Selective Background Monte Carlo Generation

feat. Deep Full Event Interpretation (T. Boeckh)

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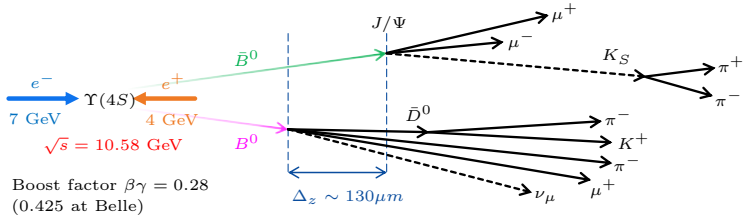
Emilio Dorigatti (LMU, Hackathon mentor)

October 1, 2019

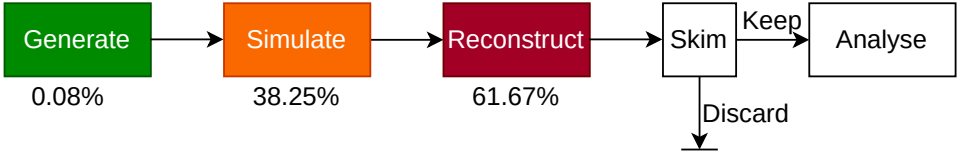
Dresden deep learning hackathon

Dresden deep learning hackathon

Project Overview



- Simulation of particle collisions computationally expensive, but most of the results are uninteresting and thrown away
- Idea: Can we figure out whether a collision is uninteresting at an early stage?



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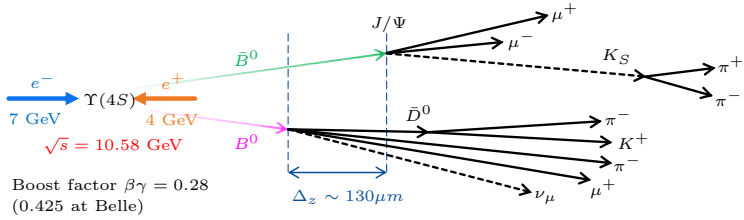

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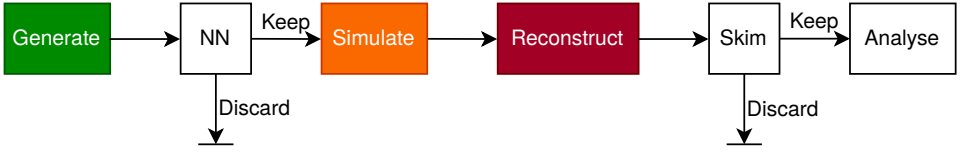
- Idea: Can we figure out whether a collision is uninteresting at an early stage?
  - **Skip expensive steps**



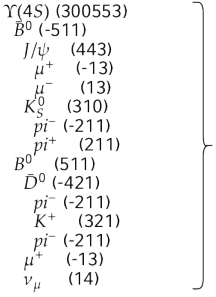
Dataset

Three categories of decay data:

- Full charged B meson reconstruction
- Full neutral B meson reconstruction
- Time-dependent CP violation

For each category:

$\sim$ 300,000 particle collision processes with binary classification labels



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

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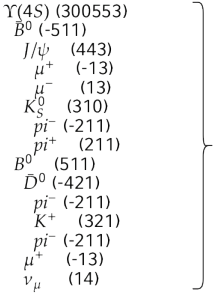

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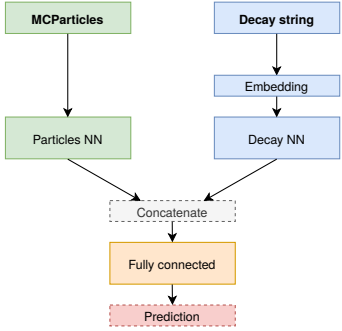
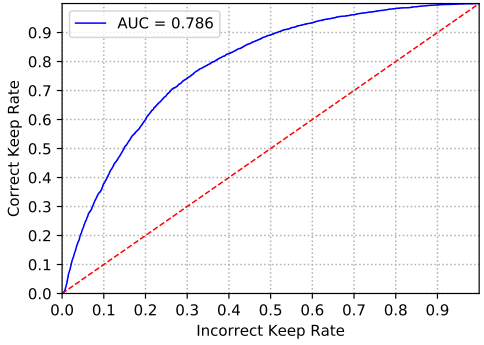
Goals

Previous work by James Kahn:

- Convolutional neural networks: residual, recurrent, vanilla...





