shows that VCNNs are generalization of standard CNNs:

**Example 4 (1D-Conv)** Assume \( \mathcal{U} = \mathcal{W} = \{[i, i+1) : i \in \mathbb{R}\} \), let \( f : \mathcal{U} \to \mathbb{R}^n \), and consider input layer \( (\mathcal{U}, f) \). Let \( \mathcal{V} = \{[0, 1), [1, 2), [2, 3)\} \), and \( \kappa : \mathcal{V} \to \mathbb{R}^{n \times m} \) be the \( \mathcal{V} \) convolution. For simplicity we denote \( f([i, i+1)) \) by \( f_i \) and denote \( \kappa([i, i+1]) \) by \( M_i \) (so \( \mathcal{V} \) convolution is defined by \( M_0, M_1, \) and \( M_2 \)). Then applying \( \kappa \) to \( (f_i) \) we get

\[
g_i = (M_0 f_i + f_{i-1} (M_0 + M_1) + f_{i-2} (M_1 + M_2) + M_2 f_{i-3})/2.
\]

Notice that this is slightly different than the 1D conus with kernel size of 3 with \( m \) filters.

**Remark 5** Note that the pooling layers in VCNN can go from any partitioning to any other partitioning. In particular, we can go from more sparse partitioning to denser partitioning.
6 Conclusion

In this note we showed how one can extend CNNs to the case where the sampling of is not done in a grid pattern. We developed our network by considering convolutions on continuous functions, and discretizing the functions on Voronoi cells. The networks we have presented here can be implemented in standard deep learning frameworks such as TensorFlow or PyTorch, under the assumption that the Voronoi cells used in each layers do not change. We note that when the cell $V$ is fairly small compared to cells $U$ and $W$, then for many choices of $U$ and $W$ we expect $K_{U,W}^V = 0$, and for cases were $U$ and $W$ have large number of cells, we need to implement an algorithm to identify those quickly for efficiency reasons. We did not investigate such algorithms in this paper.

Note that to really get the benefit of such networks, we really like to allow the points defining the Voronoi cells in each layer to move freely. To achieve that, we need to be able to compute the derivative of volume computation $K_{U,W}^V$ with respect to the Voronoi cells, which we did not undertake in this paper. On the other hand, one can treat $K_{U,W}^V$ as trained variables. In that case, the resulting network can be interpreted as a multihead attention network, where the attention of Query and Key should be interpreted as $K_{U,W}^V$. It would be interesting to see if the attention matrices in standard attention networks carry a geometric interpretation similar to the volume of Voronoi cells.

References

[1] Mark De Berg, Marc Van Kreveld, Mark Overmars, and Otfried Schwarzkopf. Computational geometry. In Computational geometry. Springer, 1997.