Convolutional Nearest Neighbors: Reinterpreting Convolution Through K-Nearest Neighbor Selection

Bowdoin

Mingi Kang, Jeova Farias Sales Rocha Neto PhD.

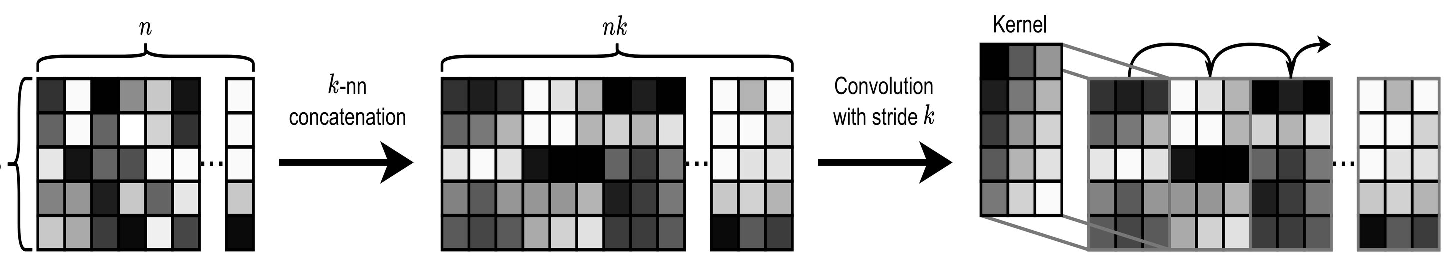
Bowdoin College, ME

INTRODUCTION

- **Convolutional Nearest Neighbor** (**ConvNN**) reinterprets convolution as k-nearest neighbor aggregation with flexible neighbor selection criteria.
- Standard convolution implicitly performs k-NN with fixed spatial distance (e.g., 3x3 kernel = k = 9 spatially-adjacent neighbors including self).
- ConvNN generalizes this by allowing neighbor selection based on:
  - Spatial distance (reduces to standard convolution)
  - Feature similarity (cosine/Euclidean)
  - Hybrid spatial-feature metrics
- Core Algorithm of ConvNN:
  1. Compute pairwise similarities between all spatial positions
  2. Select k-nearest neighbors per position via hard top-k
  3. Aggregate neighbors with learnable weights (1D convolution)

BASE ALGORITHM

ConvNN Visualization



1. Similarity Computation

$$S = XX^\top \in \mathbb{R}^{n\times n} \text{ where } S_{ij} = x_i^\top x_j$$

2. K-Nearest Neighbor Selection

$$I_k = k\text{–}argmax(XX^\top) \in \mathbb{R}^{n\times n}$$

$$\text{Neighbors} = X[I_k[i,:],:] \in \mathbb{R}^{k\times n}$$

Algorithm 1 Convolutional Nearest Neighbors 1D

Input: $\mathbf{X} \in \mathbb{R}^{B\times C\times N}$ (batch × channels × tokens)
Parameters: k (number of neighbors)
Output: $\mathbf{Y} \in \mathbb{R}^{B\times C'\times N}$

// For each batch element
Let $X = \mathbf{X}[b,:,:]^\top \in \mathbb{R}^{N\times C}$ with columns $\mathcal{X} = \{\mathbf{x}_i\}_{i=1}^N$

// Step 1: Compute similarity matrix
Assume each $\mathbf{x}_i$ is ℓ_2-normalized: $\|\mathbf{x}_i\|_2 = 1$
Compute similarity: $S = XX^\top \in \mathbb{R}^{N\times N}$ where $S_{ij} = \mathbf{x}_i^\top \mathbf{x}_j$