Goals for hackathon:

- Implement graph convolutional network
- Decorrelate network from selected kinematics

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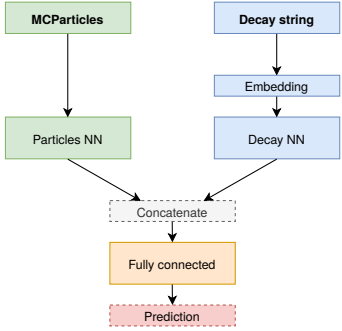
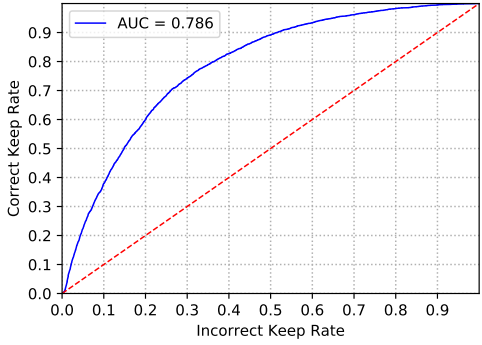




Goals for hackathon:

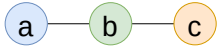
- Implement graph convolutional network
- ~~Decorrelate network from selected kinematics~~

Original Graph Convolutional Networks (GCN)

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

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

$$H^{(0)} = X$$
$$\tilde{A} = A + I_N$$
$$\tilde{D}_{ii} = \sum_j \tilde{A}_{ij}$$



$$\tilde{A}^{N\times N} = A + I = \begin{array}{c} \\ a \\ b \\ c \end{array}\begin{array}{c} \begin{array}{ccc} a & b & c \end{array} \\ \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{bmatrix} \end{array}$$

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

Modified GCN

$$H^{(l+1)} = \sigma\left(H^l\left(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}W_1^{(l)}\right)^T W_2^{(l)}\right)$$

Intuition: **custom weights for each node, considering neighbors**

- Weight vector for every node: W_1 (size: $N \times F$)
- Multiply by $\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}} \longrightarrow$ weight vector for every node as the average of the vectors of neighboring nodes (output size: $N \times F$ again)
- Transpose and multiply by $W_2 \longrightarrow$ custom dense layer for each node (W_2 size: $N \times U$, result size: $F \times U$)
- Multiply by H: transform every node in the previous layer with its own custom layer (H size: $N \times F$, result size: $N \times U$)

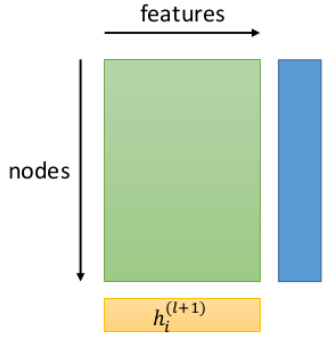
Special case of **graph isomorphism network**:
K. Xu, W. Hu, J. Leskovec, S. Jegelka, *How Powerful are Graph Neural Networks?* (CoRR 2018)

Node Aggregation

- **Soft attention** – weights given by softmax (D) and values given by $\tanh(E)$
- E, D: Independent dense layers applied to features of each node

$$h^{(l+1)} = \sum_i \left(\text{softmax}\left(D_{(i)}^{(l)} \right) \odot \tanh\left(E_i^{(l)} \right) \right)$$

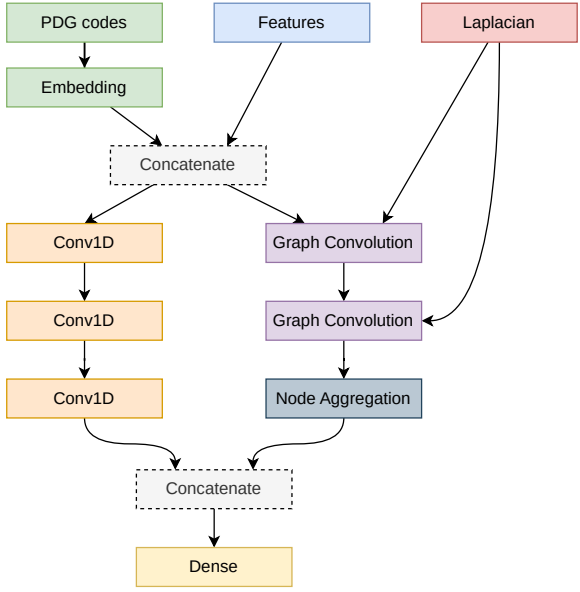
$$= \sum_i \frac{\exp D_{(i)}^{(l)}}{\exp \sum_k D_{(k)}^{(l)}} \tanh E_i^{(l)}$$



