Machine Learning at the Belle II Experiment

ML at the LHC workshop

Simon Wehle University of Nagoya 05.02.2020









Machine Learning Applications at Belle II Contents

- Charge Particle Identification
- Clustering, Cluster position, Cluster direction
- Neutral hadron/photon separation
- Image calibration
- Full Event Interpretation
- Flavour Tagging
- Disclaimer: Work from many collaborators is also presented



Introduction To Belle II



The Belle II Experiment Pushing the intensity frontier to the next level



- ~900 researchers from 30 countries, with 100+ from Germany, ~50 from DESY
- Intensity frontier flagship "B-factory" experiment: 30kHz event rate
- Precision physics and searches for (very) rare decays including Dark Matter
- First data taken 2018, data taking ongoing





Belle II Experiment

KEK, Tsukuba











Detector

Electromagnetic calorimeter (ECL):

CsI(Tl) crystals waveform sampling (energy, time, pulse-shape)

K_L and muon detector (KLM):

Resistive Plate Counters (RPC) (outer barrel) Scintillator + WLSF + MPPC (endcaps, inner barrel)

Magnet: 1.5 T superconducting

e∗ (4 GeV)

Trigger: Hardware: < 30 kHz Software: < 10 kHz

Vertex detectors (VXD):

2 layer DEPFET pixel detectors (PXD, partially installed) 4 layer double-sided silicon strip detectors (SVD)

e- (7 GeV)

Central drift chamber (CDC):

He(50%):C₂H6 (50%), small cells, fast electronics Particle Identification (PID):

Time-Of-Propagation counter (TOP) (barrel) Aerogel Ring-Imaging Cherenkov Counter (ARICH) (FWD)

> DEPFET: depleted p-channel field-effect transistor WLSF: wavelength-shifting fiber MPPC: multi-pixel photon counter



Physics Case

Motivation

 The Standard Model (SM) is very successful in describing the world at particle level

- Although many questions remain unanswered
 - Why do we have three generations of leptons and quarks? Hierarchy, masses, 22 free parameters ...
- Almost all SM predictions seem to fit experimental data precisely... Almost?



The Flavour Anomalies

(maybe only "local" anomalies...)



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(maybe only "local" anomalies...)

> 3.5 σ enhanced $B \rightarrow D^{(*)} au
u$ rates

3.3 σ suppressed branching ratio of $B_s \rightarrow \phi \mu^+ \mu^-$

 $\sim 3\sigma\,$ tension between inclusive and exclusive determination of $|V_{ub}|$

 $\sim 3\sigma\,$ tension between inclusive and exclusive determination of $|V_{cb}|$

 $> 3\sigma$ anomalies in angular distributions of $B \to K^* \ell \ell$

2.6 σ lepton flavor non-universality in $B \to K^{(*)} \mu^+ \mu^-$ vs. $B \to K^{(*)} e^+ e^-$



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The b \rightarrow s transition



The b \rightarrow s transition





The b \rightarrow s transition



B→K*II Analysis at Belle

Belle Analysis

- Similar electron and muon performance
- limited statistics
- Neural network based reconstruction in order to maximise efficiency



 $B^{+} \to K^{*+}(K^{+}\pi^{0})\ell^{+}\ell^{-} \qquad B^{0} \to K^{*0}(K_{S}\pi^{0})\ell^{+}\ell^{-} \\ B^{+} \to K^{*+}(K_{S}\pi^{+})\ell^{+}\ell^{-} \qquad B^{0} \to K^{*0}(K^{+}\pi^{-})\ell^{+}\ell^{-}$



Most simple approach: Ratio of Branching Ratios

After Moriond

- Measurements in accordance with the SM
- First measurement of R_K*+

TABLE II. Result for R_{K^*} , $R_{K^{*0}}$ and $R_{K^{*+}}$. The first uncertainty is statistical and the second is systematic.

