# Sequence Modelling of Collision Events with Convolutional Architectures

*Justin Tan*, Phillip Urquijo

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# Motivation

Processes with a variable number of intermediate/final state particles occur in many contexts, e.g.

- Analysis of flavor anomalies
- Measurements of observables in rare decays
- Vertexing
- Jet tagging

Traditionally, encode the event information in a fixed-dimensional vector as input to an ML algorithm, but this incurs some information loss.

Want a performant model that natively handles variable length sequences, while being competitive with current approaches.

# Flavor Physics

## Precision flavor physics

Compare precise experimental measurements of observables in $B$ decays with theoretical predictions; interpret discrepancies in terms of new physics.

- Look for indirect effects of heavy unknown particles in low energy observables of $B$ mesons.

Penguin processes:

Radiative: $b \to q\gamma$

Electroweak:

$b \to q\ell^+\ell^-, \quad q = s, d$

- FCNCs, forbidden at leading order → rare + hard to observe!

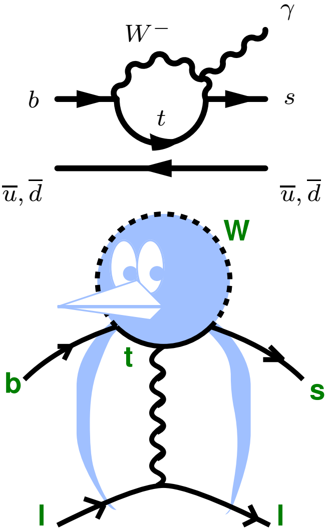


Figure 1: Radiative $b \to s\gamma$ (top) and electroweak $b \to s\ell^+\ell^-$ (bottom) penguins

# Belle II

- Next generation $B$-physics experiment at SuperKEKB, an $e^+e^-$ collider in Japan.
- Target: $50 \times 10^9$ $e^+e^- \rightarrow \Upsilon(4S) \rightarrow B\bar{B}$ events by 2024.
- Large statistics → high precision measurements of penguin decay observables: $\mathcal{B}_{s(d)\gamma}, A_{\text{CP}}$.

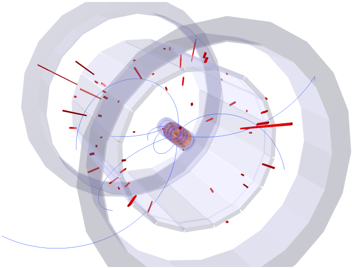


Figure 2: Belle II $e^+e^-$ collision simulation.

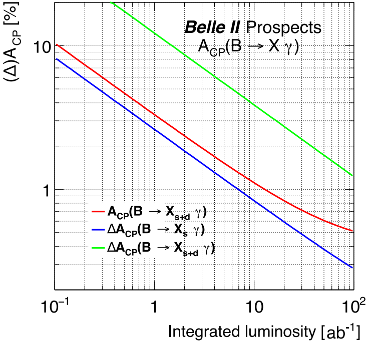
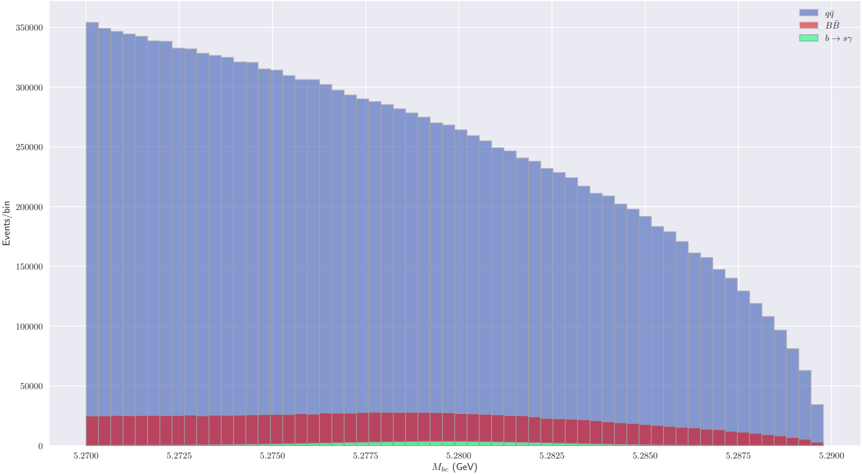


Figure 3: Sensitivity to $A_{\text{CP}}$ (red) in $b \rightarrow s(d)\gamma$ decays.

