Transfer Learning for Smart Background Simulation at Belle II

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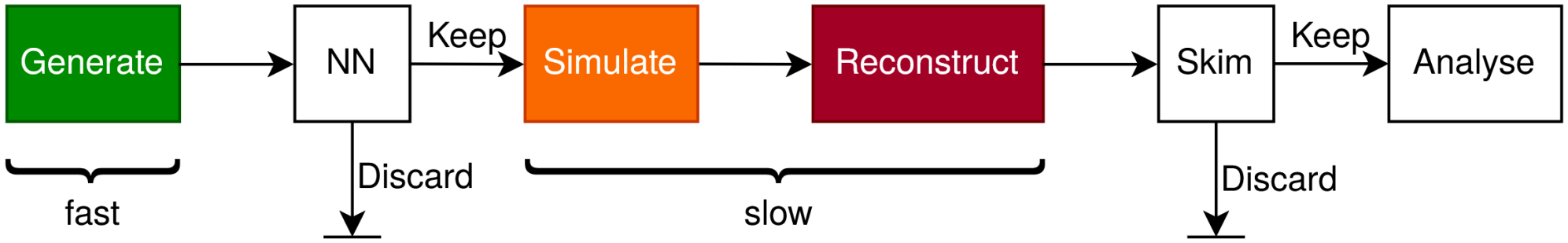
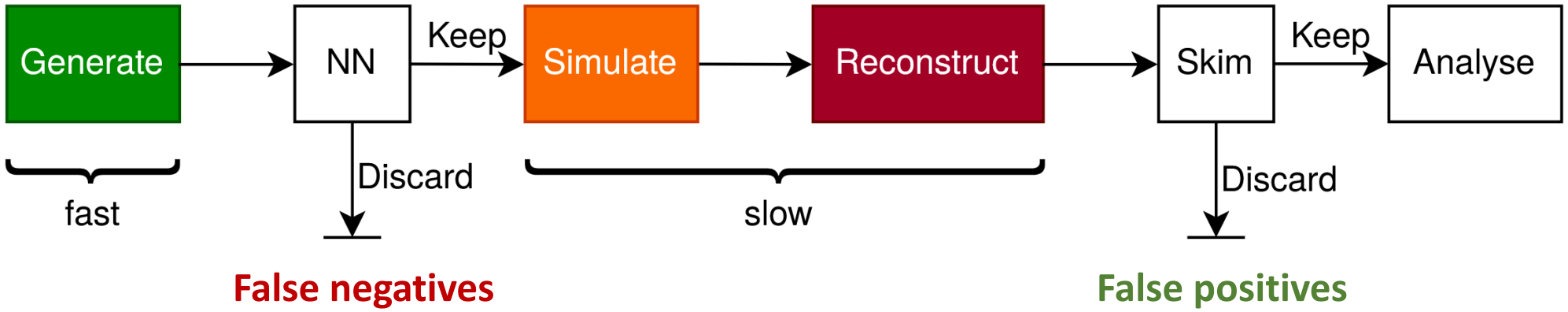
Smart Background Simulation

(Introduced in PhD Thesis by James Kahn (2019))



- **Skims** are centrally produced loose selections tailored to specific analysis types
  → Many skims throw away large fractions of costly simulated background events
- **Event generation** much faster than **detector simulation** and **event reconstruction** ($t_{slow}/t_{fast} \sim 100$)
- Typically, **no simple correlations** between features after generation and final selection criteria
- Perhaps a **neural network based classifier** can solve this issue?

Filtering procedure



- **False positives**: unproblematic (simply lower performance)
- **False negatives**: problematic!
  Discarded events are gone and may thus **bias distributions**
- Solution: **importance sampling**

Importance sampling

(Introduced in Master's Thesis by Boyang Yu (2021))

Idea:

- use NN output as **sampling probability p_i**
- **weight** each event by its **inverse probability ω_i**

→ **No bias by construction** (Disadvantage: weighted events with arbitrarily high weights)

	Probability
Event 1	0.75
Event 2	0.33
Event 3	0.01
Event 4	0.06
Event 5	0.50

	Weight
Event 1	1.33
Event 2	3.00
Event 3	X
Event 4	16.67
Event 5	X

Evaluation metric: speedup

- Goal: Train NN to achieve highest **speedup** (t_{noNN}/t_{NN}) for the same effective sample size
- **Effective sample size:**
  - := size of an unweighted sample that would yield the same **relative statistical uncertainty**
  - Estimate for number of expected events: $\mathrm{N_{exp}} = \sum_i \omega_i$
  - Estimate for variance: $\sigma^2 = \sum_i \omega_i^2$
  - Effective sample size: $\frac{\sqrt{N_{eff}}}{N_{eff}} = \frac{\sqrt{\sum_i \omega_i^2}}{\sum_i \omega_i} \Rightarrow N_{eff} = \frac{\left(\sum_i \omega_i\right)^2}{\sum_i \omega_i^2}$

