

# In-process Diagnostic methods for Entity Representation Learning on Sequential Data at Scale

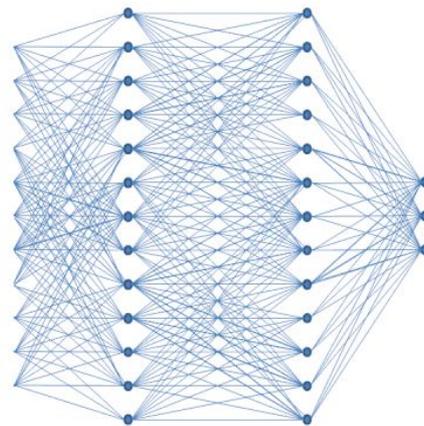
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PhD Proposal Presentation: **Diego Garcia-Olano**  
Advisor: **Dr. Joydeep Ghosh**

**June 15, 2020**

# Explainable AI for Sequential Data

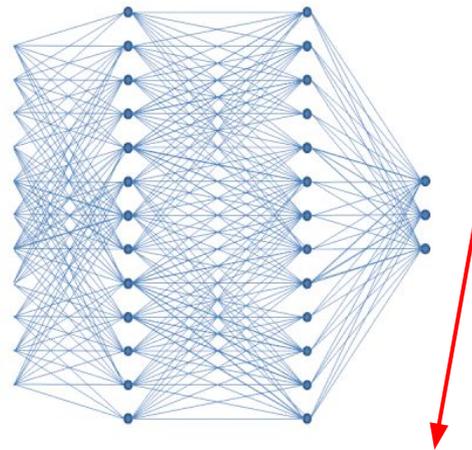
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# Explainable AI for Sequential Data

For image, text and time series data tasks, deep learning neural nets have become the default modeling choice.

Their ubiquity necessitates **transparency** into how such models arrive at the predictions they make in order that they be deemed **trustworthy** for use in critical domains.



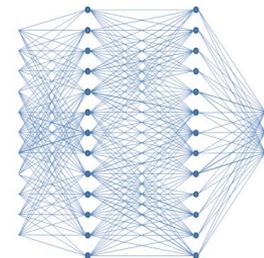
**The human torch  
was denied a  
bank loan.**

In Anchorman: The Legend of Ron Burgundy

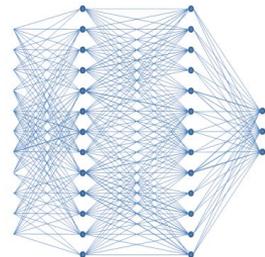
By Ron Burgundy

GIFQUOTES.COM

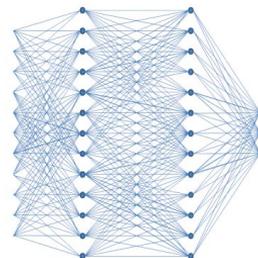
- **Who** are we explaining to:  
End user? Expert/Researcher?  
Model developers? Other Models?



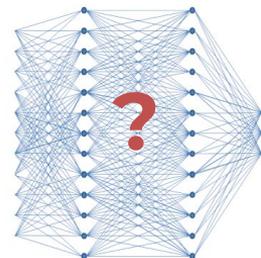
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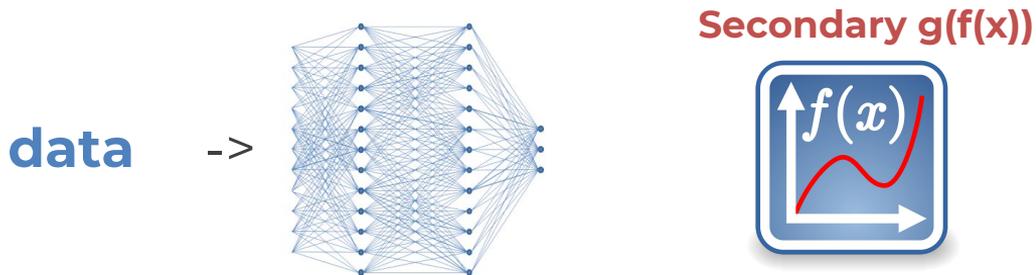
- **White Box vs Black Box:**  
 Do we have access to the model internals?  
 The data it was trained on?



**VS**

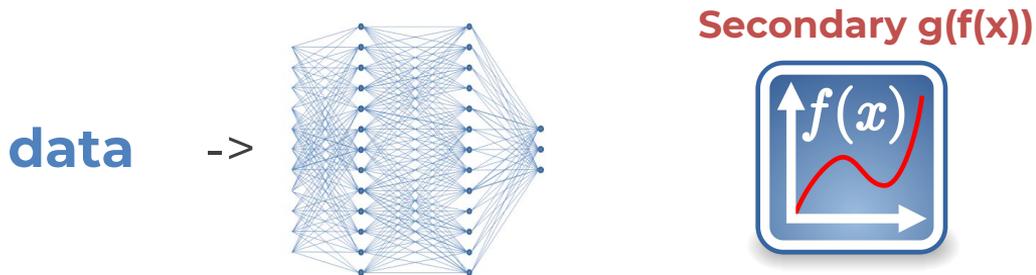


- Explaining from what point in model process:**  
 Pre-model, In-Process or Post Hoc



Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead ( Rudin, et al, 2019 Nature )

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Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead ( Rudin, et al, 2019 Nature )

- **Global** model vs **Individual** instance based explanations

## Post Hoc

**Feature Attribution:** which features contributed most to a model's output

- Path Integrated Gradients ( IG )
- Shapley Additive Explanations ( SHAP )
- Interpretability with Differential Masking

**Influential examples:** which training data most influenced a model's output

- Influence Functions
- Representer Point Selection for Explaining Deep Neural Networks

**Counterfactuals:** minimal change that would have led to a different output

**BERT probing:** assess how well a LM encodes semantic/syntactic properties of language by evaluating ("probing") on downstream tasks

## Issues with Post Hoc secondary model explainers

### **Feature importance**/saliency methods

- Need Baselines ( Shap / IG )
- Are local/linear approximations of the actual model faithful explanations?
- Can we interpret Attention weights as explanations?

