FRONTIERS IN MACHINE LEARNING FOR PHYSICS

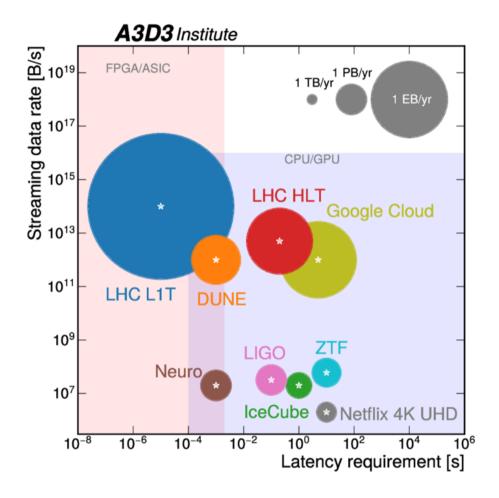
Deven Misra

November 21, 2025



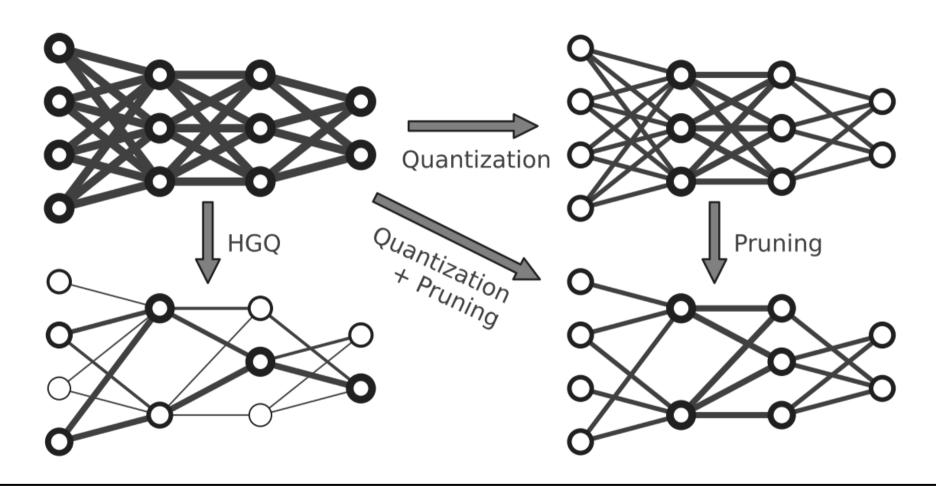
I. Fast Machine Learning

REAL-TIME DATA PROCESSING



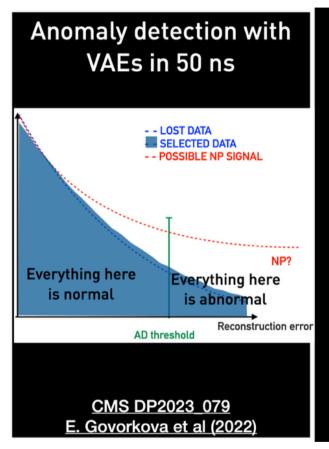
Goal: Reduce model size and inference time while preserving performance

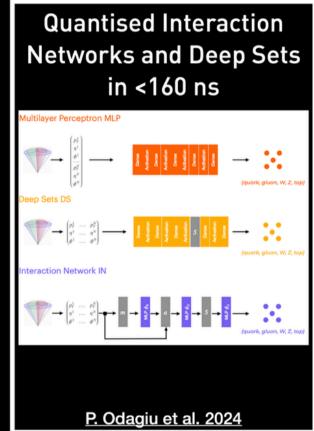
NEURAL NETWORK QUANTIZATION KERAS → HGQ2 | PYTORCH → BREVITAS

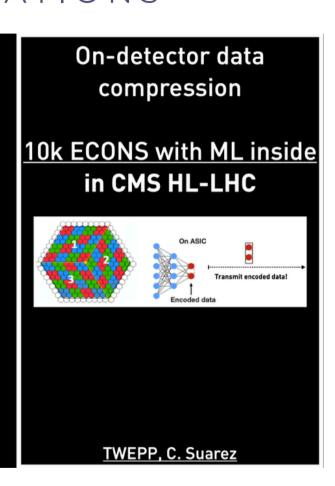


C. Sun *et al.*, *Gradient-Based Automatic Mixed Precision Quantization for Neural Networks On-Chip*, arXiv:2405.00645 **[cs.LG]**, Aug. 2024