q^2 in GeV^2/c^4	All modes	B^0 modes	B^+ modes
[0.045, 1.1]	$0.52^{+0.36}_{-0.26} \pm 0.05$	$0.46^{+0.55}_{-0.27} \pm 0.07$	$0.62^{+0.60}_{-0.36} \pm 0.10$
[1.1, 6]	$0.96^{+0.45}_{-0.29} \pm 0.11$	$1.06^{+0.63}_{-0.38} \pm 0.13$	$0.72^{+0.99}_{-0.44} \pm 0.18$
[0.1, 8]	$0.90^{+0.27}_{-0.21} \pm 0.10$	$0.86^{+0.33}_{-0.24} \pm 0.08$	$0.96^{+0.56}_{-0.35} \pm 0.14$
[15, 19]	$1.18^{+0.52}_{-0.32} \pm 0.10$	$1.12^{+0.61}_{-0.36} \pm 0.10$	$1.40^{+1.99}_{-0.68} \pm 0.11$
[0.045,]	$0.94^{+0.17}_{-0.14} \pm 0.08$	$1.12^{+0.27}_{-0.21} \pm 0.09$	$0.70^{+0.24}_{-0.19} \pm 0.07$



arXiv:1904.02440

Belle 1 Angular Analysis

Results

- LHCb sees the largest deviation in the low q² region
- Atlas and Belle can confirm the anomaly with less significance
- CMS is in good agreement with SM

 $Q^{()}$

 ℓ^{-}



 π

 K^*

 K^+

Flavour Anomalies in b->sll

New Physics or systematic problem?



The neutrino case

Golden mode for Belle II



The neutrino case

Golden mode for Belle II



- Sensitive to similar NP as tension in C9:
 - $b \rightarrow s$ transition shows signs of NP
- Theoretically very clean (no charm loops)

The neutrino case

Golden mode for Belle II















Missing Energy Channels

Full Event Interpretation (FEI)

- Hierarchical approach
 - Multivariate classifier for each state
 - Gather all information in the signal probability
- FEI can provide hadronic and semileptonic final states

Maximum reconstruction efficiency				
Tag	FR @ Belle	FEI @ Belle	FEI @ Belle II	
Hadronic B ⁺	0.28 %	0.49 %	0.61 %	
Semileptonic B^+	0.67 %	1.42 %	1.45 %	
Hadronic B ⁰	0.18 %	0.33%	0.34 %	
Semileptonic B ⁰	0.63 %	1.33%	1.25 %	



Improving the sensitivity: Deep Full Event Interpretation



Deep Full Event Interpretation

Similar to Inclusive Tagging Approach



Deep Full Event Interpretation

Similar to Inclusive Tagging Approach



Deep Full Event Interpretation

Dense Deep Neural Network


Deep Full Event Interpretation

Convolutional Neural Network



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First Results

Study performed for an example rare decay of B mesons

- Result on simulated data:
 - Order of magnitude better Performance
 - Only slight loss of information on the tag candidate
- Many "golden modes" for Belle II need tagging
- The baseline of the traditional tagging methods is ~1%
- Detailed constrain of tag-side 4-vector lost
- Improvements of only a few percent to the method can increase the statistics corresponding to years of data taking!



Excursion: Attention and Transformer Networks







Applications of RNNs

Excursion: Attention and Transformer Networks

Translation

Caption Generation



• Sentiment analysis

• But: information of whole sentence stored in fixed-length context vector

Recurrent Neural Networks (RNN)



Excursion: Attention and Transformer Networks

internal state
$$h_t = f(W_{hx}x_t + W_{hh}h_{t-1} + b_h)$$

output $y_t = g(W_{yh}h_t + b_y)$





(a) LSTM



• internal state / "memory" $h_n \rightarrow$ learn context

BUT require sequence

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slow computation

long-range dependencies are tricky

Recurrent Neural Networks (RNN)

Sequence to Sequence

Neural Machine Translation

SEQUENCE TO SEQUENCE MODEL



Credit: Jay Alammar

Recurrent Neural Networks (RNN)

Sequence to Sequence



Adding Attention

Attention is all you need

Neural Machine Translation SEQUENCE TO SEQUENCE MODEL WITH ATTENTION



am

am

Neural Machine Translation



Credit: Jay Alammar

student

а

а

Adding Attention

Attention is all you need



Attention is All You Need

DESY.