### **Influence functions:**

- Expensive to compute
- Correlation to true influence for deep architectures

### **Counterfactuals:**

- Semantic distance and meaning with text?

### **BERT probing:**

- Don't generalize past probing tasks and don't "explain" model decisions

## In-Process

**Prototypes:** learn “prototypical” representations

- Deep Learning for Case-Based Reasoning through Prototypes

**Deep k-NN models:** utilize layer representations as additional “clustering” features

- Deep k-Nearest Neighbors: Towards Confident, Interpretable and Robust DL

**Concept Bottlenecks:** layer specific additional task loss

- Concept bottleneck models
- On completeness-aware concept-based explanations in deep neural networks

**Retrieval as Explanation:** for tasks involving entity retrieval as an intermediate step

- REALM: retrieval-augmented language model pre-training
- Entities as experts: Sparse memory access with entity supervision

**Feature Importance as an auxiliary loss during training:**

- Incorporating Priors with Feature Attribution on Text Classification

Require access and modifications to the underlying model ...

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Require access and modifications to the underlying model ...  
**which is fine for critical applications!**

## **In-process explainable models for Sequential Data**

- **are an Useful & Under-explored area for sequential data modeling**
- **provide Interpretable and Faithful explanations of model decisions**
- **allow for model “diagnosis” and intervention at inference time.**

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**Entity Representation learning** allows for an additional interesting and underexplored explainability aspect that grounds models.

**Scalability** is vital to the adoption of models in practice  
Both play a central role in this work.

# Completed Work

- Learning Dense Representations for Entity Retrieval. (CoNLL 2019)
- Deep Classification of Time-Series Data with Learned Prototype Explanations. (ICML time series workshop 2019 *joint work with Alan Gee*)
- Biomedical Interpretable Entity Representations. (ACL-IJCNLP 2021)

# Completed Work

Learning Dense Representations for Entity Retrieval. (CoNLL 2019)

Constructed a **dual mention-entity encoder** that learns dense representations for efficient neural **Entity Retrieval** with an **in-process, iterative hard negatives procedure** for **model learning and inference time inspection**.

Deep Classification of Time-Series Data with Learned Prototype Explanations. (ICML 19)

Adapted a **prototypical autoencoder** classifier to be compatible with **time series data** and allow for **tunable prototype diversity** leading to improved accuracy and **global and instance level explanations**.

Biomedical Interpretable Entity Representations. (ACL-IJCNLP 2021)

Learned a distantly supervised entity type system and data set for use in training a **Biomedical Interpretable Entity model** whose representations exist in a **semantically meaningful vector space** & whose **predictions may be interpreted and diagnosed** with an oracle method.

# Learning Dense Representations for Entity Retrieval

Gillick, D., Kulkarni, S., Lansing, L., Presta, A., Baldrige, J., Ie, Eugene., Garcia-Olano, D.  
“Learning Dense Representations for Entity Retrieval”. Proceedings of the 23rd Conference on  
Computational Natural Language Learning (CoNLL), Hong Kong, China, 2019.

## Entity Resolution:

Predict the most probable “entity”  
in a knowledge graph ( Wikipedia )  
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Predict the most probable “entity” in a knowledge graph ( Wikipedia ) that a “mention” links to given its surrounding “context.”

**Example Query:**      What is George Harrison’s favorite Nintendo game?

**Mention:** George Harrison

**Context:** What is \_\_ favorite Nintendo Game ?

**Entity:** ????

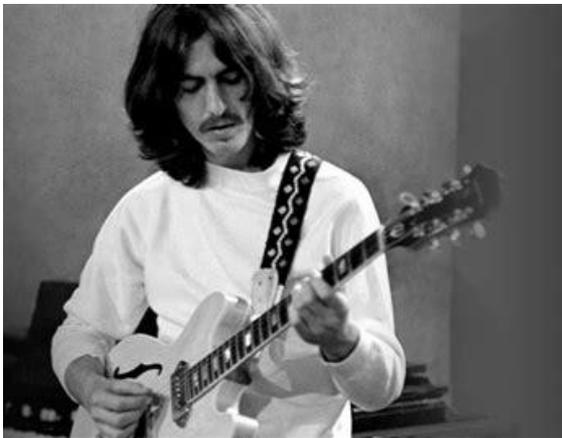
**5.7 million entities** to choose from in Wikipedia (considering only english)

Finding the **real entity** this mention resolves to allows us to **learn representations grounded in the real world.**

and to **leverage structured data** from the knowledge graph.