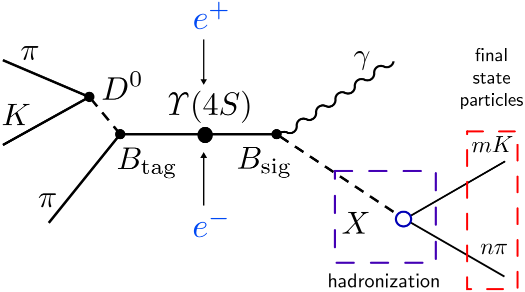
# Penguin hunting

Mass distribution for 1 $\mathrm{ab}^{-1}$ of simulated $e^+e^-$ collisions at Belle II.
Background: $e^+e^- \to q\bar{q}, \quad q = u, d, s, c$ + $e^+e^- \to b\bar{b}$
Signal: $b \to s\gamma$



# Event Reconstruction

- Reconstruct $B_{\text{sig}} \to X\gamma$ from combining the radiative photon $\gamma$ with the hadronic final state $X$
- Hadronic $X$ is explicitly reconstructed in as many final states as possible ($\approx 50$)

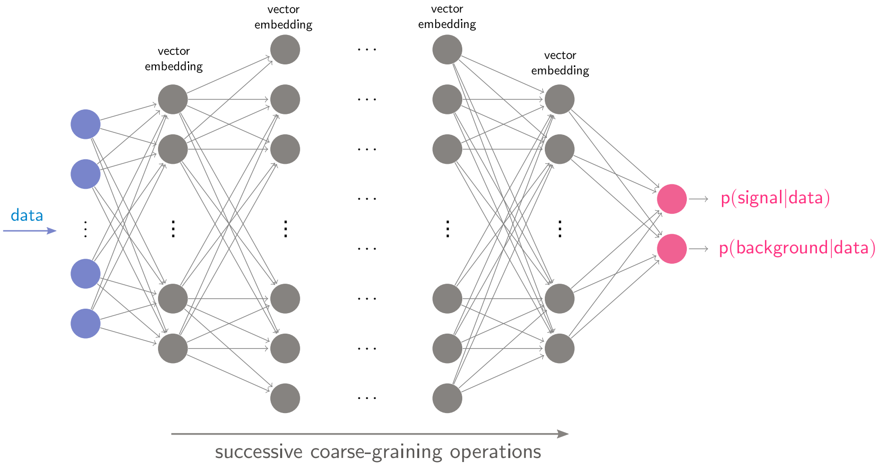


$$X = K^+\pi^+\pi^-$$
$$\text{or } (K^0_S \to \pi^+\pi^-)\ \pi^+\pi^-$$
$$\text{or } \pi^+(\pi^0 \to \gamma\gamma)(\eta \to \gamma\gamma), \text{etc.}$$

How can we capture the full event information of variable-length decay sequences?

# Neural Networks

Identify 'relevant' degrees of freedom, iteratively integrate out 'irrelevant' degrees of freedom.



# Natural Language

Condition on the entire sequence to infer a distribution over some property.

Prediction $p(\cdot|\text{Luke went to the beach and caught a})$

Translation $p(\text{some English} \mid \text{du français})$

Classification $p\left(\textit{positive} \mid \text{Despite the constant negative press covfefe}\right)$

Modern approach:
Introduce a learnable projection of each word into a continuous vector space, condition on the **learnt representation**, $\mathcal{R}$, usually the output of a neural network acting over the embedded words.

**Donald J. Trump** @realDonaldTrump · 38m
Despite the constant negative press covfefe

# Natural Language x Particle Physics

see also arXiv:1702.00748

Collision event ↔ sentence, particle ↔ word

Particles are words in our 'language', described by a vector of 'morphemes':

$$\mathbf{x}_{particle} = (p^{\mu}, \{r, \theta, \phi\}) \leftarrow \text{kinematic + topological features}$$

e.g. Rare decay $B^{+} \rightarrow \rho^{+}\gamma$, where $\rho^{+} \rightarrow \pi^{+}\pi^{0}$ and $\pi^{0} \rightarrow \gamma\gamma$, represent event as an ordered sequence of particle vectors

$$\{\mathbf{x}\}_{\text{input}} = \left[ \left( \mathbf{x}_{B}, \mathbf{x}_{\rho}, \mathbf{x}_{\gamma}, \mathbf{x}_{\pi^{+}}, \mathbf{x}_{\pi^{0}}, \ldots \right)^{T} \right]_{|\mathbf{p}|\text{-ordered}}$$

Given the observed particle sequence, how probable is this correctly reconstructed signal?

$$p\left( \textit{positive} \mid \text{Despite the constant negative press covfefe} \right) \ll 1$$

$$p\left( \textit{signal} \mid \{\mathbf{x}_{B}, \mathbf{x}_{\rho}, \mathbf{x}_{\gamma}, \ldots\} \right) = \,?$$