Adding Attention

Attention is all you need



Visualisation

















Transformer

Vaswani et al. 2017

DESY.



Credit: Jay Alammar

Transformer

Vaswani et al. 2017

- Multiple stacks of attention
- Implements "Self-Attention"
- Handel long range relations
- Computationally efficient
- State of the art performance



Transformer Applications in Belle II





Deep FEI Developments

Future work

- Learn generic decay reconstruction by example
- Currently FEI contains hard-coded subdecays
- Utilising self-attention maps to cluster particles
- Implemented $B \rightarrow D(\rightarrow K \pi \pi 0)\pi$ reconstruction with transformer network
- Utilising permutation invariant loss function: Kuhn-Munkres/Hungarian algorithm (shipped with SciPy)





Deep FEI Developments

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Attention Is All You Need

Other Deep NN Applications at Belle II



DEEP Flavour tagger

Flavour Tagging



- Quantum Entanglement:
 - Neutral B mesons are entangled in flavour with their production
 - With mixing, the possible outcomes are $B\bar{B}$, BB, $\bar{B}\bar{B}$

DEEP Flavour tagger

Flavour Tagging





- Deep neural network approach using track information in Input
- Simple approach already outperforms "classical" method $Belle (MC) J/\Psi K_S^0 0.293 \pm 0.01^1 0.3442 \pm 0.0009$

Credit: Jochen Gemler





Problem



- Approach at Belle:
 - Background MC ≈ 10 × data
- Infeasible at Belle II → still require high statistics

- Skims
 - Physics working-group specific datasets (26)
 - General selections applied to discard trivial backgrounds
 - Retain O(0.1–10%) of full dataset





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Selective Event Reconstruction

- Proposed Solution:
 - Let ML algorithm decide before time intensive steps
- Use Graph NN for classification





Exploring Graph Neural Networks

Selective background Monte Carlo simulation at Belle II





Graph terminology

- Nodes = Particles
- Node attributes = Particle properties
- Edges = Parent-daughter relations (decays)
- Graph type = Tree

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https://github.com/deepmind/graph_nets

Exploring Graph Neural Networks

Selective background Monte Carlo simulation at Belle II



$$X^{(l+1)} = \mathcal{A} X^{(l)} W^{(l)}$$

X = Feature matrix W = Weight matrix

Original Graph Convolutional Networks (GCN)

Propagation rule of layer activations $H^{(I)}$

$$H^{(l+1)} = \sigma \left(\tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)} \right)$$



Thomas N. Kipf, Max Welling, Semi-Supervised Classification with Graph Convolutional Networks (ICLR 2017)

Dataset

 \sim 300, 000 particle collision events with binary classification labels:

- Hadronic B+ meson reconstruction ($\sim 5\%$)
- Time-dependent *CP* violation ($\sim 0.2\%$)



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$\Upsilon(4S)$ (300553) B^0 (-511)	Feature	Definition
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	PDG code Mother PDG code Mass Charge Energy Momentum Production time Production vertex	Identifier of particle type and charge. Particle parent PDG code. Particle mass in GeV/c ² . Electric charge of the particle. Particle energy in GeV. Three momentum of the particle in Gev/c. Production time in ns relative to $\Upsilon(4S)$ production. Coordinates of particle production vertex.
	Status bit	Bitmask representing MC production conditions.