**Example Query:**      What is George Harrison's favorite Nintendo game?

George Harrison



Q2643

George Harrison

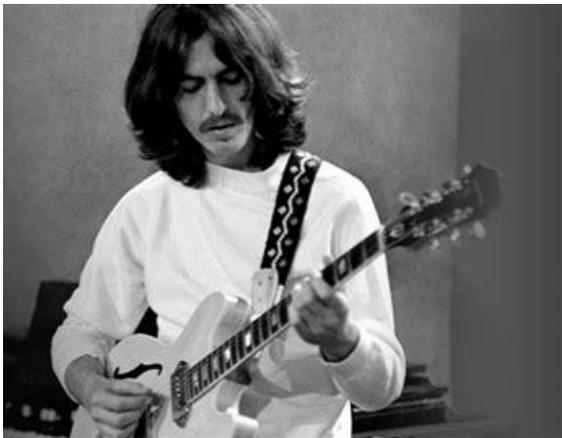


Q5540278

**Example Query:**      What is George Harrison's favorite Nintendo game?

Beatles Guitarist

Highest Popular Prior



Q2643

Former Senior VP of Marketing  
at Nintendo of America.



Q5540278

Prior State of the Art for Entity Resolution:

- Train on ( **Mention**, **Context**, **Entity** ) Triples.

## 2 Stages

### (1) Retrieve Candidates

- Construct a **Mention** to **Entities** Lookup **“Alias” Table**.  
 9.8 Million unique mention strings  
 5.7 Million unique entities

### (2) Re-Rank them

- **Limitations**

- 1) Low Recall
- 2) Context not considered. Can't predict unseen entities



Define a **novel dual encoder architecture** for learning **entity** and **mention encodings** suitable **for retrieval**

Describe a fully **unsupervised, iterative hard-negative mining** algorithm that greatly improves retrieval performance and can be used to track and **explain model learning**.

**Approximate nearest neighbor** search yields quality candidate entities efficiently.

**Outperform discrete retrieval baselines** ( alias table, BM25 ) and gives results competitive with the best reported accuracy on TACKBP-2010.

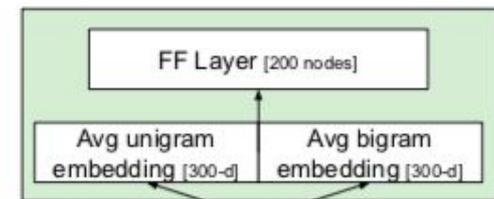
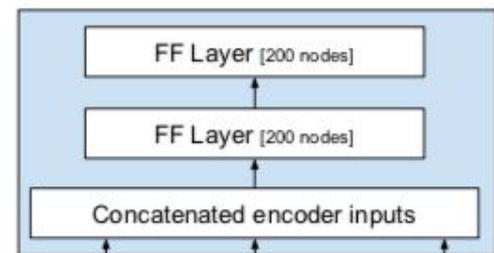
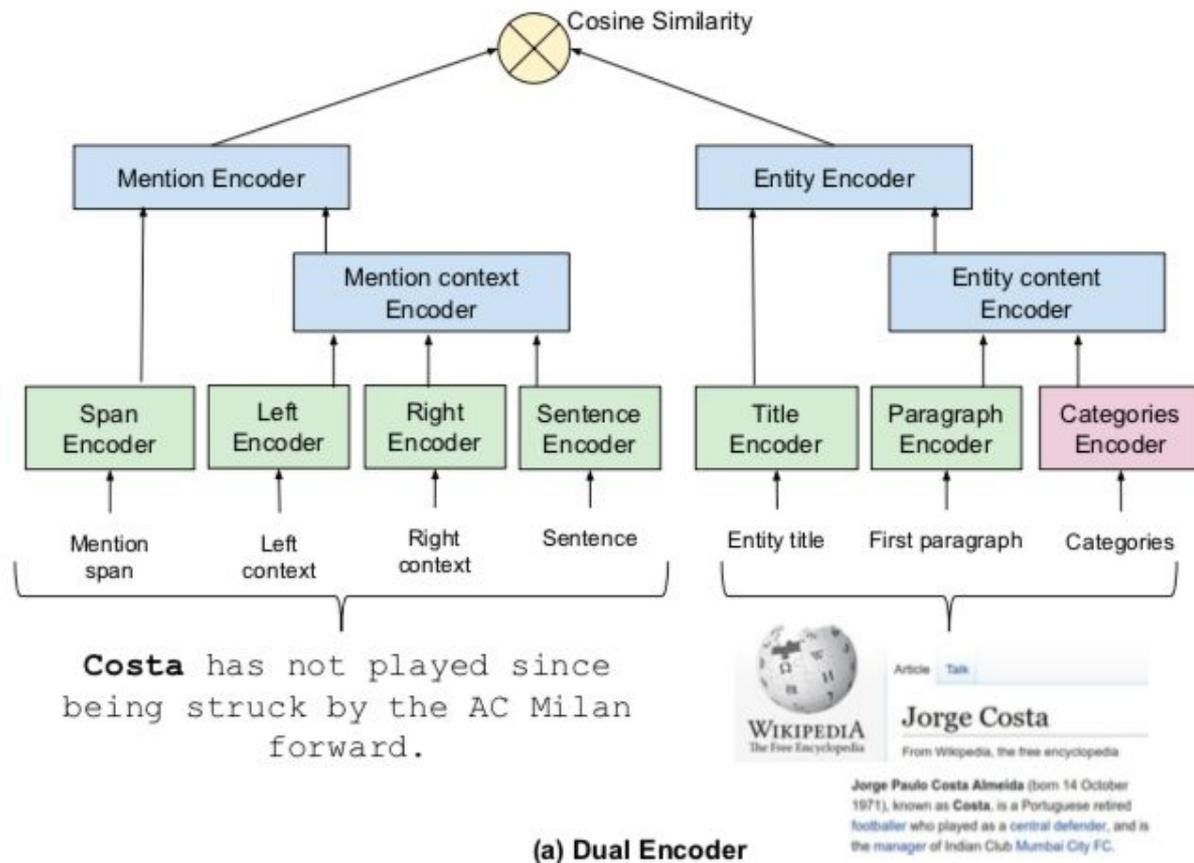


Figure 1: Architecture of the dual encoder model for retrieval (a). Common component architectures are shown for (b) text input, (c) sparse ID input, and (d) compound input joining multiple encoder outputs. Note that all text encoders share a common set of embeddings.