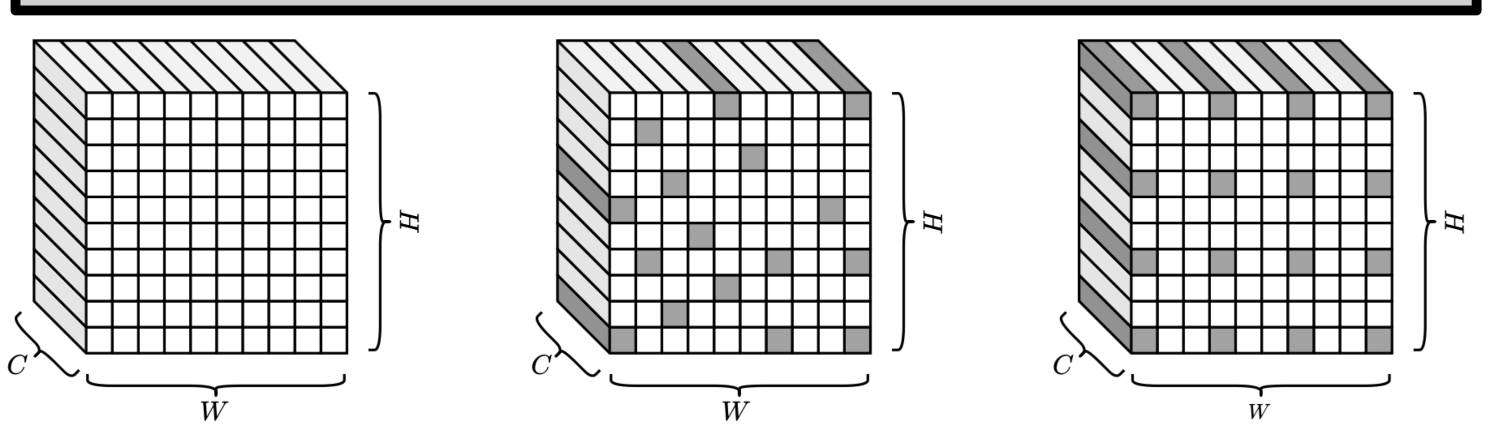
// Step 2: Find k-nearest neighbors
$I_k = argmax_k(S) \in \{0,1\}^{N\times N}$

// Step 3: Gather features
for $i \in [1, N]$ **do**
  $\mathcal{N}_k(\mathbf{x}_i) = X[I_k[i,:],:] \in \mathbb{R}^{k\times C}$
  $\mathbf{V}_{prime}[:,:,i\cdot k : (i+1)\cdot k] = \mathcal{N}_k(\mathbf{x}_i)^\top$
end for

// Step 4: Convolve
$\mathbf{Y} = \text{Conv1D}(\mathbf{V}_{prime}, \text{kernel\_size} = k, \text{stride} = k)$

return Y

SIMILARITY COMPUTATION SPEED-UPS



(a) Input Tensor (b) After Random Sparsification $n = 16$ (c) After Spatial Sparsification $n = 4$

- To reduce $O(N^2)$ complexity of all to all similarity computation, we introduce two sampling methods: Random Sparsification and Spatial Sparsification.
- Trade-off between computational efficiency and neighbor selection quality is controlled by sampling parameter n.

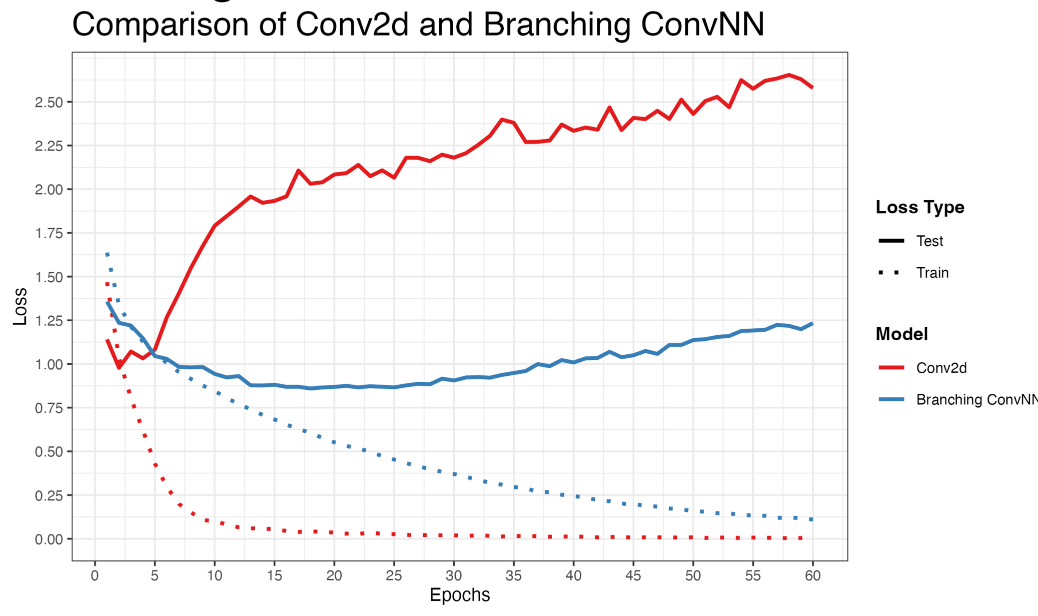
ARCHITECTURE AND TRAINING

- **Architecture**: VGG-11 with Conv2d layers replaced by ConvNN and branching layers
- **Dataset**: CIFAR-10 image classification
- **Training**: 60 epochs with AdamW (lr=1e-5, wd=1e-6), StepLR scheduler (gamma=0.95, step=2)
- **Variants tested**:
  - Location-only (spatial distance)
  - Feature-only (cosine similarity)
  - Hybrid (weighted combination)
  - Branching with ratio (e.g., 50% Conv2d + 50% ConvNN)