EXPERIMENTAL PARTICLE PHYSICS REAL-TIME INFERENCE APPLICATIONS



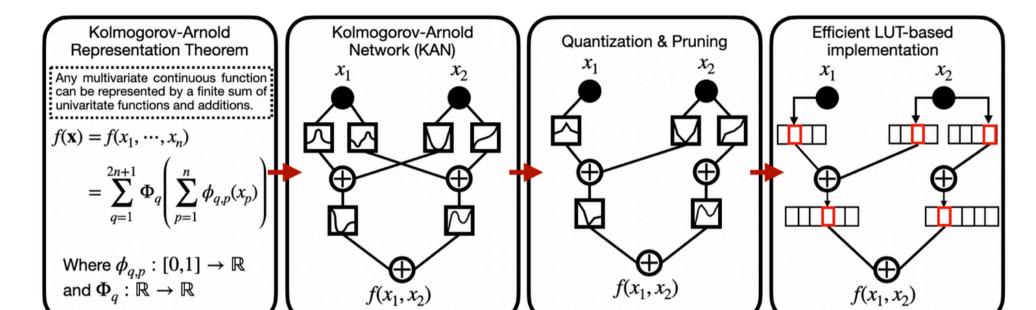




T. Arrestad, EPS-HEP 2025

EXPERIMENTAL PARTICLE PHYSICS

KAN-LUT



D. Hoang, A. Gupta, P. Harris, and V. Loncar, "FPGA-optimized Kolmogorov-Arnold Networks (KANs) via LUT-based design", Fast Machine Learning for Science Conference, Sept. 2025

EXPERIMENTAL PARTICLE PHYSICS

HEPT

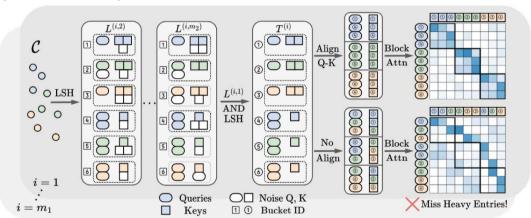
- Central idea: reduce computations in the attention kernel
- Locality sensitive hashing using E2LSH is used to sort points into buckets
- Attention only computed for elements in same bucket

$$\mathbf{x} \in \mathbb{R}^d, h_{\mathbf{a},b}(\mathbf{x}) = \lfloor \frac{\mathbf{a} \cdot \mathbf{x} + b}{r} \rfloor, \mathbf{a} \sim \mathcal{N}(0, \mathbf{I}), b \sim \mathcal{U}(0, r)$$

Attention kernel choice to exhibit local inductive bias:

$$k\left(\mathbf{q}_{u}, \mathbf{k}_{u}\right) = \exp\left(-\frac{1}{2}||\mathbf{q}_{u} - \mathbf{k}_{u}||^{2}\right)$$

- Achieves a local attention mechanism with linear complexity
- Lower inference latency compared to GNNs by > 10x
- Best resource scaling out of all proposed point cloud transformer models



@ ⑤

Efficient

Sequence Model

S. Miao *et al.*, "Locality-Sensitive Hashing-Based Efficient Point Transformer with Applications in High-Energy Physics, Proceedings of the 41st International Conference on Machine Learning", PMLR **235**, 2024

GRAVITATIONAL WAVE ASTRONOMY PARAMETER ESTIMATION

Accelerated Gravitational Wave Parameter Estimation with Reduced Order Modeling [1]

Rapid Parameter Estimation of Gravitational Waves from Binary Neutron Star Coalescence using Focused Reduced Order Quadrature [2]

Bayesian Parameter Estimation using Conditional Variational Autoencoders for Gravitational-Wave Astronomy [3]

Real-Time Gravitational-Wave Science with Neural Posterior Estimation [4]

Rapid localization and inference on compact binary coalescences with the Advanced LIGO-Virgo-KAGRA gravitational-wave detector network [5]