Evaluation metric: speedup

- Goal: Train NN to achieve highest **speedup** (t_{noNN}/t_{NN}) for the same effective sample size
- Speedup also depends on:
  - **Assumed times** for generation t_{fast}, NN inference t_{NN} and simulation/reconstruction t_{slow} (roughly $t_{fast} : t_{NN} : t_{slow} \sim 1 : 1 : 100$)
  - **Skim efficiency** (retention rate)
    → lower retention increases potential speedup

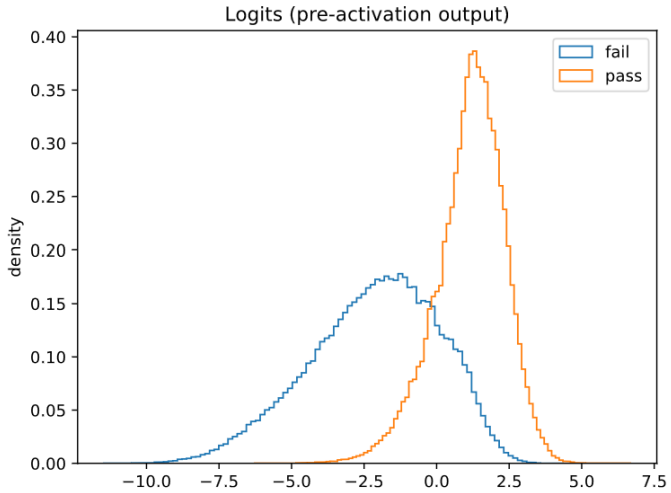
Evaluation metric: speedup

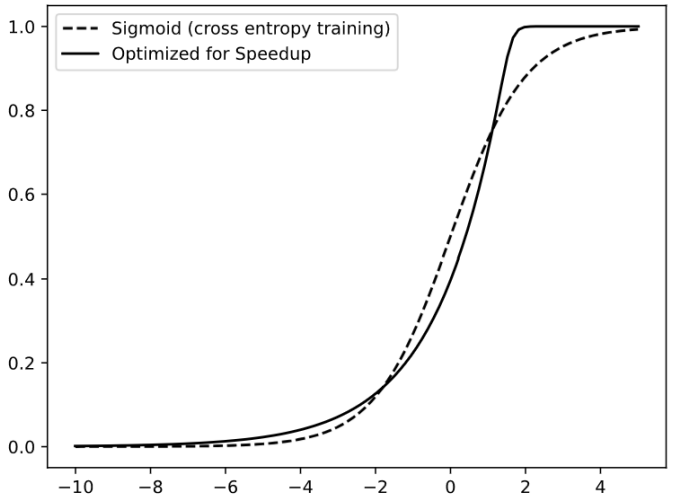
- Speedup $= t_{noNN}/t_{NN}$
- Define:
  - $t_1 \coloneqq t_{fast} + t_{NN} + t_{slow}$ (events accepted by NN)
  - $t_2 \coloneqq t_{fast} + t_{NN}$ (events rejected by NN)
  - $t_3 \coloneqq t_{fast} + t_{slow}$ (events with no NN)
- Use:
  - $t_{noNN} = t_3 \cdot N_{eff}$
  - $t_{NN} = t_1 \cdot (N_{TP} + N_{FP}) + t_2 \cdot (N_{FN} + N_{TN})$
- Some algebra later…

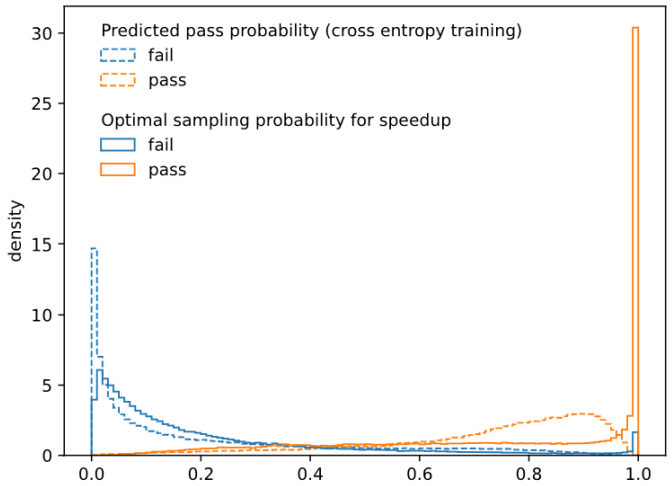
	Pass skim	Fail skim
NN accepts	TP	FP
NN rejects	FN	TN

$$\text{Speedup} = \frac{t_3/E[\omega_i]}{(\varepsilon\, f_{TP} + (1-\varepsilon)\, f_{FP})\, t_1 + (\varepsilon\, f_{FN} + (1-\varepsilon)\, f_{TN})\, t_2}$$