# Natural Language x Particle Physics

Decays can be very short ☺

$$B \to K^+\pi^-\gamma, \quad \text{input: } \left[\left(\mathbf{x}_B, \mathbf{x}_{K^+}, \mathbf{x}_{\pi^-}, \mathbf{x}_\gamma\right)^T\right]_{|\mathbf{p}|\text{-ordered}}$$

Or very long ☹

$$B \to [K_S^0 \to \pi^+\pi^-][\pi^0 \to \gamma\gamma][\pi^0 \to \gamma\gamma]\pi^+\pi^-\gamma$$

$$\text{input: } \left[\left(\mathbf{x}_B, \mathbf{x}_{K_S^0}, \mathbf{x}_{\pi^+}^{K_S^0}, \mathbf{x}_{\pi^-}^{K_S^0}, \mathbf{x}_{\pi^0_{(1)}}, \mathbf{x}_{\pi^0_{(2)}}, \mathbf{x}_{\gamma_1}^{\pi^0_{(1)}}, \mathbf{x}_{\gamma_2}^{\pi^0_{(1)}}, \mathbf{x}_{\gamma_1}^{\pi^0_{(2)}}, \mathbf{x}_{\gamma_2}^{\pi^0_{(2)}}, \mathbf{x}_{\pi^+}, \mathbf{x}_{\pi^-}, \mathbf{x}_\gamma\right)^T\right]_{|\mathbf{p}|\text{-o}}$$

Challenging because of combinatorics for high-multiplicity states!

Instead of having a fixed ('global') representation of features present in all events, we use a variable-sized event representation to encode more information.

# Event Representations

## Classical representation

- Reliance on low-dimensional engineered features - information loss
- Can only use restrictive global event information - input is unordered set of features common to all event types
- No a priori knowledge of intrinsic structure of collision event

## Sequential representation

- Inclusion of elementary kinematic features should contain all information needed to derive high-level features ✔
- Condition network response on all particle candidates in event → less information discarded ✔
- Introduce prior over event structure (composed of discrete units with related attributes) ✔

Two approaches to sequence analysis - *recurrent* and *convolutional*.

# Recurrency

arXiv:1303.5778

**Recurrent models** compress the entire history into a fixed-length vector, allowing long-range correlations to be understood.

- Read input sequence $X = (\mathbf{x}_1, \ldots, \mathbf{x}_T)$
- Accumulate information in the hidden state $h = (\mathbf{h}_1, \ldots, \mathbf{h}_T)$ through repeated matrix operations/nonlinearities

The **hidden state** $h_n$ encodes knowledge about all particles encountered up to step $n$.

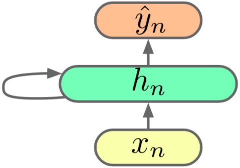


Figure 4: Network state factorizes into repeated application of hidden function $\mathcal{H}$.

# Recurrency

The last hidden state $h_T$ is a learnable encoding of the entire event.

- Input sequence: $X = (\mathbf{x}_1, \dots, \mathbf{x}_T)$
- Compute hidden vector sequence $h = (\mathbf{h}_1, \dots, \mathbf{h}_T)$

$$\begin{aligned} h_n &= \mathcal{H}\left(V\left[x_n \oplus h_{n-1}\right] + b_h\right) \\ y_n &= W h_n + b_n, \quad |y_n| = \#\text{ classes} \\ p(c|X) &= \text{softmax}(y_T), \quad \text{softmax}(v)_i = \frac{\exp v_i}{\sum_j \exp v_j} \end{aligned}$$

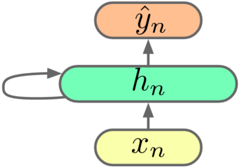
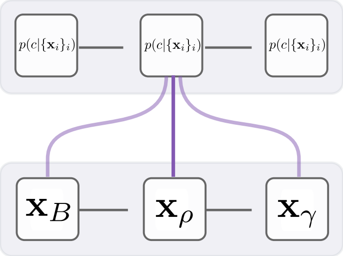


Figure 5: Network state factorizes into repeated application of hidden function $\mathcal{H}$.