The dual encoder learns a **mention encoder**  $\varphi$  and **an entity encoder**  $\psi$ , where the **score** of a mention-entity pair  $(m, e)$  is:

$$\mathbf{s}(m, e) = \cos( \varphi(m), \psi(e) )$$

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	e1	e2	e3	e4	e5
m1					
m2					
m3					
m4					
m5					

These pairs constitute only positive examples, so we use **in-batch random negatives** (Henderson et al., 2017;):

We build the **all-pairs similarity matrix** for all mentions & entities **in a batch**. & **optimize a softmax loss** on each row of the matrix.

We do this **sampled softmax** (Jozefowicz et al, 2016) in place of a full softmax because the normalization term is **intractable** to compute over all 5.7M entities.

$$\sigma(\vec{z})_i = \frac{e^{z_i}}{\sum_{j=1}^K e^{z_j}}$$

For each training pair  $(m_i, e_i)$  in a batch of  $B$  pairs, the loss is computed as:

$$L(m_i, e_i) = -f(m_i, e_i) + \log \sum_{j=1}^B \exp(f(m_i, e_j))$$

where  $f(m_i, e_j) = a \cdot s(m_i, e_j)$

We track **in-batch recall@1** accuracy on val set and stop training after the metric flattens out (about 40M steps).

Recall@1 means for each instance, the model gets a score of 1 if the correct entity is ranked above all in-batch random negatives, 0 otherwise.

Hyperparams: **batch size of 100**, fixed learning rate 0.01  
SGD with Momentum of 0.9,

**Random negatives are not enough** to train an accurate entity resolution model

So after learning an initial model using random negatives,  
we identify more challenging **“hard negatives”** via the following:

1. Encode all mentions and entities found in training pairs using current model.
2. For each mention, retrieve the most similar 10 entities (i.e., its nearest neighbors).
3. Select all entities ranked above the correct one as negative examples.

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We merge these new hard negative mention/entity pairs  
with the original positive pairs to construct an additional task  
& resume training the dual encoder using logistic loss on them.

For a pair  $(m, e)$  with label  $y \in \{0, 1\}$ , the **hard negative loss** is defined as:

$$L_h(m, e; y) = -y \cdot \log f(m, e) - (1 - y) \cdot \log(1 - f(m, e))$$

$$\text{where } f(m, e) = g(a_h \cdot s(m, e) + b_h)$$

The hard negative task is mixed with the original random negatives task

$$L_{multi} = L_{orig} + L_{hard}$$

<b>System</b>	<b>R@1</b>	<b>Entities</b>
AT-Prior	71.9	5.7M
AT-Ext	73.3	5.7M
Chisholm and Hachey (2015)	80.7	800K
He et al. (2013)	81.0	1.5M
Sun et al. (2015)	83.9	818K
Yamada et al. (2016)	85.2	5.0M
Nie et al. (2018)	86.4	5.0M
Barrena et al. (2018)	87.3	523K
<b>DEER (this work)</b>	87.0	5.7M

Table 1: Comparison of relevant TACKBP-2010 results using Recall@1 (accuracy). While we cannot control the candidate entity set sizes, we attempt to approximate them here.

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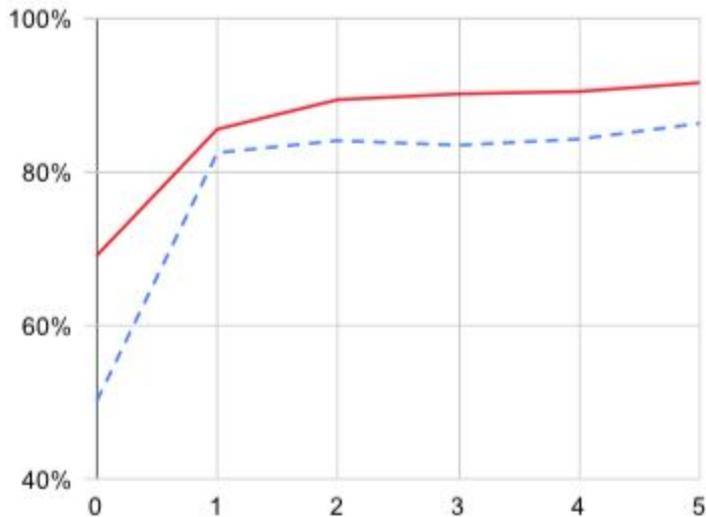