Optimizing for speedup







- Model trained with **cross entropy loss** and final sigmoid activation
- Idea: optimal **classification probability** for cross entropy should be related to optimal **sampling probability** for speedup by **monotonic function**

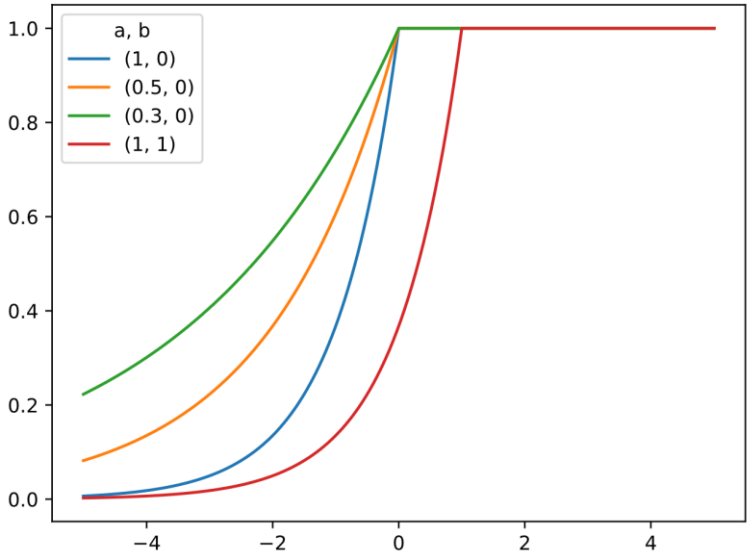
→ **Replace sigmoid activation by fitted “skewed” sigmoid optimized for speedup**

Optimizing for speedup

- Turns out generic skewed sigmoid $\left(1 + ae^{-c(x-b)}\right)^{-1/a}$ has too many parameters (no unique maximum)
- Tradeoff: shorter time ↔ narrower weight distribution
- Narrow weight distribution desirable → empirically leads to the following function:

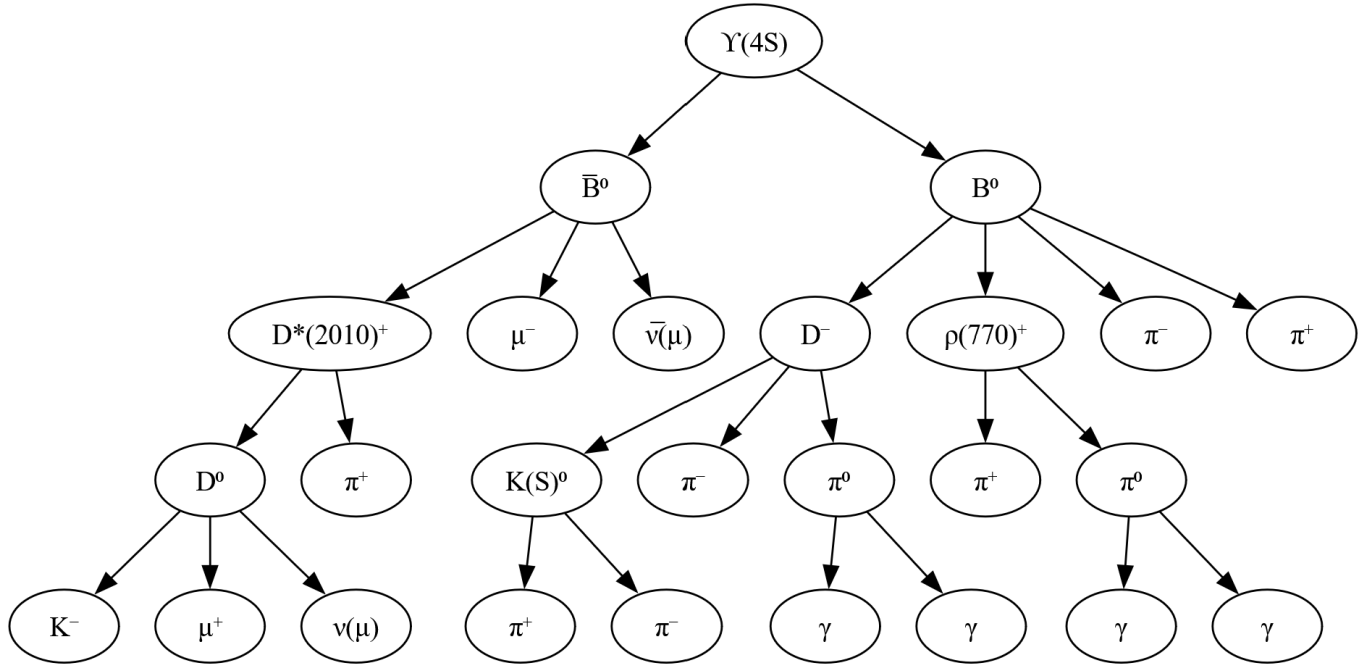
$$\min\left(e^{a(x-b)}, 1\right)$$

Two parameters:
- Scale a
- Shift b



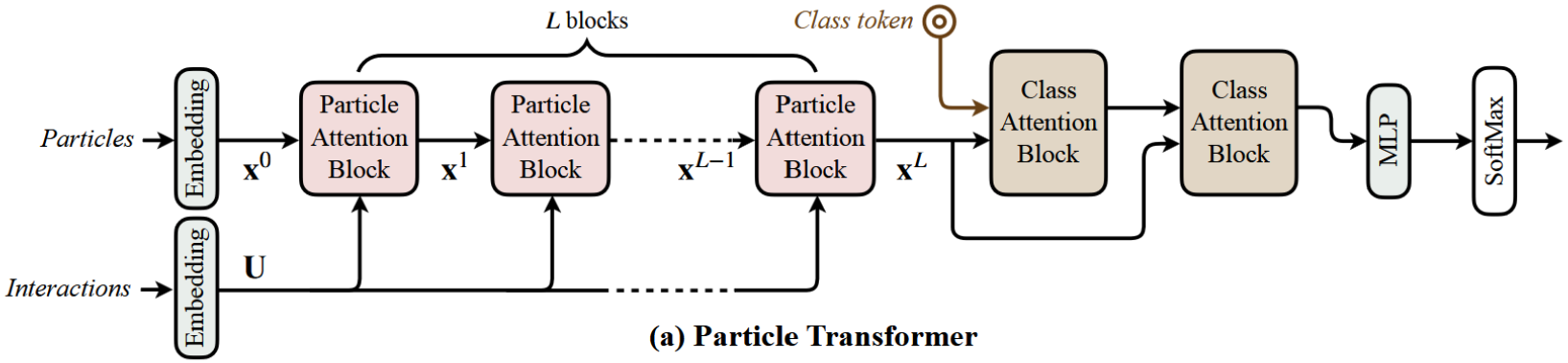
Dataset

- Generator level MC particles (hadrons, no gluons/quarks)
- List of particles with decay structure information (mother-daughter relations)
- Particle features:
  - PID
  - 4-momentum
  - Production 4-vertex