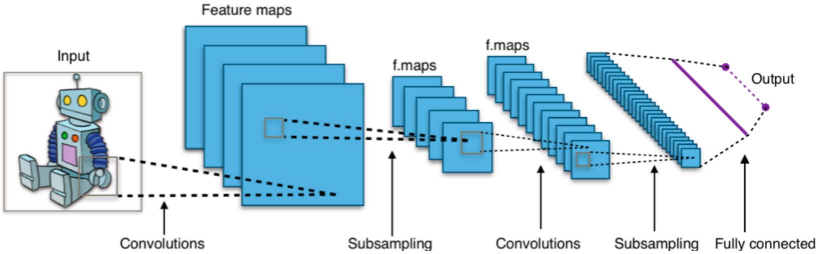
# In practice: Recurrent networks

arXiv:1409.0473

- Depth: Multiple layers increases memory and representational capacity with linear computational increase
- Bidirectionality: Observe 'future' and 'past' context at each stage
- Attention: Impractical to encode all information about the sequence in a fixed size vector. Focus on subsets of information (different particles / features in the input collision) during prediction.
- But: Sequential operations cannot exploit parallelization ...



# Convolutional Networks



| | |
|---|---|
| Convolution: | Capture local correlations between features in small regions of the input. |
| Subsampling: | Coarse-graining: Extract important features from localalized input regions. |

Stacking convolutional layers: Build high-level features from first order local features → hierarchical feature development. Useful where local correlations in the input are crucial to prediction of global properties (e.g. computer vision, speech generation).

# Convolutions

arXiv:1404.2188

Image: [height, width, colors]
Collision: [1, # particles, features]

- Define filters which project raw features ('colors') into an embedding space to capture local correlations.
- Each filter runs over *n* adjacent particles simultaneously, projecting features from different particles into a common embedding space.
- Convolve filters across the input width, operating over each 'particle *n*-gram' (groups of *n* adjacent particles) in the sequence.
- Each filter is only aware of a local region of the input width, stack convolutional + subsampling layers to derive higher-order correlations/features

# Convolutions

Input: Sequence $X = (\mathbf{x}_1, \dots \mathbf{x}_T) \in \mathbb{R}^{1 \times T \times n_{\text{features}}}$

- Slide over particle $n$-grams with kernel $\mathbf{k}^{(n)} \in \mathbb{R}^{1 \times n \times K^{(n)}}$, with $K^{(n)}$ the embedding dimension, where $n = \{2 \dots 6\}$:

$$\mathbf{c}^{(n)} = (\mathbf{k}^{(n)} \star X) \in \mathbb{R}^{1 \times (T-n) \times K^{(n)}}$$

- Subsample (max/avg pool) over 2nd dimension to extract important features:

$$\mathbf{p}^{(n)} \in \mathbb{R}^{1 \times 1 \times K^{(n)}}$$

- Concatenate along first dimension: $\mathbf{f} = \texttt{concat}(\{\mathbf{p}^{(n)}\}_n\texttt{, axis=1)}$
- $\mathbf{f} \in \mathbb{R}^{1 \times j \times K}, \leftarrow$ stack of extracted feature maps, $j = |\text{filters}|$
- Subject $\mathbf{f}$ to further $[3, 1]$ convolutions to understand correlations between different feature maps, flatten + dense layer for final classification

# Experiments

Run over simulated $e^+e^-$ collisions at Belle II, with $\sqrt{s} = 10.58$ GeV.

Signal: Radiative penguin $b \to s\gamma$ ($B \to X_s\gamma$)

Background: $e^+e^- \to q\bar{q}$ and $e^+e^- \to B\bar{B}$, where both $B$ mesons undergo non-penguin decay.

- Train: $\approx 23 \times 10^6$, test fraction 0.1
- Validation: $\approx 2 \times 10^6$

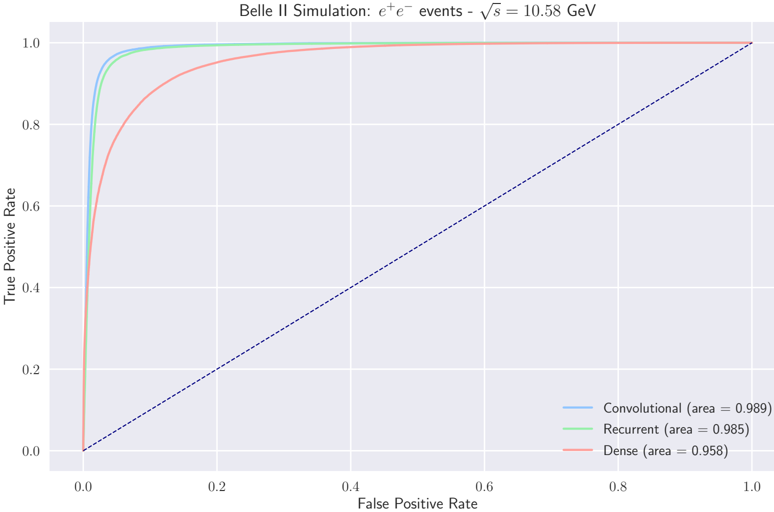
Represent the same events in two ways:

Fixed feature vector: Input to dense network

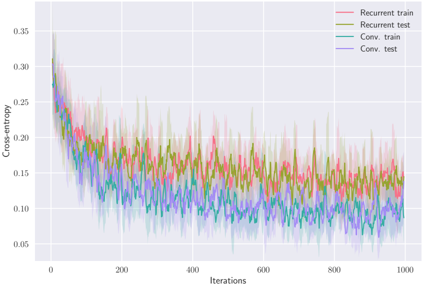
Variable-length sequence of vectors: Input to convolutional / recurrent nets

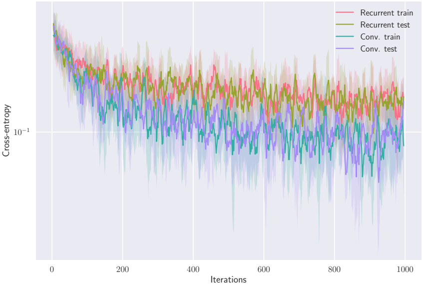
Recurrent architectures tend to overfit, but convolutional networks exhibit good generalization even with no explicit regularization.

# Results


Belle II Simulation: $e^+e^-$ events - $\sqrt{s} = 10.58$ GeV
True Positive Rate
False Positive Rate
0.0
0.2
0.4
0.6
0.8
1.0
0.0
0.2
0.4
0.6
0.8
1.0
Convolutional (area = 0.989)
Recurrent (area = 0.985)
Dense (area = 0.958)

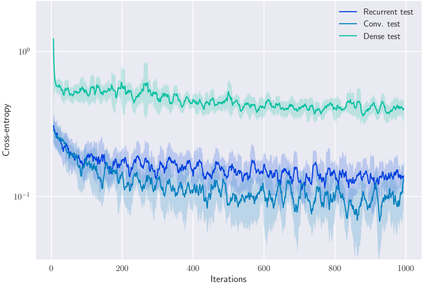
# Convergence





Kernel weight sharing in convolutional networks have a strong regularizing effect.

# Convergence



# Performance

## Learnable parameters

Kernel weight sharing in CNNs + parameter-less pooling layers → reduced learnable parameters relative to recurrent/dense networks.

## Computation Time

Recurrent architectures perform sequential computation → unable to exploit the parallelization capabilities of modern GPUs.

TensorFlow 1.7 | CUDA 9.0 | 2 Tesla P100s

| Architecture | AUC† | $\frac{\text{Training time}}{\text{Conv. training time}}$ | Learnable parameters |
|---|---|---|---|
| Convolutional | $0.988 \pm 0.03$ | 1 | $\approx 4.5 \times 10^5$ |
| Recurrent | $0.985 \pm 0.04$ | 3.9 | $\approx 1.2 \times 10^6$ |
| Dense* | $0.956 \pm 0.04$ | 0.6 | $\approx 2.3 \times 10^6$ |

*Same events, but cast in sequential representation for conv./recurrent models - on average lower # features/event used for dense network.

†Training rerun 5 times with different random seeds

# Outlook

- Aim to serve as a modular part of analysis.
  - Integration into the software framework @ Belle II
- Significant mass/energy sculpting
  - Interface with adversarial training

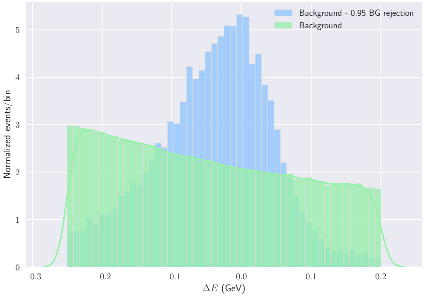


Figure 6: Standard neural network

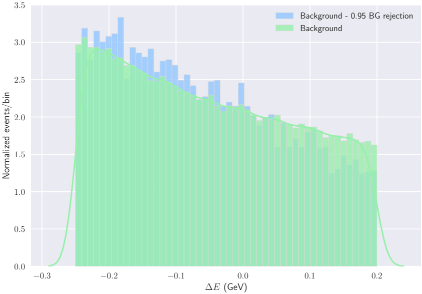


Figure 7: Adv. trained neural network

# Summary

- Draw parallels between event structure / natural language
- Represent a collision event as an ordered set of feature vectors, one for each reconstructed particle candidate
  - Capture more complete picture of event than classical approaches
- Convolutional architectures permit sequential event representation
  - Capture local interactions between particle candidates through convolution + subsampling
  - Long-range / global relations can be understood by stacking convolutional layers → increase in receptive field
- Why convolutions?
  - Fast! Exploits parallelization, unlike recurrent approaches
  - Outperforms recurrent/dense approaches

Improved background rejection → better sensitivity to new physics.