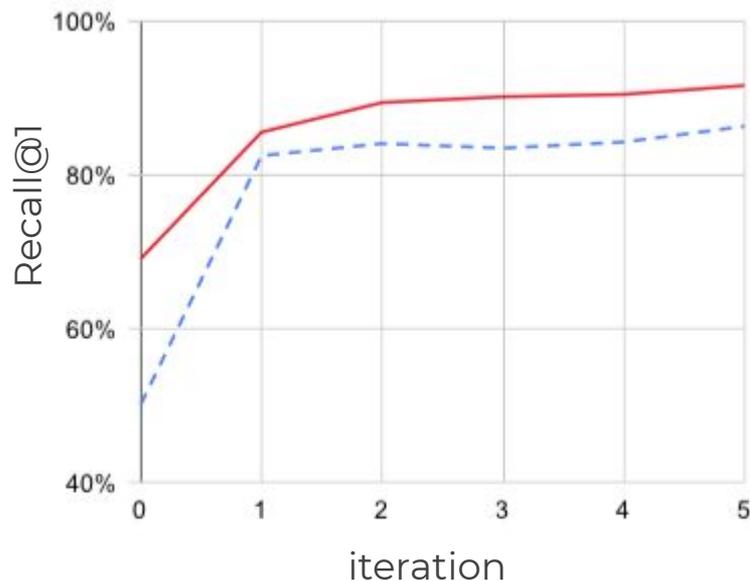
Figure 2: Recall@1 improvement for successive iterations of hard negative mining for Wikinews (solid) and TACKBP-2010 (dashed).

During each iteration of learning, we identify entities which our model assigns a higher ranking than the true entity associated with a given mention and context.

These **hard negative triples** (  $m, e', 0$  ) **can be inspected over time** during training or inference to assess the mention/contexts and entities that are added which are difficult for the model to learn ( esp. later iterations )

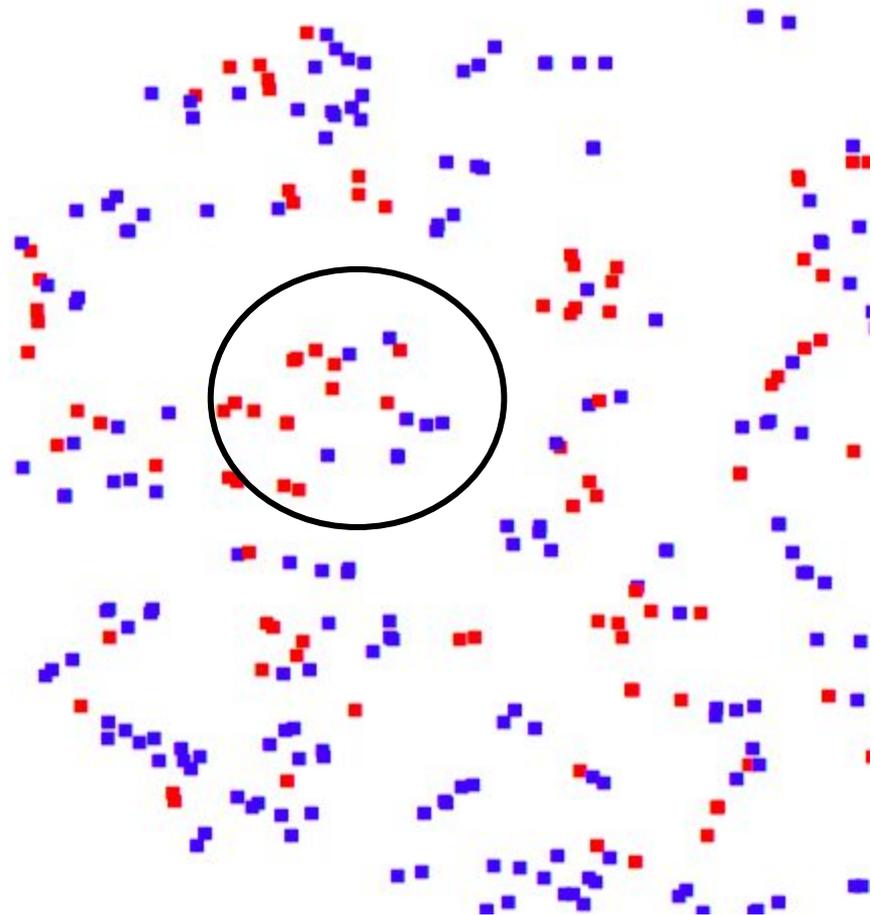
This **interpretable in-process information about the learning process** could be used to:

- improve **error analysis**,
- identify cases where **additional supervision** could be useful
- gauge **confidence** in inference time predictions



At inference time,  
given a test mention/context,

- 1) Get K nearest mention/contexts from training set
- 2) Collectively assess how each of them performed over iterations (gather the hard negatives along with the true entities)
- 3) Get top entity prediction(s) for the test mention/context via cosine similarity
- 4) Utilize 2 and 3 results to calculate confidence measures for the final entity prediction



## Inspecting Entity Encodings for Semantic Meaning



Figure 3.5: t-SNE visualization of our learned embeddings for select country Wikipedia page entities. More at [diegoolano.com/deer/](http://diegoolano.com/deer/)

Inference is done by computing cosine similarity between the test mention/context encoding and each of the cached entity encodings.

**Approximate Search** using quantization-based approaches (Guo et al. (2016) ) can be used to speed up retrieval greatly!