Adapted from: Yujia Li, Richard Zemel, Marc Brockschmidt, Daniel Tarlow, *Gated Graph Sequence Neural Networks*, (ICLR 2016)

Results

- Train with random subset of 225k processes (validate on 20%)
- Test on 75k independent processes
- Class weights
- Early stopping
- Reduce learning rate on plateau
- Model checkpoint – save only best



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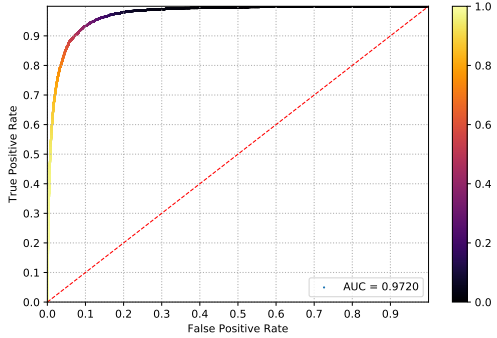
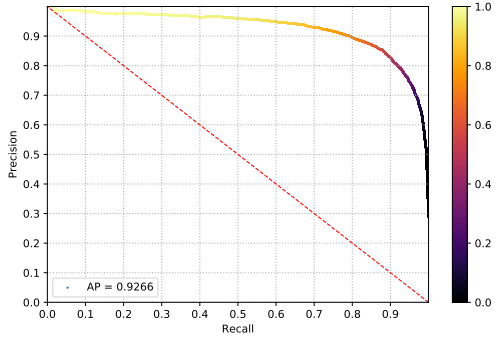
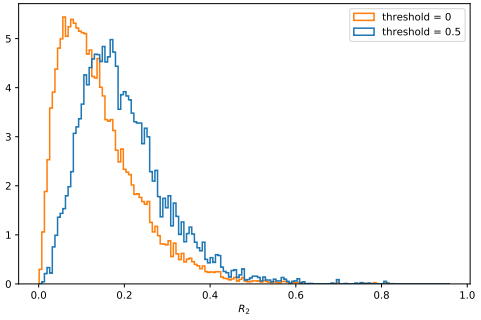


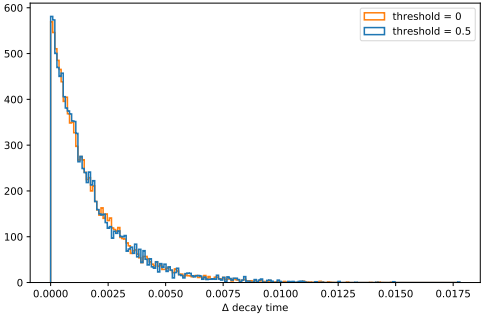


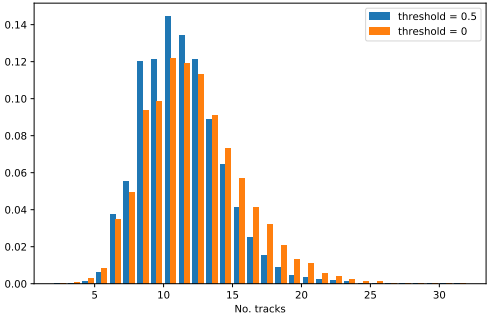
Current work

Bias control

- Studying impact of NN on resulting physics
- Selected event-level kinematic variables
- Implementing adversarial decorrelation







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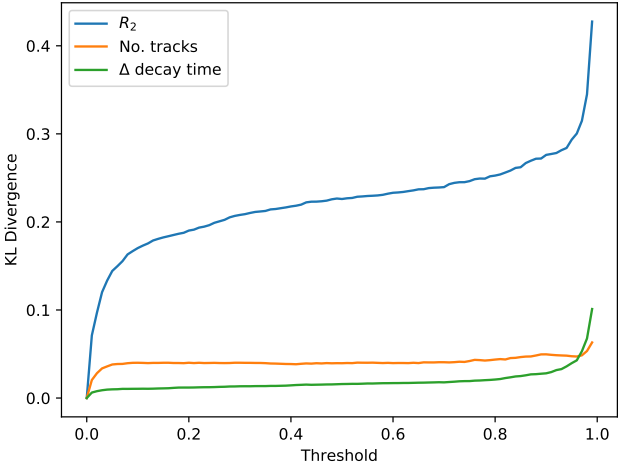