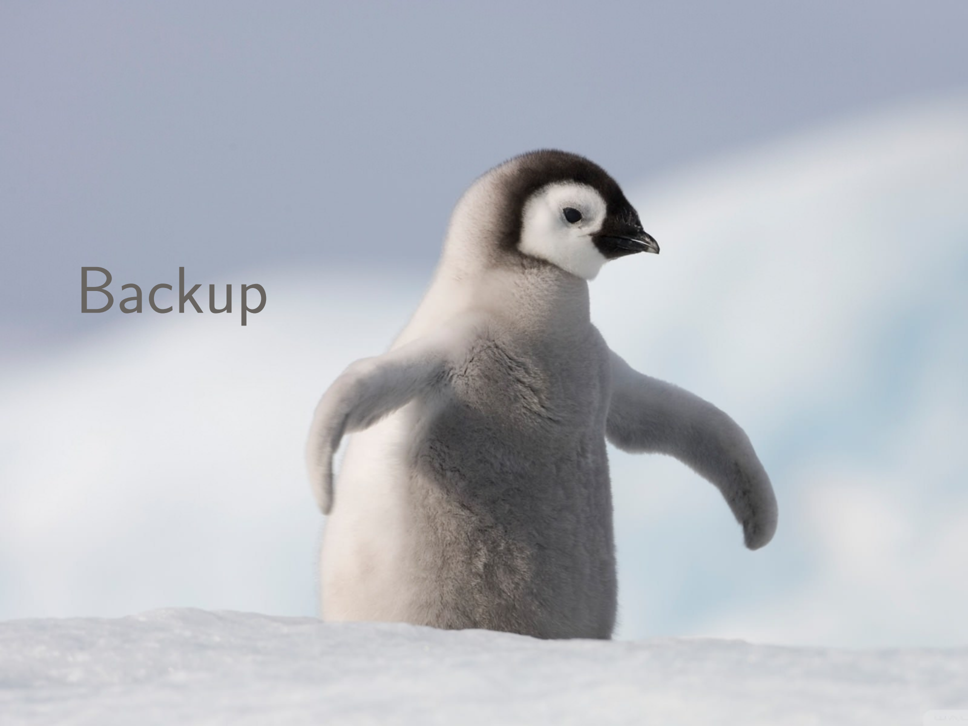
# Thanks for listening

Code + Docs

`github.com/Justin-Tan/particle2seq`

`justin.tan@coepp.org.au`

# Backup



# Implementation

  - Data collection: `ROOT`
  - To Python: `uproot`
  - Preprocessing: Spark/Pandas

- Workflow scalable to $\mathcal{O}(100)$ GB worth of training data.
- TensorFlow:
  - Open-source: No black boxes. ✔
  - Fine-grained control over entire architecture. ✔
- Train:
  - 64 epochs, scheduled annealing
  - SGD + Nesterov momentum

# Motivation

- Non-SM contributions enter through hypothetical new TeV-scale particles running within the loop → interference with known amplitudes.
- Strong constraints on NP by measurement of inclusive/exclusive BR, CP asymmetries

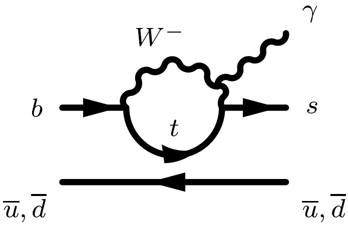


Figure 8: Example of SM radiative penguin decay for $b \to s\gamma$ [2]

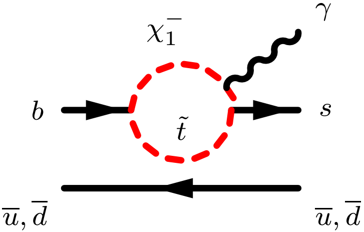


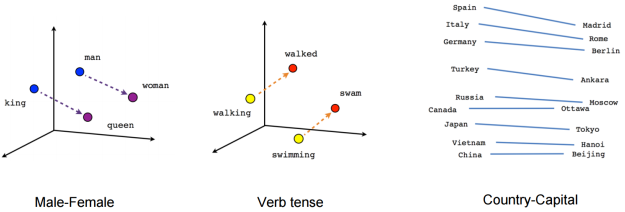
Figure 9: Example of hypothetical SUSY contribution to radiative decay [2]

# Words as Vectors

**Distributional Hypothesis:** Words that occur in the same context share semantic meaning.

- Represent words in a continuous vector space to group semantically similar words.
  - Learned vectors explicitly encode linguistic regularities and patterns: $\vec{v}(Madrid) - \vec{v}(Spain) + \vec{v}(France) \approx \vec{v}(Paris)$
  - Inability to represent idiomatic phrases $\vec{v}(California) \neq \vec{v}(Golden) + \vec{v}(State)$ - overcome with phrase based models.