RESULTS

Training and Test Loss

Comparison of Conv2d and Branching ConvNN



Branching ConvNN = Branching with branching ratio 0.500, kernel_size = 3, K = 9, Feature Similarity and Aggregation.

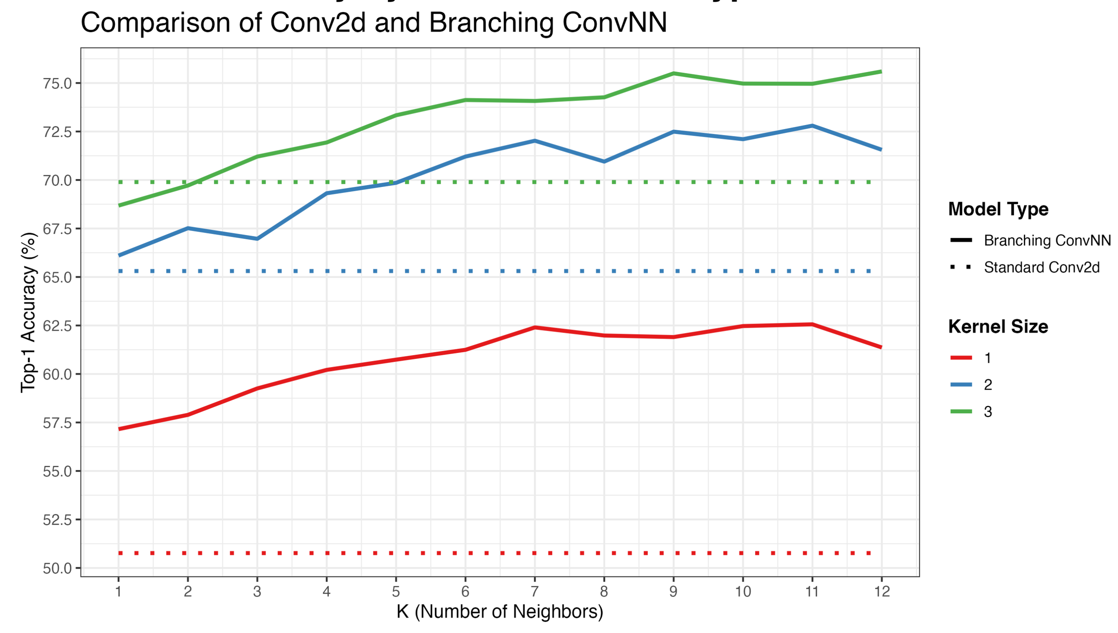
Table 1: CIFAR10 ConvNN Branching Ratio (Color Similarity and Color Aggregation)

Models	Branching Ratio (λ)	Params	Top-1 Acc.	Test Loss	GFlops
Conv2d	0.000	$130.015M$	69.78%	2.57	0.293
Branching	0.125	$130.015M$	**73.49%**	1.81	0.325
Branching	0.250	$130.015M$	**74.32%**	1.56	0.325
Branching	0.500	$130.015M$	**73.61%**	1.23	0.325
Branching	0.750	$130.015M$	68.63%	1.23	0.325
Branching	0.875	$130.015M$	65.66%	1.33	0.325
ConvNN	1.000	$130.015M$	50.250%	1.84	0.325

VGG 11 Architecture with kernel_size = 3 (Conv2d), K = 9 (ConvNN)
Branching Models: $\lambda \times \text{ConvNN} + (1-\lambda) \times \text{Conv2d}$

Model Accuracy by Kernel Size and Type

Comparison of Conv2d and Branching ConvNN



Branching ConvNN = Branching with branching ratio 0.250, Location + Feature Similarity and Aggregation.