<b>Method</b>	<b>Mean search time (ms)</b>	<b>Wikinews R@100</b>
Brute force	291.9	97.88
AH	22.6	97.22
AH+Tree	3.3	94.73

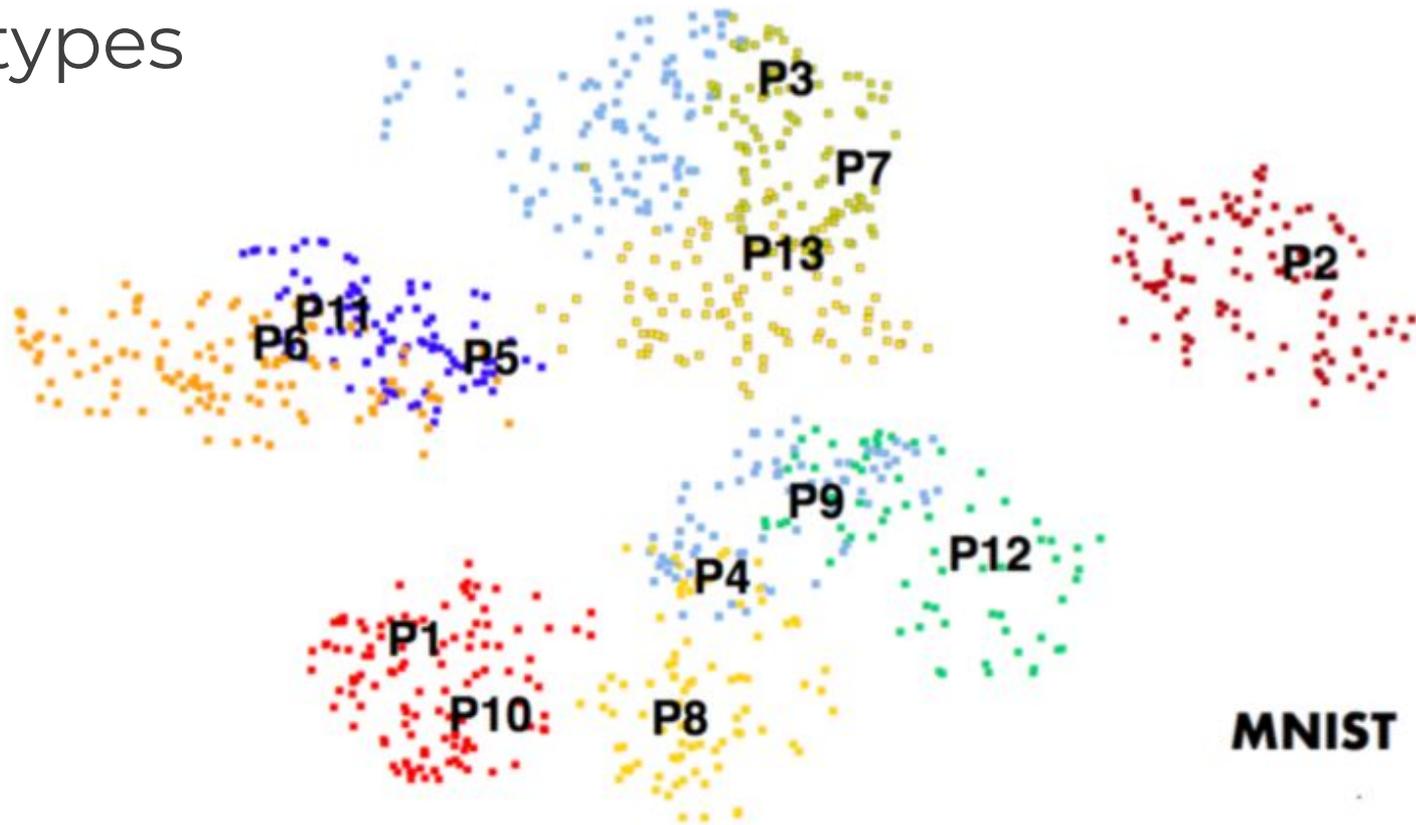
Table 3: Comparison of nearest-neighbor search methods using the DEER model. The benchmark was conducted on a single machine. AH indicates quantization-based asymmetric hashing; AH+Tree adds an initial tree search to further reduce the search space.

# Explaining Deep Classification of Time-Series Data with Learned Prototypes

Garcia-Olano, D.\*, Gee, A.\*, Ghosh, J., Paydarfar, D. “Deep Classification of Time-Series Data with Learned Prototype Explanations”. International Conference on Machine Learning (ICML 2019 time series workshop)