Rapid Likelihood Free Inference of Compact Binary Coalescences using Accelerated Hardware [6]

[1] P. Canizares et al., Phys. Rev. Lett. 114, 7 (2015)

[2] S. Morisaki and V. Raymond, Phys. Rev. D 102, 10 (2021)

[4] H. Gabbard et al., Nat. Phys. 18, 112-117 (2022)

[3] M. Dax et al., Phys. Rev. Lett. 127, 24 (2023)

[5] S. Morisaki *et al.*, Phys. Rev. D 108, 12 (2023)

[6] D. Chatterjee et al., MLST 5, 4 (2024)

GRAVITATIONAL WAVE ASTRONOMY NOISE REDUCTION

Noise reduction in gravitational-wave data via deep learning [7]

Demonstration of machine learning-assisted low-latency noise regression in gravitational wave detectors [8]

Coherence DeepClean: Toward autonomous denoising of gravitational-wave detector data [9]

DETECTION

GWAK: Gravitational-Wave Anomalous Knowledge with Recurrent Autoencoders [10]

A Machine-Learning Pipeline for Real-Time Detection of Gravitational Waves from Compact Binary Coalescences [11]

ML4GW

[7] R. Ormiston et al., Phys. Rev. Research 2, 3 (2020)

[8] M. Saleem et al., Class. Quantum Grav. 41, 19 (2024)

[9] C. Reissel et al., arXiv:2501.04883 [gr-qc] (2025)

[10] R. Raikman et al., MLST 5, 5 (2024)

[11] E. Marx et al., Phys. Rev. D 111, 4 (2025)

II. Geometric Methods

NON-EUCLIDEAN SPACES

RIEMANNIAN MANIFOLDS

Let \mathcal{M} be a smooth manifold. For $\mathbf{x} \in \mathcal{M}$, define the **tangent space** $\mathcal{T}_{\mathbf{x}}\mathcal{M}$ to be the first order approximation of \mathcal{M} around \mathbf{x} , which is locally Euclidean. The **Riemannian metric**,

$$g_{\mathbf{x}}(\cdot,\cdot):\mathcal{T}_{\mathbf{x}}\mathcal{M} imes\mathcal{T}_{\mathbf{x}}\mathcal{M}
ightarrow\mathbb{R},$$

defines an inner product on the tangent space $\mathcal{T}_{\mathbf{x}}\mathcal{M}$.

The tuple (\mathcal{M}, g) is called a **Riemannian manifold**.

For $\mathbf{x} \in \mathcal{M}$,

$$\exp_{\mathbf{x}}(\cdot): \mathcal{T}_{\mathbf{x}}\mathcal{M}
ightarrow \mathcal{M}$$

$$\log_{\mathbf{x}}(\cdot): \mathcal{M}
ightarrow \mathcal{T}_{\mathbf{x}} \mathcal{M}$$

GeoOpt

- [1] S. Bonnabel, "Stochastic Gradient Descent on Riemannian Manifolds", IEEE Transactions on Automatic Control 58, 2013
- [2] G. Becigneul and O-E. Ganea, "Riemannian Adaptive Optimization Methods", 7th International Conference on Learning Representations (ICLR), 2019
- [3] S. Gruffaz and J. Sassen, "A Review on Riemannian Metric Learning", arXiv:2503.05321 [stat.ML] (2025)

NON-EUCLIDEAN SPACES

SELFMGNN

Given a graph $G=(V,E,\mathbf{X})$, the problem of **self-supervised graph representation learning** in the mixed-curvature space is to learn an encoding function $\Phi:V\to P$ that maps the node \mathbf{v} to a vector \mathbf{z} in a mixed-curvature space P that captures the intrinsic complexity of graph structure without using any label information.