**Takeaway:** Encode semantic relationships in directions in induced vector space.



Male-Female Verb tense Country-Capital

Figure 10: Semantic relationships as approximate linear relations (projected into 3D)

# Stacking Recurrent Layers

A Deep RNN increases memory and representational capacity with linear scaling.

- The output sequence of one layer forms the input sequence for the next

$$h_t^{(n)} = \mathcal{H}\left(V^{(n)}\left[h_t^{(n-1)} \oplus h_{t-1}^{(n)}\right] + b_h^{(n)}\right)$$

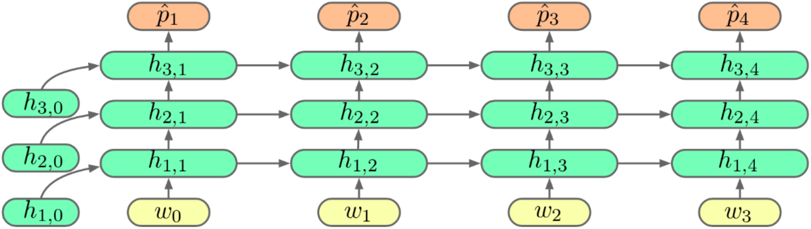
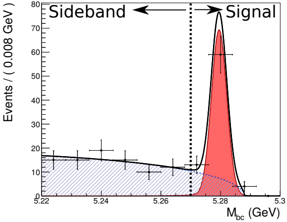


Figure 11: Hidden state of layer $n$ accepts hidden state of layer $n-1$ as input [5]

# Signal Identification

- Identify signal peak in:
    - $\Delta E = E_{beam} - E_B$
    - $M_{bc} = \sqrt{E_{beam}^2 - |\vec{p}_B|^2}$
- Background processes not fully captured by simulation
- Rely on interpolation of smooth background spectrum from sidebands beneath signal peak



Learning algorithms preferentially select signal-like events → background spectrum distortion → uncontrollable systematic uncertainties

# Background Sculpting

Classifier output $f(X;\theta_f) \sim \text{p(signal}|\text{data)}$. Only accept events above a given posterior probability.

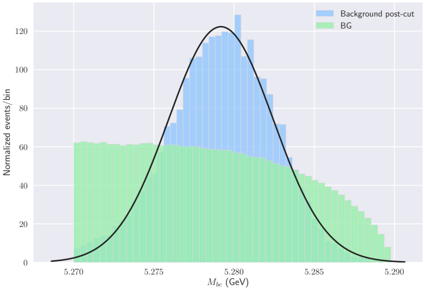


Figure 12: Continuum $M_{bc}$ before (green) and after (blue) suppression

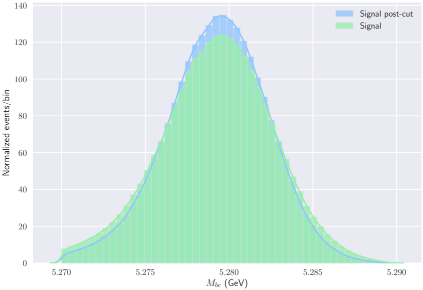


Figure 13: Signal $M_{bc}$ before (green) and after (blue) suppression

Background looks like signal post-selection.

**Tension between optimal discrimination and reduced systematics!**

# Controlling Systematics

- Physics variables of interest: $z \in \mathcal{Z}$ (e.g. $\Delta E, M_{inv}$)
- Classification function: $f(X; \theta_f)$ gives probabilities of data $X$ being signal events.
- $f(X; \theta_f)$ and $z$ should be independent random variables

$$p(f(X; \theta_f) = s | z) = p(f(X; \theta_f) = s | z')$$

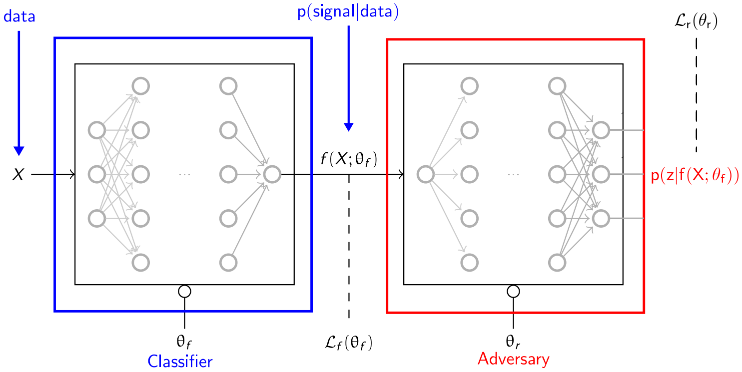
Q: How can we enforce independence of $f(X; \theta_f)$ and $Z$?