Table 2: CIFAR10 ConvNN Branching Ratio (Location + Color Similarity and Color Aggregation)

Models	Branching Ratio (λ)	Params	Top-1 Acc.	Test Loss	GFlops
Conv2d	0.000	$130.015M$	69.78%	2.57	0.293
Branching	0.125	$130.015M$	**72.92%**	1.92	0.331
Branching	0.250	$130.015M$	**74.20%**	1.52	0.331
Branching	0.500	$130.015M$	**73.16%**	1.24	0.331
Branching	0.750	$130.015M$	**69.98%**	1.22	0.331
Branching	0.875	$130.015M$	64.77%	1.33	0.331
ConvNN	1.000	$130.015M$	52.70%	1.80	0.331

VGG 11 Architecture with kernel_size = 3 (Conv2d), K = 9 (ConvNN)
Branching Models: $\lambda \times \text{ConvNN} + (1-\lambda) \times \text{Conv2d}$

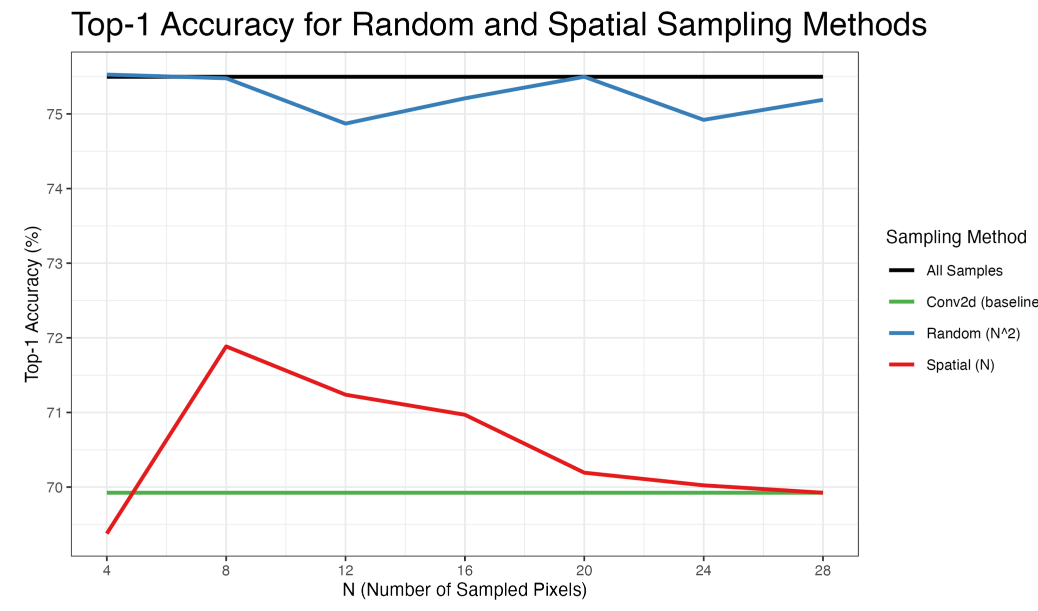
Table 3: CIFAR10 ConvNN Branching Ratio (Location + Color Similarity and Location + Color Aggregation)

Models	Branching Ratio (λ)	Params	Top-1 Acc.	Test Loss	GFlops
Conv2d	0.000	$130.015M$	69.78%	2.57	0.293
Branching	0.125	$130.021M$	**73.75%**	1.85	0.331
Branching	0.250	$130.028M$	**75.22%**	1.46	0.331
Branching	0.500	$130.040M$	**74.52%**	1.17	0.331
Branching	0.750	$130.052M$	69.49%	1.15	0.331
Branching	0.875	$130.059M$	66.14%	1.25	0.325
ConvNN	1.000	$130.065M$	60.09%	1.44	0.325

VGG 11 Architecture with kernel_size = 3 (Conv2d), K = 9 (ConvNN)
Branching Models: $\lambda \times \text{ConvNN} + (1-\lambda) \times \text{Conv2d}$