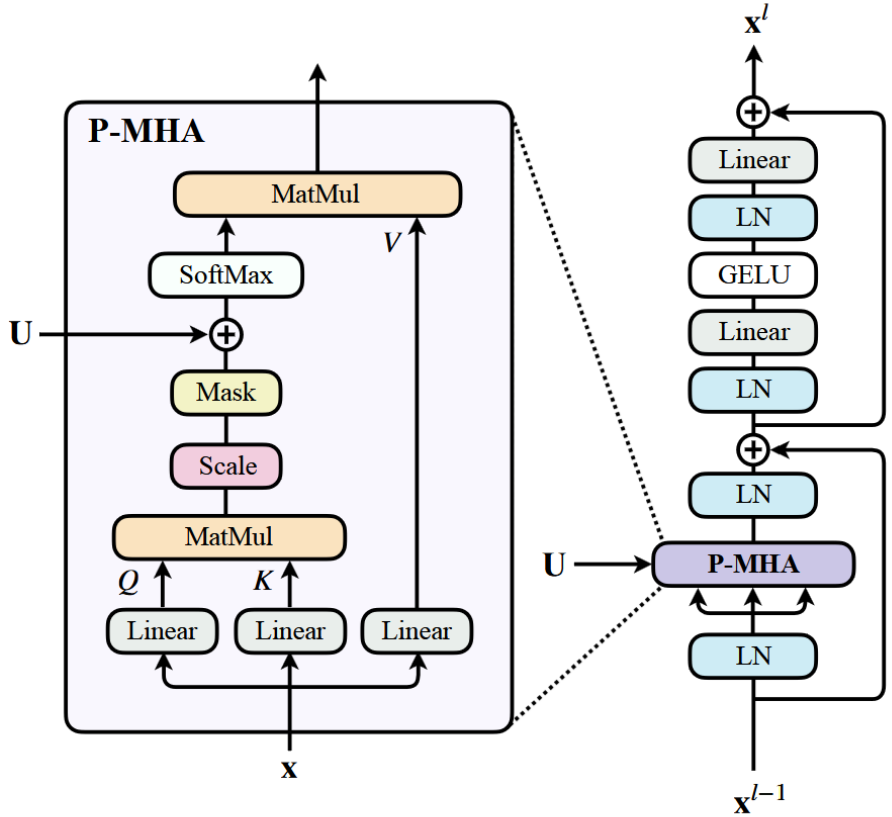


Model architecture

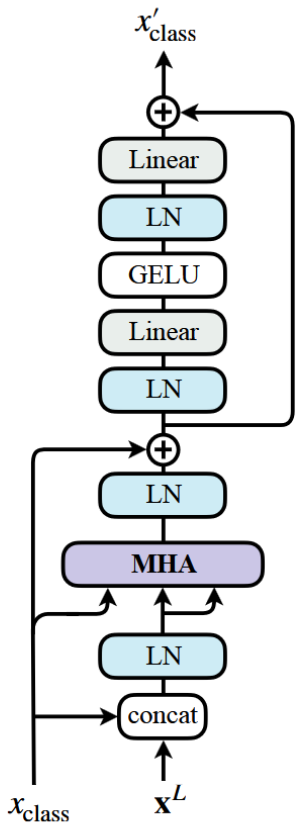
- Based on **ParT** (Particle Transformer for Jet Tagging, arxiv:2202.03772)
  → State-of-the-art performance in jet tagging by **pre-training** on large dataset and subsequent **fine-tuning** (e.g. for top tagging)
- Very generic architecture (essentially just a transformer)
- Supports edge features:
  - Adjacency matrix of decay graph
  - Two-particle invariant masses and angles
- 10 layers, $\sim$2 million parameters



(a) Particle Transformer



(b) Particle Attention Block



(c) Class Attention Block

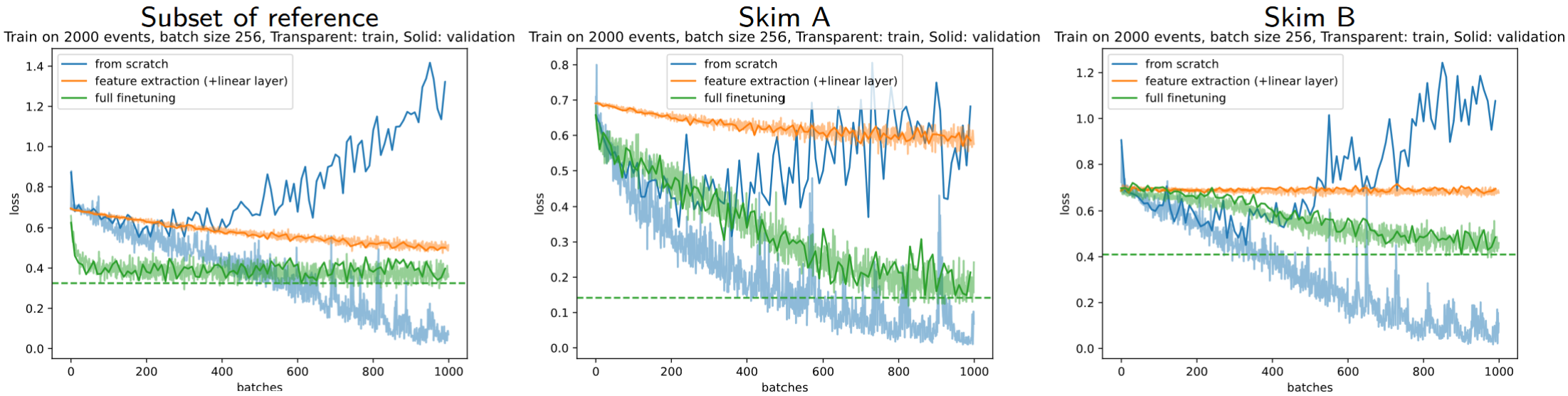
Transfer learning

- Fundamental problem:
  - Training transformer requires **large dataset**
  - But if a large dataset for a skim is already available: **what do I need the model for?**
- Solution: pre-trained models!
- Two approaches:

Feature extraction:
- Remove final layer and retrain only that
- Perhaps even just re-fit final sigmoid activation
- Only feasible for highly correlated skims

Whole model fine-tuning:
- Start with pre-trained model but adjust all parameters
- Perhaps reinitialize last layer (if output shape changes)
- Promising results in ParT paper