Next steps

- Implementation and timing in analysis framework
- Hyperparameter optimisation
- Training on large dataset and other skims
- Talk accepted at CHEP2019 (Computing in High Energy Physics) – proceedings

Bias Mitigation/Decorrelation:
Many approaches being explored:

- Divergence term in loss
- Adversarial setup
- Distance decorrelation (G. Kasieczka)
- Mutual information regularization (J. Tan, Belle II)
- ...

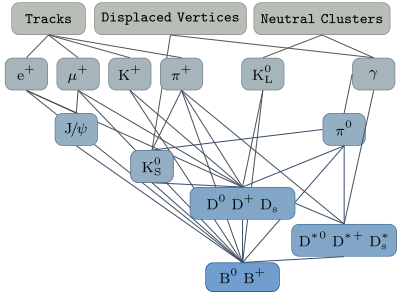
Common problem in physics ML usage

Deep Full Event Interpretation (deepFEI)

Overview

Existing generic reconstruction algorithm at Belle II:

- Hierarchical approach
- Reconstruct multiple *hard-coded* decay channels per particle
- Stacked boosted decision trees
- $\epsilon(B_{\mathrm{SL}}) = \mathcal{O}(1\%)$, $\epsilon(B_{\mathrm{H}}) = \mathcal{O}(0.1\%)$



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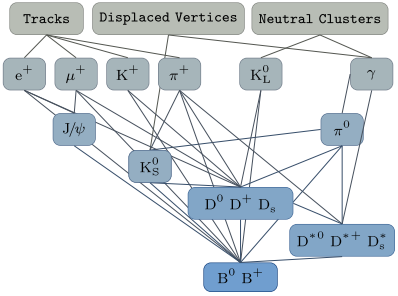
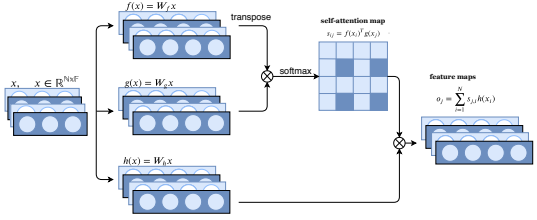
deepFEI:

- Generic solution to learn common decays by example
- Stacked self-attention maps to group particles – interpret as parent

Addresses generic problem:
How to build a tree from the leaves alone?



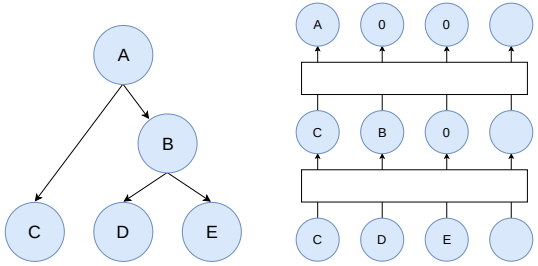


Deep Full Event Interpretation (deepFEI)

Progress

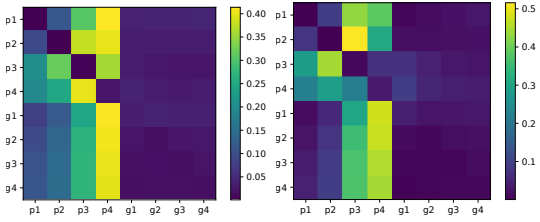
Implemented at hackathon:

- Transformer network setup
- Reconstruct $B \to D(\to K\pi\pi^0)\pi$ decays
- Permutation invariant loss function: *Kuhn-Munkres/Hungarian algorithm* (shipped with SciPy)



Results:

- Difficult to interpret attention maps
- No clear way to identify candidate decay chains
- Converging on **graph-based** solution



Closing remarks

Experiences from machine learning in Belle II:

- Sharing individual project progress interesting but ultimately not useful (without a lot of personal effort)
- Abstraction to generic, situational solutions significantly more useful
- Difficult to get overview of (latest) machine learning landscape