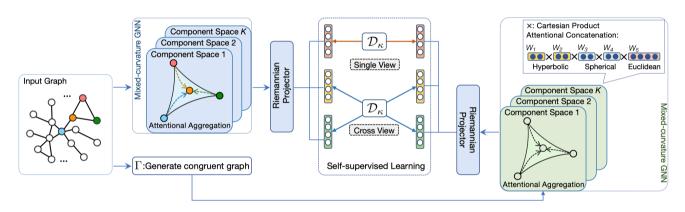
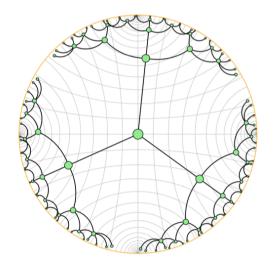
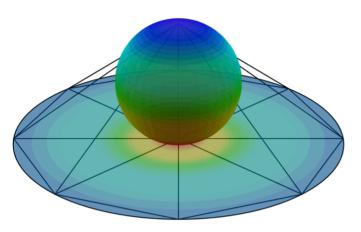


Figure 1: Overall architecture of Selfmgnn: In Selfmgnn, we first introduce a mixed-curvature Gnn to learn graph representations. Specifically, we perform attentional aggregation within the component space where the triangle is to show its geometry, e.g., triangles curve inside in \mathbb{H} , and attentional concatenation among component spaces whose example with learnable weights is on the top right. Then, to enable self-supervised learning, we design a Riemannian projector to reveal different views of the mixed-curvature space, and utilize a well-designed Riemannian discriminator \mathcal{D}_{κ} to contrast samples for single- and cross-view contrastive learning, shown in the middle. In practice, we feed the graph and its congruent augmentation, generated by $\Gamma(\cdot)$, for the contrastive learning as specified in Algo. 1.

NON-EUCLIDEAN SPACES PRODUCT MANIFOLDS



(a) A rooted tree with a branching ratio of 3 and a depth of 4 is plotted in the 2D Poincaré Disk, illustrating the exponential growth of area and volume characteristic of hyperbolic spaces.



(b) Stereographic projection of 2D sphere onto 2D plane with coloring according to stereographic mapping.

$$\mathcal{P} = \mathcal{M}_{\kappa_1}^{d_1} imes \mathcal{M}_{\kappa_2}^{d_2} imes \cdots imes \mathcal{M}_{\kappa_n}^{d_n}$$
 (Product Space)

"... \mathcal{PM} representations generally achieve comparable or superior performance with the most pronounced improvements observed for highly hierarchical jets."

NON-EUCLIDEAN SPACES COLLIDER PHASE SPACE

The volume form for four-dimensional, on-shell, massless, N-body phase space in the center-of-mass frame is

$$\mathrm{d}\Pi_N = 2\pi^{4-3N} \left[\prod_{i=1}^N \mathrm{d}^4 p_i \delta^+(p_i^2)
ight]\! \delta^{(4)} \left(Q - \sum_{i=1}^N p_i
ight)$$

where Q=(0,0,0,0) and $\delta^+(p_i^2)=\delta(p_i^2)\Theta(p_i^0)$. The phase space Π_N can be separated as

$$\Pi_N\cong \Delta_{N-1} imes S^{2N-3}$$

where Δ_{N-1} is the N-1 dimensional simplex, and S^{2N-3} is the 2N-3 dimensional (hyper)sphere [1]. Furthermore, it is shown that the product space can be equipped with global coordinates which allow for the explicit construction of a Riemannian metric on Π_N ,

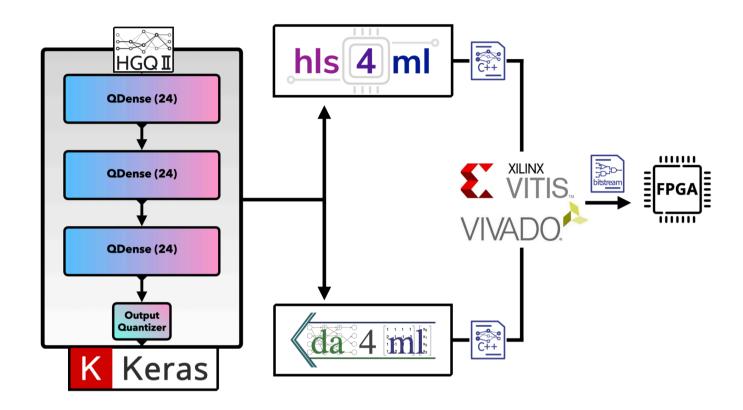
$$\mathrm{d}_{\Pi}(ec{
ho}_A,ec{v}_A';ec{
ho}_B,ec{v}_B') = rac{1}{2\pi}\sqrt{rac{1}{4}\Big(rac{c}{4}\Big)^{rac{3-2N}{3N-4}}}\mathrm{d}_{\Delta}^2(ec{
ho}_B,ec{
ho}_B) + \Big(rac{c}{4}\Big)^{rac{N-1}{3N-4}}\mathrm{d}_{S}^2(ec{v}_A',ec{v}_B').$$