Transfer learning - Prestudy



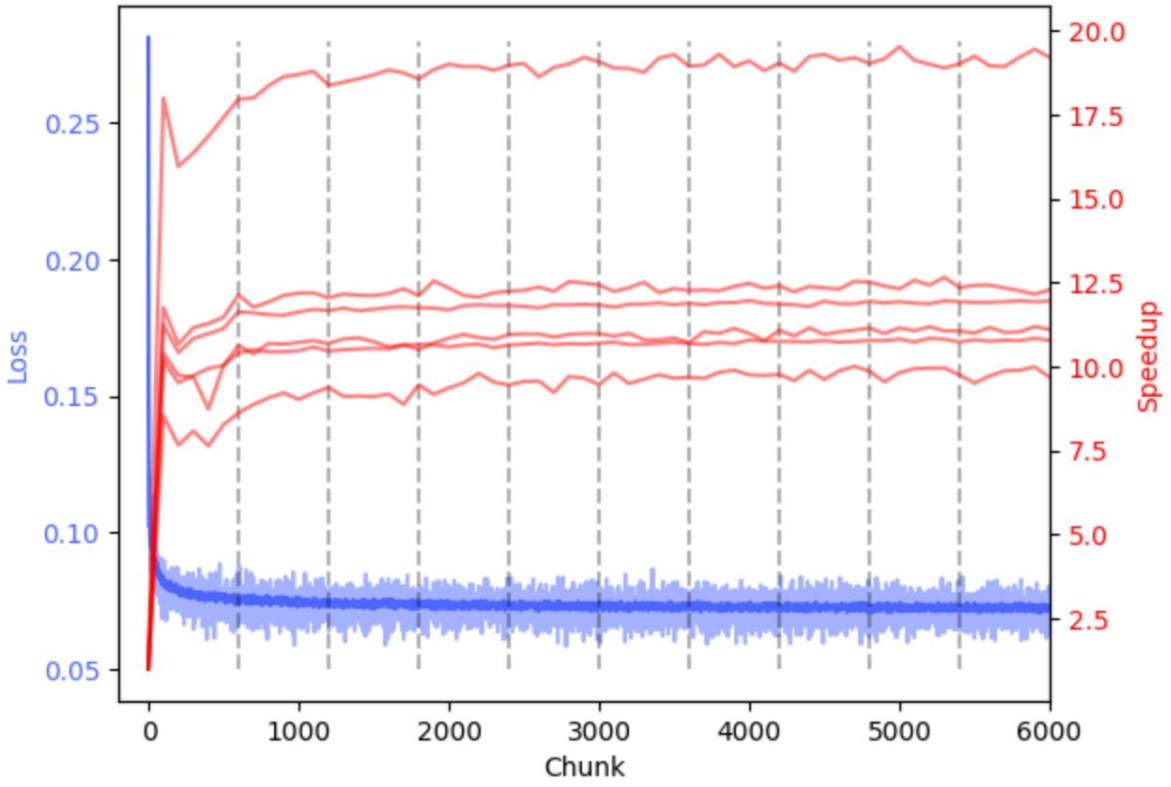
- Model trained on reference skim, then fine-tuned on 2000 events of new skim
- Feature extraction works poorly, especially with low correlations between skims (A and B)
- Training from scratch overtrains very quickly on small dataset
- Full fine-tuning looks promising, consistently yielding the best validation loss

Large scale training

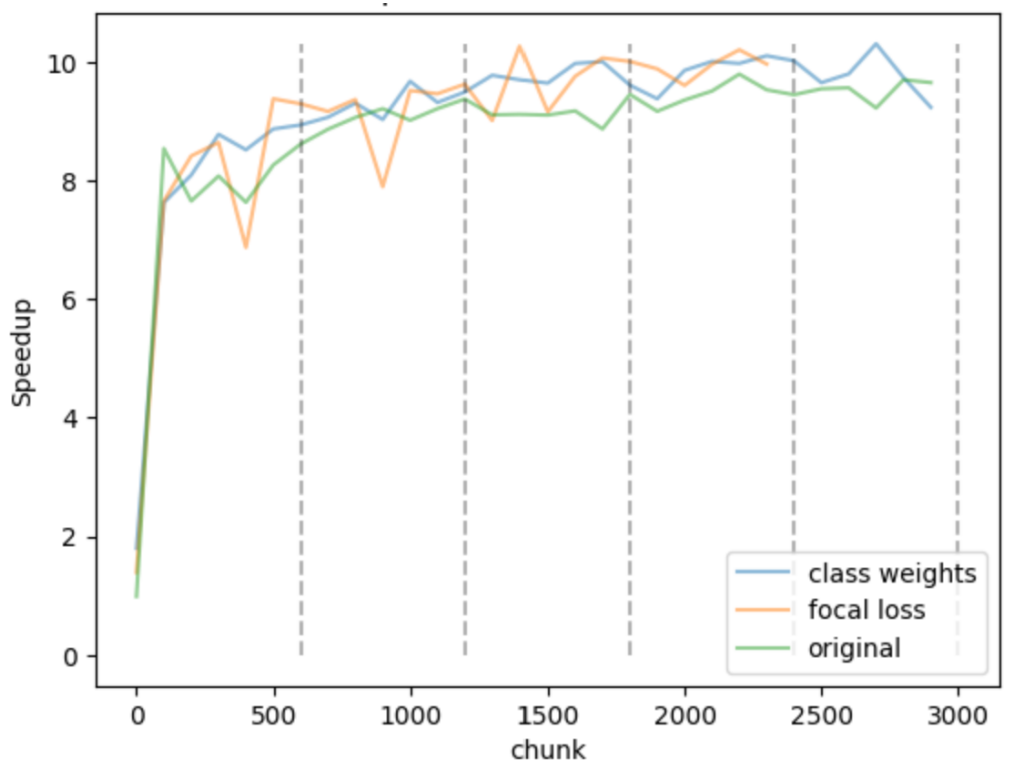
- Idea: to make flexible fine-tuning possible, pre-train model on **all available skims** at once
  - Currently samples for 51 centrally produced skims available
- 7 background types (useful for many analyses): $e^+e^- \to B^+B^-$, $B^0\bar{B}^0$, $q\bar{q}$ (q=u,d,s,c), $\tau^+\tau^-$
  - Condition model on background type
- Dataset balanced between different types, containing ~ 180 million events or $\sim 20 \mathrm{fb}^{-1}$
- Training
  - Without class weights (original)
  - With class weights
  - With class weights and empirical *focal loss* emphasizing difficult training examples