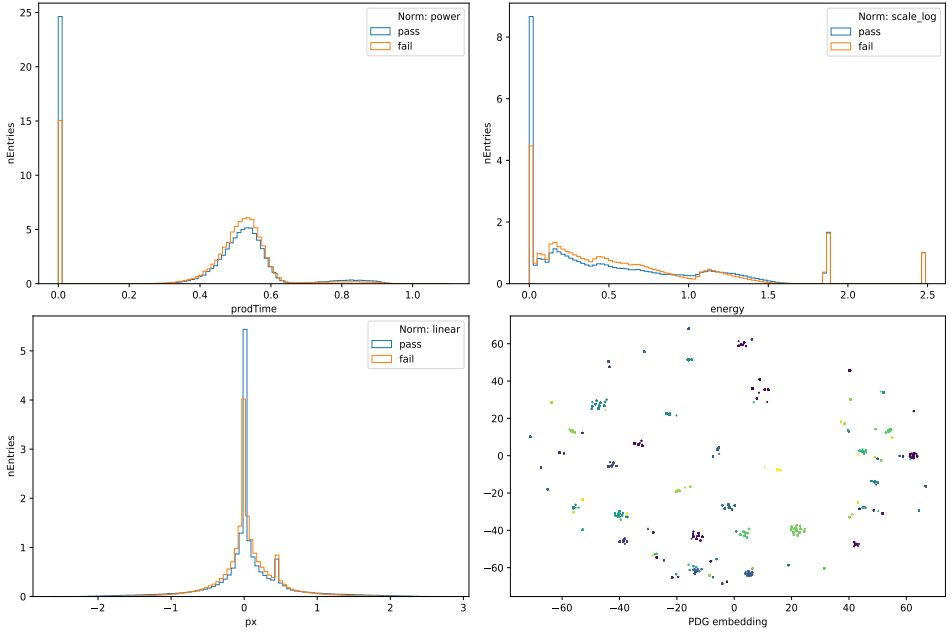
Example recurring topics:

- Quantifying systematic uncertainties
- Decorrelating network outputs
- Variable or irregular-shape inputs

Thank you

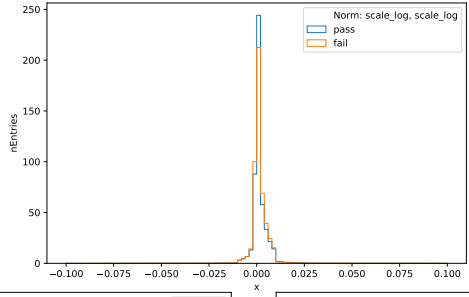
Backup

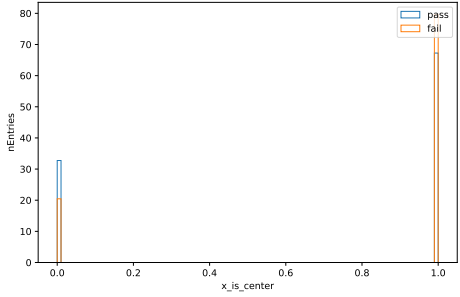
Features

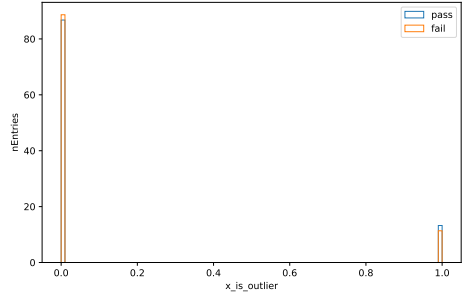

Norm: power
pass
fail
nEntries
prodTime
Norm: scale_log
pass
fail
nEntries
energy
Norm: linear
pass
fail
nEntries
px
PDG embedding