Graph Isomorphism Network

Node N update rule of layer ℓ (Red = trainable):

- Custom weights for parent (W_p) , node (W), daughters (W_d)
- Independent of daughter ordering
- Normalise adjacency matrix
 - Prevent over-representation in high multiplicity decays

Special case of:

K. Xu, W. Hu, J. Leskovec, S. Jegelka, How Powerful are Graph Neural Networks? (CoRR 2018)

 $N^{(\ell+1)} = \mathsf{MLP}^{(\ell)} \left(W_p^{(\ell)} N_p^{(\ell)} + W^{(\ell)} N^{(\ell)} + W_d^{(\ell)} \sum_{\text{daughters}} N_d^{(\ell)} \right)$

Normalised
Laplacian
$$\tilde{A} = A + I_N$$

 $\tilde{D}_{ii} = \sum_j \tilde{A}_{ij}$
 $\tilde{L} = \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}}$



Training

- Train on 250k events (validate on 10%)
- Test on 50k independent events
- Batch normalisation, dropout, class weights, early stopping, reduce LR on plateau, model checkpoint (save only best), ...
- Additional convolutional 1D for full reconstruction dataset





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Bias check

Compare event-level kinematics:

- Pass skim = True
- Pass skim and NN = True positive

Kullback-Leibler divergence of Q from P: $D_{\text{KL}}(P \parallel Q) = -\sum_{x \in \mathcal{X}} P(x) \log \left(\frac{Q(x)}{P(x)}\right)$





Selective Skim Performance

- Graph NN classification
 - > 90% accuracy on test skim
 - Orders of magnitude speed-up possible
 - Inspect event-level kinematics for bias (Kullback-Leibler divergence)
 - Presented at <u>CHEP</u> (James Kahn)





Detector based ML


Charged PID using ECL images

Clustering



Preprocessing: Image rotation, normalization, thresholds

Charged PID using cluster images

First proof-of-concept

- Seedless clustering around extrapolated
 track
- **Preprocessing** to correct charge asymmetries and background fluctuations
- Image recognition using convolutional networks
- **Future:** Add non-image information to the fully connected layers, use asymmetric images, use high dimensional image information (7×7×3..9) from digitized waveforms.



Muon/pion separation for low pt tracks ML with the Belle II calorimeter

- Low transverse momentum muons do not reach outer muon detector → Large fake rate from pions
- Particle ID based on calorimeter: E/p, BDT, or CNN?
- Design goals:
 - Separation power
 - Robustness against varying beam background
 - Flat efficiency as function of polar angle



ECL Photon position reconstruction

ML with the Belle II Calorimeter

- Crystal calorimeter: most information contained in central crystal.
- Problem: Very sparse information leads to strong bias towards towards central crystal in non-ML approaches.
- Current ML approach uses "brute force" input 5×5×3 (energy, θ, Φ) and two targets θTruth and ΦTruth. Barrel only (fully connected approach only)
- Move to generalised local position + bias reconstruction next



ECL cluster shape calibration

Wasserstein Generative Adversarial Network: WGAN

- High level user analysis is performed on reduced datasets with several expert-engineered shower shape variables per shower
 - Used to separate photons and neutral hadrons
- Differences in data and simulation of shower shapes reduces experimental precision by introducing multiple ad-hoc corrections (one per shower shape)
- Under study: Use Wasserstein refiner networks to calibrate shower images instead, before further analysis steps

CL cluster shape calibration

Wasserstein Generative Adversarial Network: WGAN



Wasserstein Generative Adversarial Network: **WGAN** (with supervised auxiliary constrainers: AC-WGAN) Wasserstein Refiner Network

ECL cluster shape calibration

Wasserstein Generative Adversarial Network: WGAN



Semi-supervised learning: Wasserstein GAN learns to create 'fake' images that look like real Belle II images.