In this form, d_{Δ}^2 is the line element on the simplex, d_S^2 is the line element on the sphere, and c is a dimensionless parameter which reweights the simplex and sphere contributions to the distance between events [2].

- [1] A. Larkoski and T. Melia, "Covariantizing Phase Space", Phys. Rev. D 102, 9 (2020)
- [2] T. Cai et al., "The Phase Space Distance Between Collider Events", J. High Energ. Phys. 2024, 54 (2024)

Backup

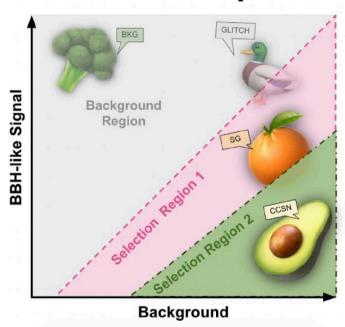
EXAMPLE FASTML WORKFLOW



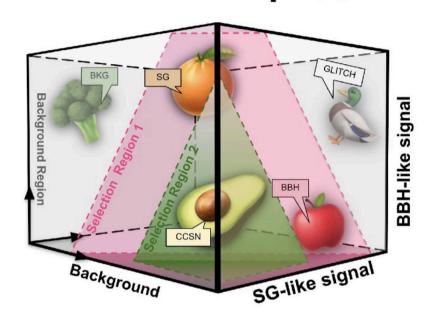
- 1. Train model using open-source framework (Keras v3 + HGQ2)
- 2. Translate model to C++ via high-level synthesis (hls4ml and/or da4ml)
- 3. Transpile HLS code to generate register-transfer level implementation
- 4. Generate bitstream and program device

A CLOSER LOOK AT GWAK

2D GWAK Space

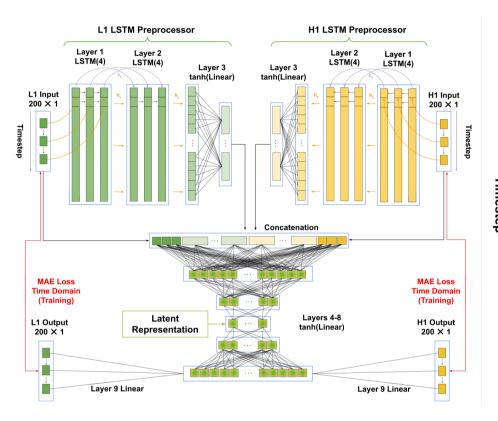


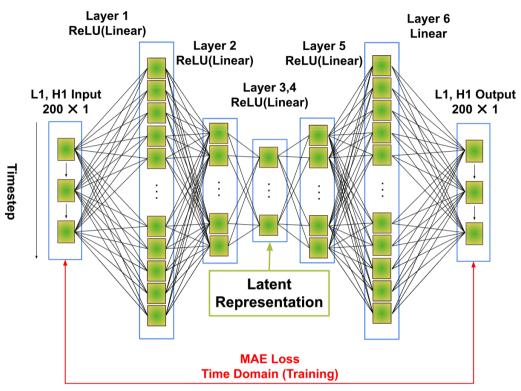
3D GWAK Space



The semi-supervised method is manifested by using simulated signals as approximations for anomalous-unmodeled signals in the GWAK embedded space. A graph representation of this embedded space is shown in figure 1 for the case of two (left) and three (right) different dataset classes.

A CLOSER LOOK AT GWAK





A separate unsupervised autoencoder network is then trained on each class of samples separately, resulting in a low-dimensional 'GWAK' space consisting of the coherence metrics between the autoencoder inputs and outputs for each autoencoder, which is then used to search for anomalous signals.