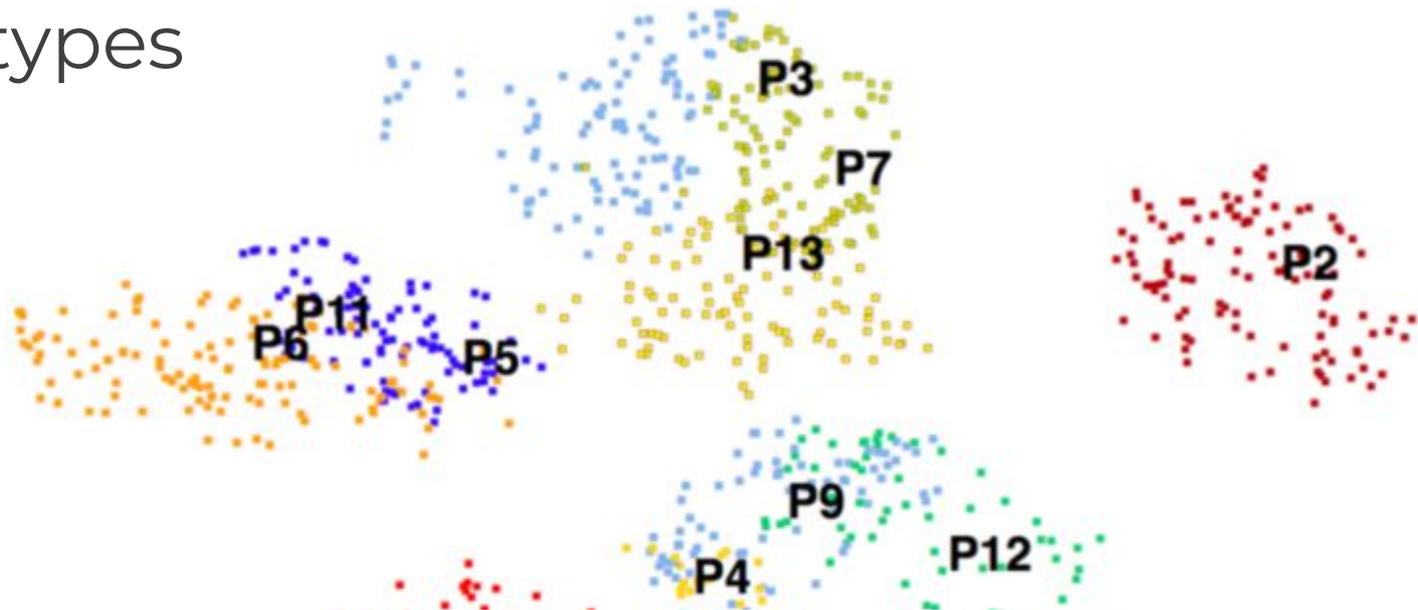
\* *equal contribution*

## Prototypes



\*Li et al. Deep learning for case-based reasoning through prototypes. (2017)

## Prototypes

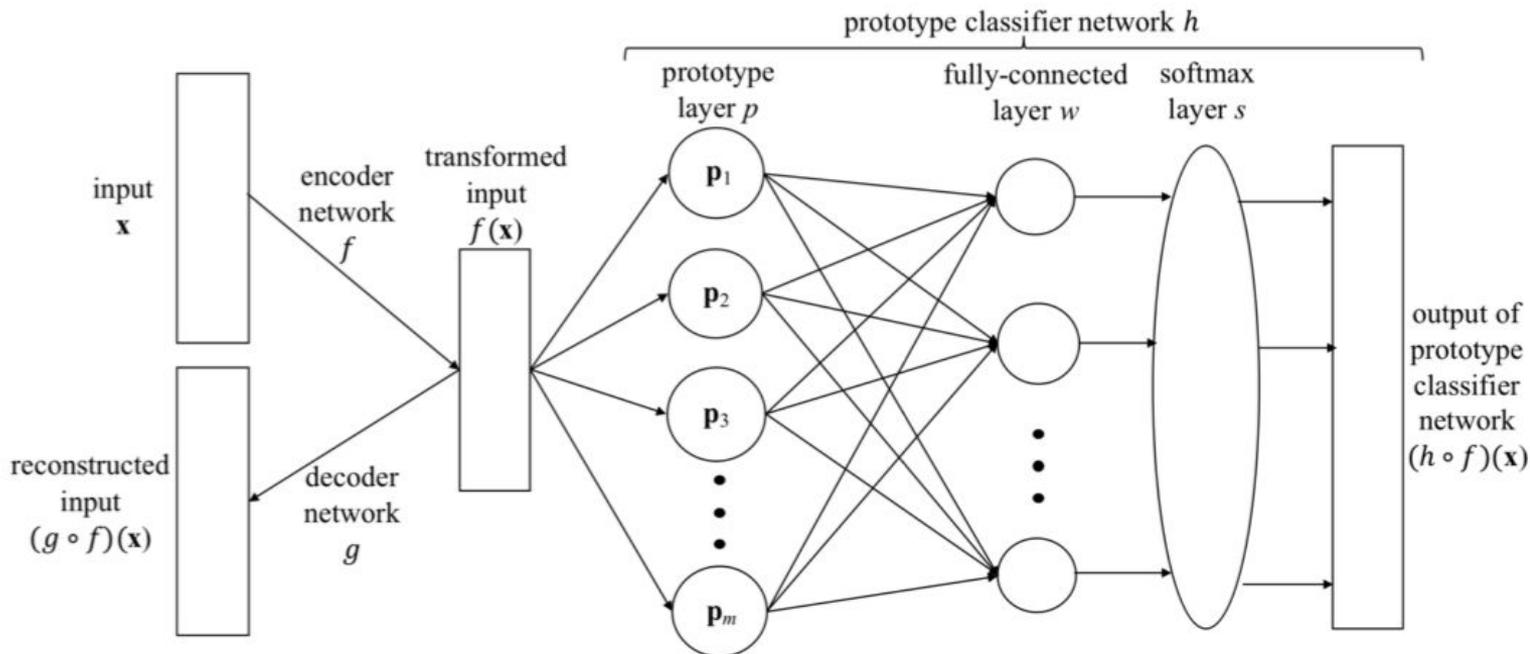


**MNIST**

totypes. (2017)