A: Set up a game between two competing players, $f$ and $r$. Independence arises at the Nash equilibrium.

Train $f$ and $r$ simultaneously by minimax optimization of

$$\hat{\theta}_f, \hat{\theta}_r = \arg \min_{\theta_f} \left( \max_{\theta_r} \left( \mathcal{L}_f(\theta_f) - \mathcal{L}_r(\theta_r) \right) \right)$$

# Adversarial Neural Networks



Adversary $r$ attempts to infer $z$ from p(signal|data) emitted by the classifer $f$, increasing the loss function $E = \mathcal{L}_f(\theta_f) - \mathcal{L}_r(\theta_r)$.

$f$ circumvents penalization by decorrelating p(signal|data) with $z$.

# Adversarial Neural Networks

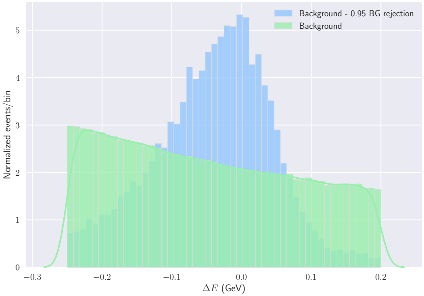


Figure 14: Standard neural network

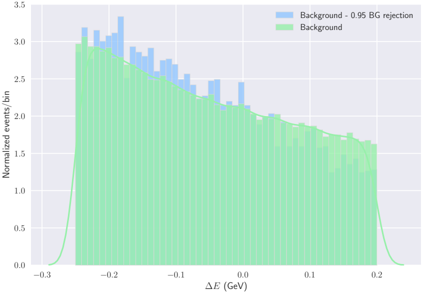


Figure 15: Adv. trained neural network

- Enforce 95% BG rejection
- Signal: $b \to s\gamma$
- Background: $e^+e^- \to q\bar{q}$

Smooth interpolation from sideband ✔

# Adversarial Neural Networks

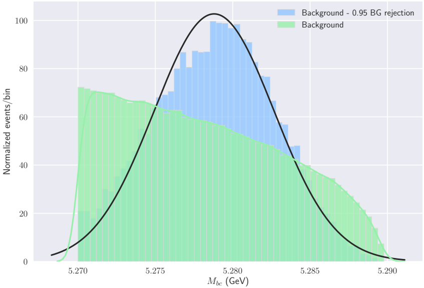


Figure 16: Standard neural network

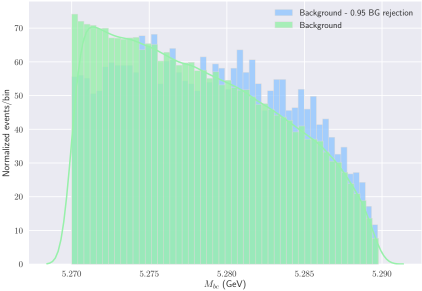


Figure 17: Adv. trained neural network

- Enforce 95% BG rejection on 1 $ab^{-1}$ of simulated $e^+e^-$ collisions at Belle II
- Signal: $b \to s\gamma$
- Background: $e^+e^- \to q\bar{q}$

Smooth interpolation from sideband ✔

# No Free Lunch

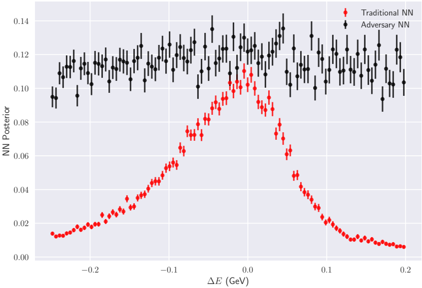


Figure 18: Posterior p(signal|data) versus $\Delta E$

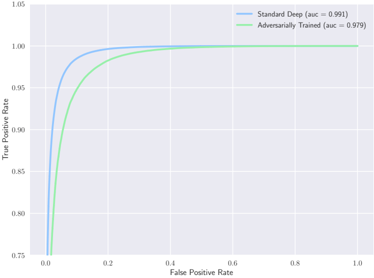


Figure 19: Competition reduces separation power

- Posterior probabilities relatively uniform ✔
- Tradeoff between optimal discrimination and reduced systematic error. ✗