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Photon calibration samples using CycleGANs

ML with the Belle II calorimeter

- Difficult to get very pure photon calibration sample of low-medium energy at Belle II
- Train CycleGAN to convert electrons into photons: Same physics, different curvature due to magnetic field
- Visually appealing, but is the physics right? (Same question for GANs)
- Design goals:
 - Proof of concept for a use case of CycleGANs in HEP





CLUSTER OF EXCELLENCE QUANTUM UNIVERSE

 New "Cross disciplinary" project within the Quantum Universe cluster: Belle II (intensity frontier) and SuperCDMS (low background frontier)

Fast inference for L1 trigger

ML with the Belle II calorimeter

- 8910₁ current 4×4 trigger cell Belle II: Real time photon identification for merged clusters and - 8910 5 (θ) Belle II Simulation signal-like low threshold Dark Photon searches ≙ Amplitude [a.1 0688 0668 0668 Calorimeter background Crystal Photon 1 Photon 2 Azimuthal SuperCDMS: Ultra-low threshold 8870 triggers for light ALP searches 8860 (a) Simulated ALP $\rightarrow \gamma \gamma (m_{ALP} =$ 8850 energy depositions in the Belle II calor currently used example trigger cell (m KINTEX. Please get in touch if you are 8840 Figure 1: Example inpu interested. 8830 SuperCDMS data **Belle II Simulation** CDMS SNOLAB to not saturate 8820 3 5 Polar Crystal ID (ϕ) for the DAQ system is to be dea Time [ms] means the hardware level trigge A way to lower the threshold in the presence of LFN noise while keeping the DAQ deadtime free is to identify LFN noise in real-time. LFN traces do not have a unique pulse Machine Learning at the Belle II Experiment | Simon Wene 105.02.2020 stypically differ from signal-like pulses. We will work to-Credit: Torben Ferber 63 wards replacing the existing threshold–based amplitude triggers by an ML classification

Final Excursion: Fallacies and Prospects

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- Deep learning methods sometimes have extraordinary amount of free parameters (VC dimensions >> data)
- Learned "features" of the data is not always obvious

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EXPLAINING AND HARNESSING Adversarial Examples

 $+.007 \times$

Ian J. Goodfellow, Jonathon Shlens & Christian Szegedy Google Inc., Mountain View, CA {goodfellow, shlens, szegedy}@google.com





=

 $x + \epsilon sign(\nabla_x J(\theta, x, y))$ "gibbon" 99.3 % confidence

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(a) Husky classified as wolf

Figure 11: Raw data and explanation of a bad model's prediction in the "Husky vs Wolf" task.

Re-Interfere model response on the input may help understand the expertise

"Why Should I Trust You?": Explaining the Predictions of Any Classifier Marco Tulio Ribeiro, Sameer Singh, Carlos Guestrin

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- These problems often can't be spotted with classical test and training data sets





Heatmaps showing the class evidence extracted from of each part of the image.

Approximating CNNs with Bag-of-local-Features models works surprisingly well on ImageNet <u>Wieland Brendel</u>, <u>Matthias Bethge</u>

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Plans for the Future of ML at Belle II



Graph Neural Network

Plans for the Future of ML at Belle II

- GNNs might be applicable in many parts of our analyses
 - Deep Full Event Interpretation
 - Skimming of Data
 - Tracking

HEP.TrkX project



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 $o_i = \sum s_i$

Systematic Uncertainties and Deep Learning

Plans for the Future of ML at Belle II

- Systematic uncertainty on multivariate methods are a serious challenge
 - How to propagate uncertainties
- Bayesian Neural Networks are more and more used in HEP



Conclusion

Prospects for machine learning

- "Classical" ML is very successful in Belle II analyses already
- Potential of Deep Learning is explored in many studies like simulation, reconstruction and analyses
 - Is the problem well described?
 - Does it get the physics right?
 - There is for sure a lot room for improvement
- GraphNN approaches offer interesting new opportunities
 - Work in progress
 - Promising approaches exist already from industry and other experiments



Credit: Google DeepMind













Thank you very much for your attention!

Contact

DESY. Deutsches Elektronen-Synchrotron

www.desy.de

Simon Wehle Belle & Belle II simon.wehle@desy.de +49 40 4994 3789