Training curves

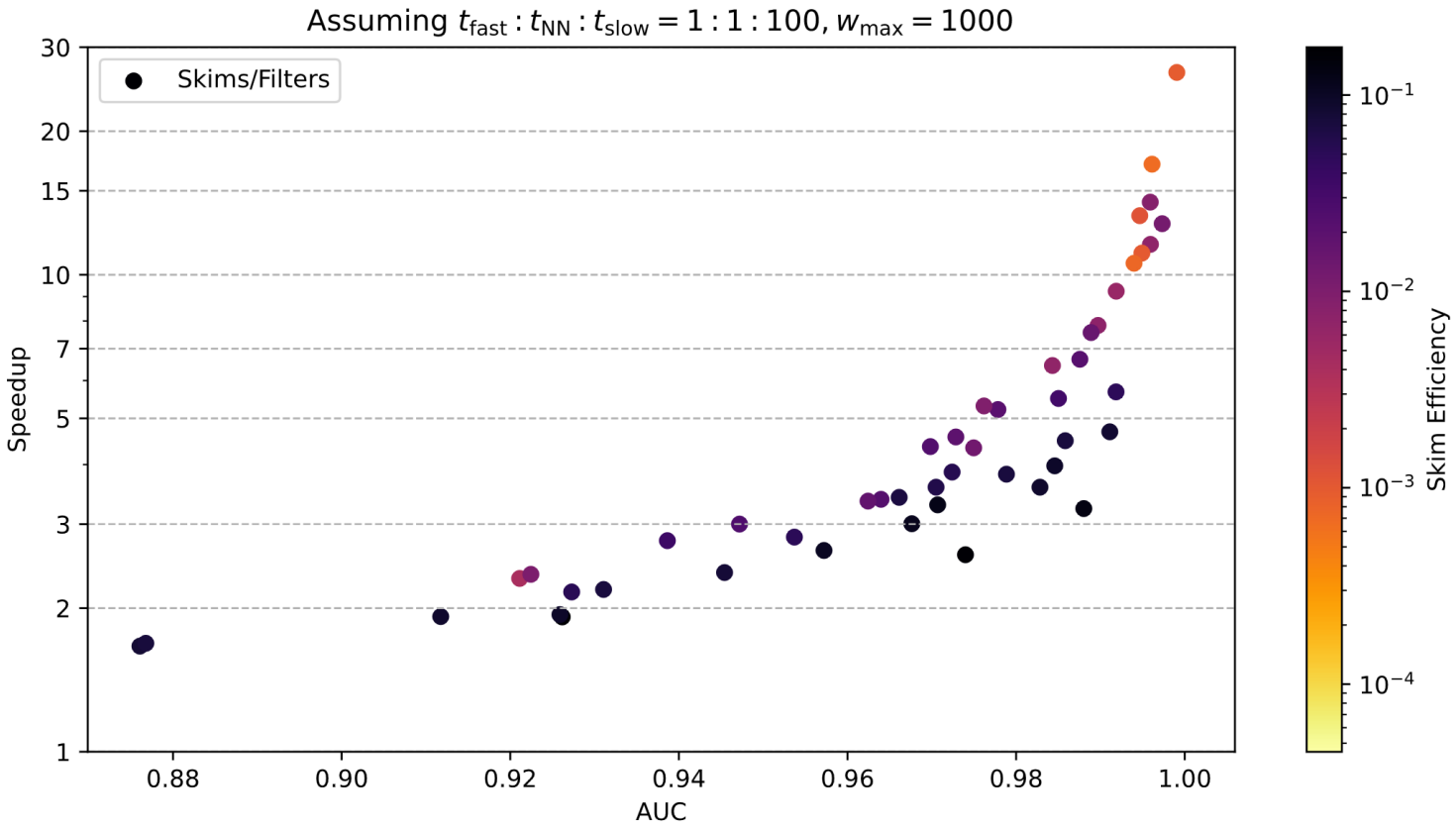
Original training



Training Comparison (example skim)