Features II

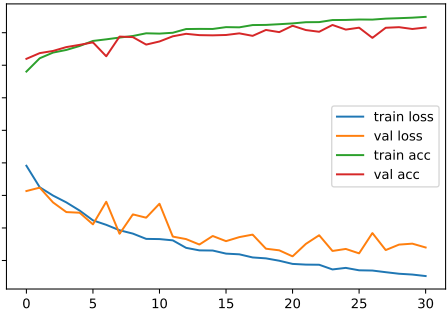
x, y, z coordinates: Hard to normalize

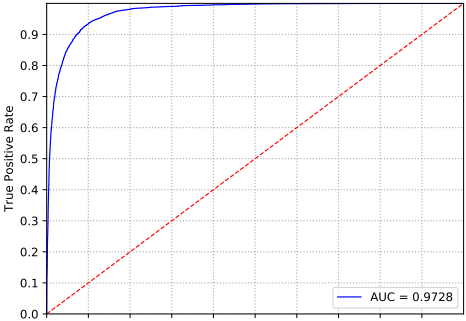


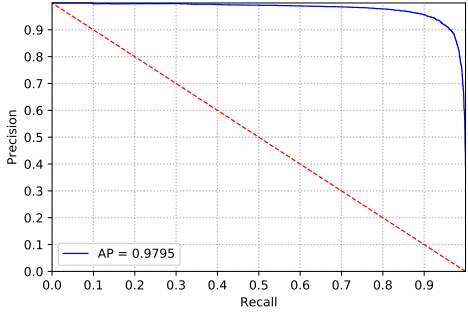




Results (Smaller network)







Adjacency matrix

Add my plot from notebook

Architecture

```
p = GraphConvolution(128, kernel_regularizer=regularizers.l2(l2_strength))([feature_input, laplacian_input])
p = layers.LeakyReLU()(p)
p = GraphConvolution(128, kernel_regularizer=regularizers.l2(l2_strength))([p, laplacian_input])
p = layers.LeakyReLU()(p)
p = NodeAggregation(256, kernel_regularizer=regularizers.l2(l2_strength))(p)

m = layers.Concatenate()([pdg_l, feature_input])
m = layers.LeakyReLU()(layers.Conv1D(128, 5)(m))
m = layers.LeakyReLU()(layers.Conv1D(128, 5)(m))
m = layers.LeakyReLU()(layers.Conv1D(128, 5)(m))
m = layers.GlobalAveragePooling1D()(m)

l = layers.Concatenate()([m, p])

l = layers.Dropout(0.5)(l)
l = layers.LeakyReLU()(layers.Dense(512, kernel_regularizer=regularizers.l2(l2_strength))(l))
l = layers.LeakyReLU()(layers.Dense(256, kernel_regularizer=regularizers.l2(l2_strength))(l))
l = layers.Dropout(0.3)(l)
l = layers.LeakyReLU()(layers.Dense(128, kernel_regularizer=regularizers.l2(l2_strength))(l))
l = layers.LeakyReLU()(layers.Dense(32, kernel_regularizer=regularizers.l2(l2_strength))(l))

output_layer = layers.Dense(1, activation='sigmoid')(l)
```

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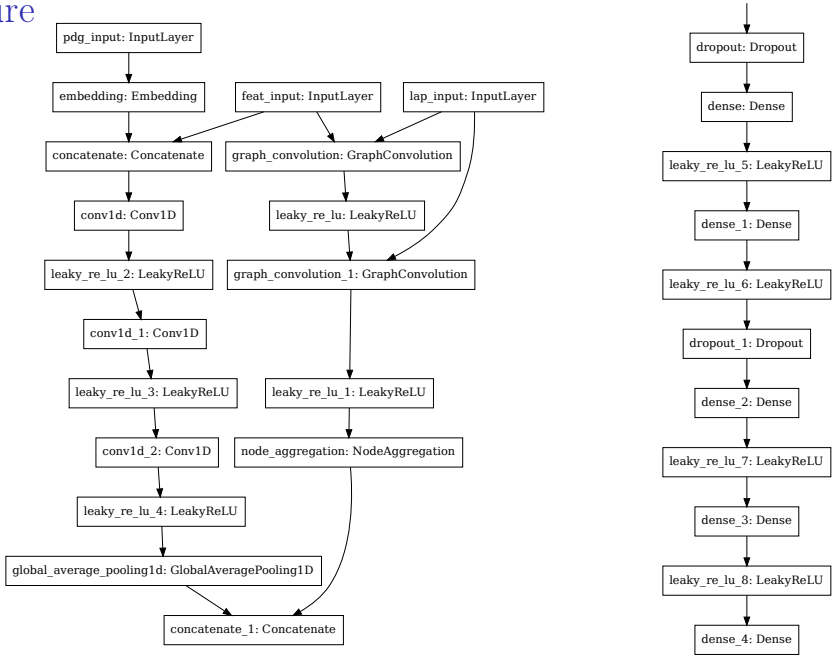

Architecture