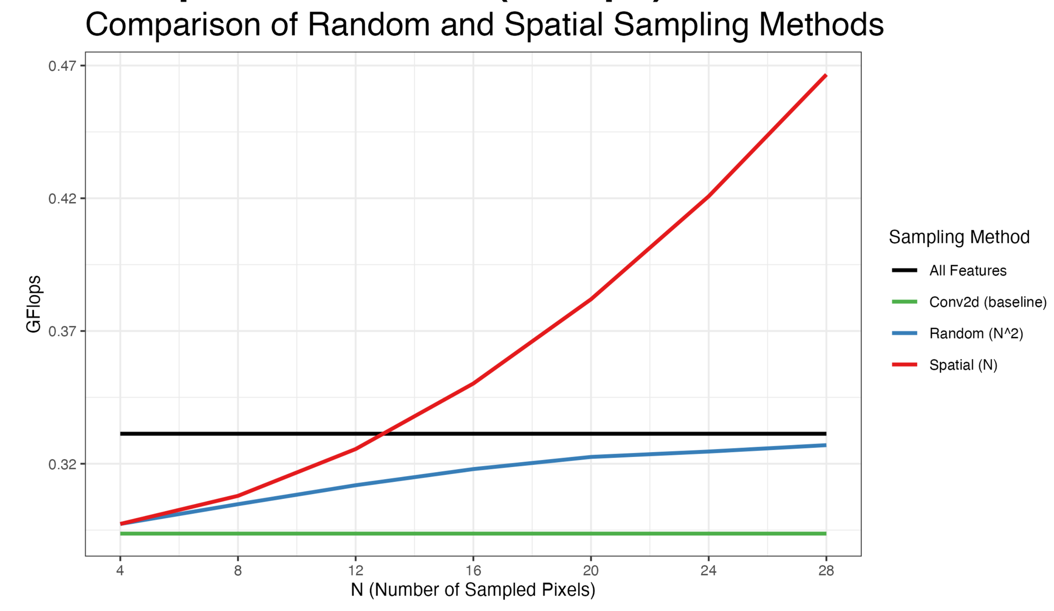
Model Performance vs. N

Top-1 Accuracy for Random and Spatial Sampling Methods



Computational Cost (GFlops) vs. N

Comparison of Random and Spatial Sampling Methods



Branching ConvNN = Branching with branching ratio 0.250, Location + Feature Similarity and Aggregation. Spatial Sampling = $N = N\times N$ sub grid 3, Random Sampling = N^2 pixels.

CONVOLUTION AND ATTENTION

1. Convolution

$$S = D = 2(1 - X^\top X) \in \mathbb{R}^{n\times n} \text{ where } D_{ij} = \| x_i - x_j \|_2^2 = 2(1 - x_i^\top x_j)$$

$$I_k = k\text{–}argmax(2(1 - X^\top X)) \in \mathbb{R}^{n\times n}$$

$$\text{Neighbors} = X[I_k[i,:],:] \in \mathbb{R}^{k\times n}$$

2. Convolutional Nearest Neighbor

$$S = XX^\top \in \mathbb{R}^{n\times n} \text{ where } S_{ij} = x_i^\top x_j$$

$$I_k = k\text{–}argmax(XX^\top) \in \mathbb{R}^{n\times n}$$

$$\text{Neighbors} = X[I_k[i,:],:] \in \mathbb{R}^{k\times n}$$

3. Attention

$$QK^\top \in \mathbb{R}^{n\times n} \text{ where } Q = w_Q X, K = w_k X$$

$$A(Q,K) = \text{softmax}\left(\frac{QK^\top}{\sqrt{d_k}}\right) \in \mathbb{R}^{n\times n}$$

$$\text{Attention}(Q,K,V) = A(Q,K)V \text{ where } V = w_v X$$

DISCUSSION

- **Hybrid similarity** (spatial + feature) outperforms pure spatial or pure feature selection
- **Branching architecture** achieves best performance by combining ConvNN's global context with Conv2d's spatial locality.
- ConvNN unifies convolution and attention as neighbor aggregation differ:
  - Spatial-only → standard convolution
  - All positions with soft weights with linear projection → self-attention
  - ConvNN occupies the middle ground with hard, content-aware selection
- **Feature work**: Extend to Vision Transformers, explore learnable similarity metrics, investigate soft vs. hard selection.

REFERENCES

- A. Buades, B. Coll and J. . -M. Morel, "A non-local algorithm for image denoising," *2005 IEEE Computer Society Conference on Computer Vision and Pattern Recognition (CVPR'05)*, San Diego, CA, USA, 2005, pp. 60-65 vol. 2, doi: 10.1109/CVPR.2005.38.
- Singh, Sidak Pal, and Martin Jaggi. "Model fusion via optimal transport." *Advances in Neural Information Processing Systems* 33 (2020): 22045-22055.
- Plötz, Tobias, and Stefan Roth. "Neural nearest neighbors networks." *Advances in Neural information processing systems* 31 (2018).
- Wang, Xiaolong, et al. "Non-local neural networks." *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2018.
- Vaswani, Ashish, et al. "Attention is all you need." *Advances in neural information processing systems* 30 (2017).