Speedups



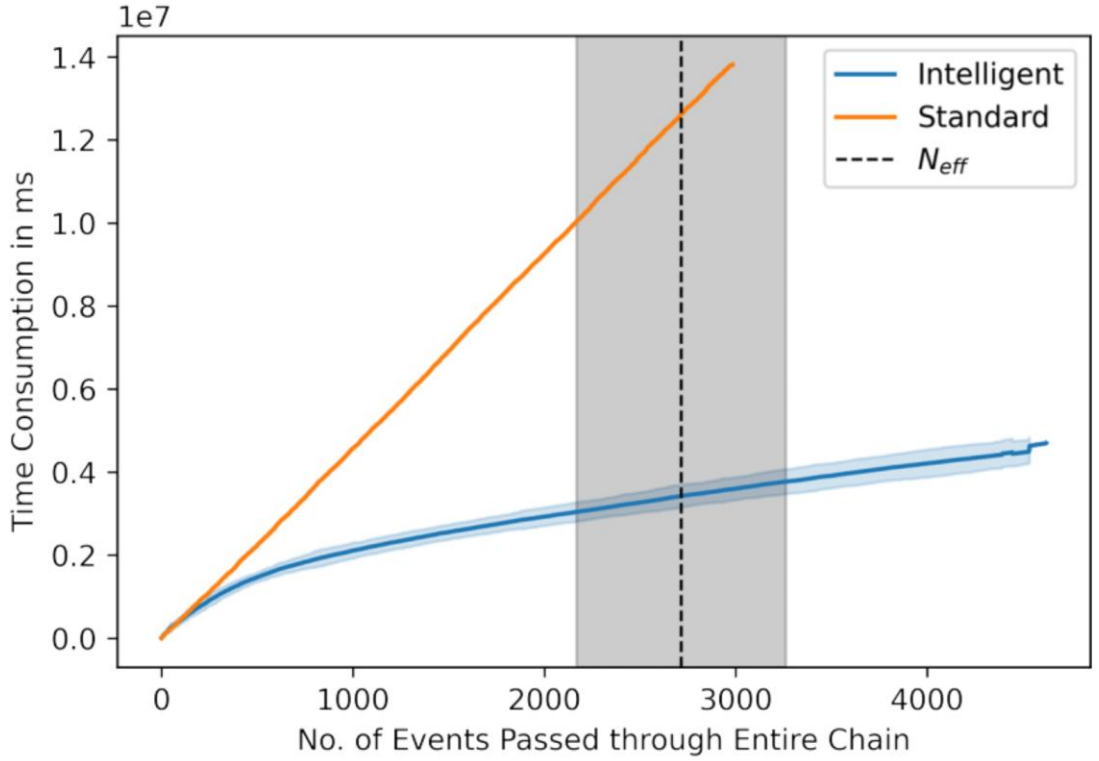
Achievable speedups **correlate with**

- **Separation power**
  (as measured by the area under the ROC curve)
- **Skim efficiency**
  (lower retention rates → higher potential for speedup)

Adaptive/Reinforcement Learning

(Introduced in Bachelor's Thesis by Daniel Pollmann (2024))

- Another possible idea:
  - Train model while producing data and running skim
  - Model becomes successively better, producing data more efficiently
- Pro: Overall time-saving, on-the-fly procedure in one step
- Contra: Requires implementing training loop in Belle II production software



Current work and outlook

Currently three main objectives:

- **Test** pre-trained model on already known skim under **different data taking conditions**
  - E.g. reprocessed data under a new software release or with more realistic beam background from so-called run-dependent MC
- **Fine-tune** and evaluate pre-trained model on **entirely new skim**
- Implement model inference in Belle II software to test model in an **actual skim production** and evaluate realistic speedup

Thank you for your attention!

Backup

Speedup derivation

- $t_{noNN} = t_3 \cdot N = t_3 \cdot \frac{\left(\sum_i \omega_i\right)^2}{\sum_i \omega_i^2} = t_3 \cdot \frac{\left(\varepsilon\, N_{gen}\right)^2}{\varepsilon^2\, N_{gen}\, E[\omega_i]} = \frac{t_3\, N_{gen}}{E[\omega_i]}$
- $t_{NN} = t_1 \cdot (N_{TP} + N_{FP}) + t_2 \cdot (N_{FN} + N_{TN}) = t_1 \cdot N_{gen}\,(\varepsilon\, f_{TP} + (1-\varepsilon)\, f_{FP}) + t_2 \cdot N_{gen}\,(\varepsilon\, f_{FN} + (1-\varepsilon)\, f_{TN})$

$$\text{Speedup} = \frac{t_3 / E[\omega_i]}{(\varepsilon\, f_{TP} + (1-\varepsilon)\, f_{FP})\, t_1 + (\varepsilon\, f_{FN} + (1-\varepsilon)\, f_{TN})\, t_2}$$

Hyperparameters

- Largely based on ParT:
  - 8 self attention blocks
  - 2 class attention blocks
  - 8 heads per multi-head attention block
  - Embedding size 128

  → Roughly 2 million parameters
- Differences:
  - Fewer norm layers
  - Embeddings for PDG ID and background type
  - Using 3 pair features (adjacency matrix, pair mass and angle)