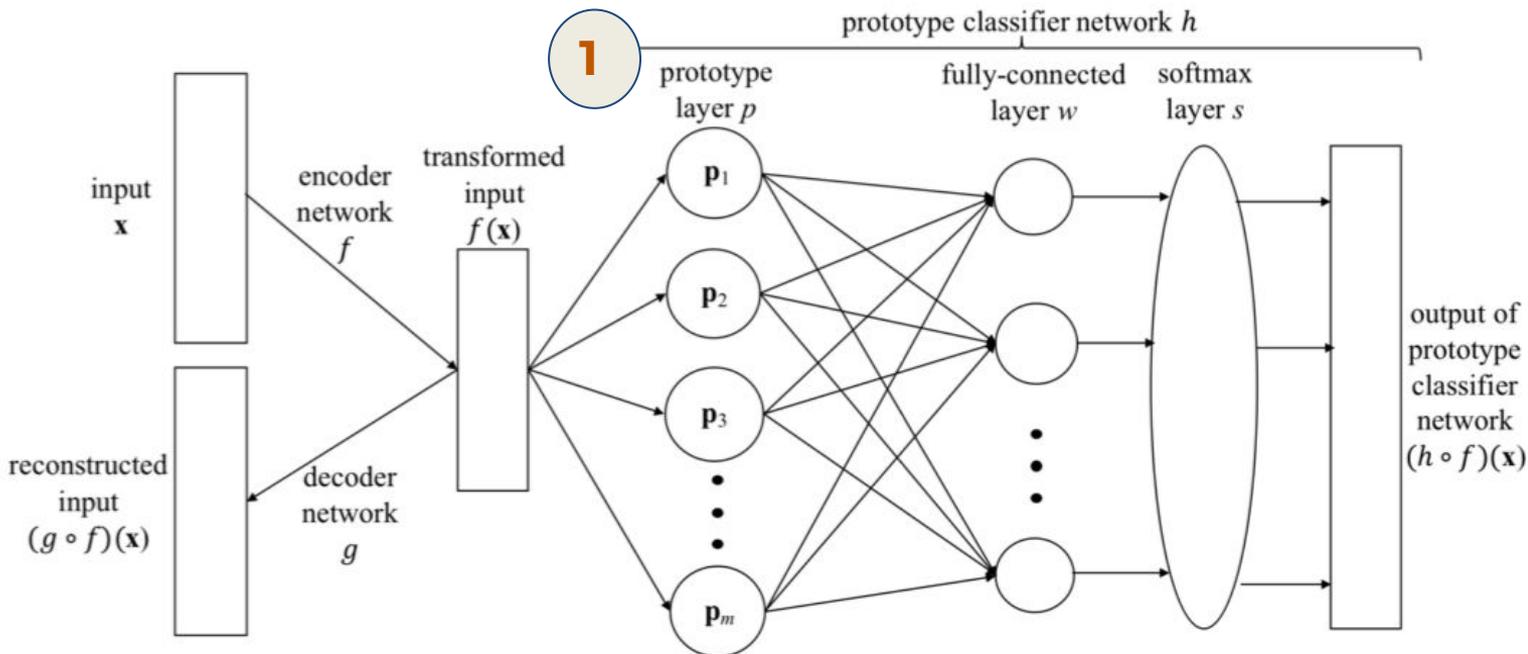
## Prototype Classifier Network

$n$  data points  
 $m$  prototypes



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$n$  data points  
 $m$  prototypes



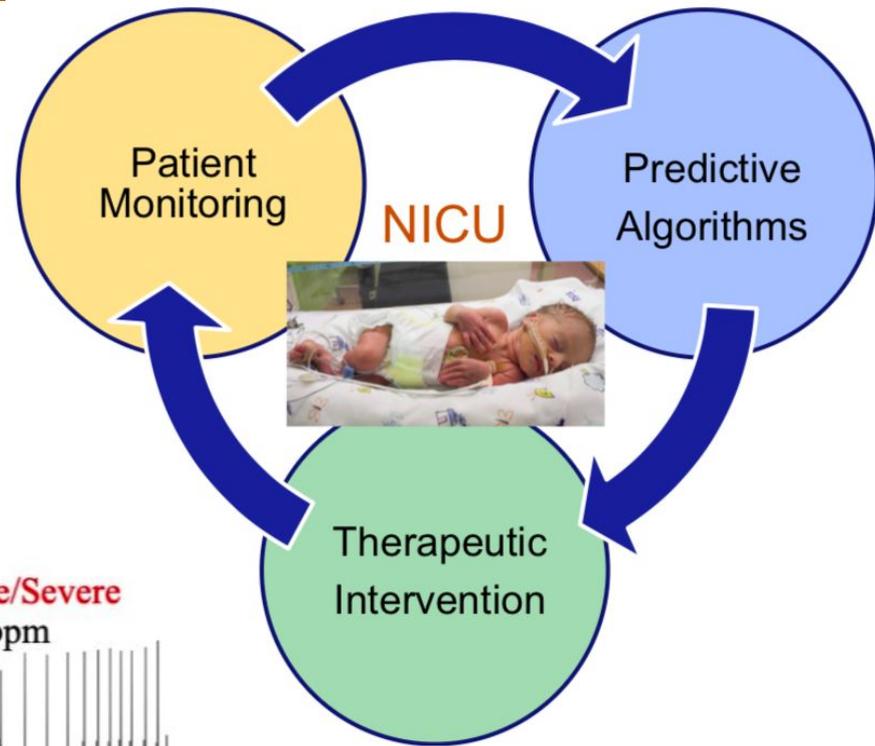
Feature Vector  
 $f(\mathbf{x}) \in \mathbb{R}^q$

Prototypes  
 $\mathbf{p}_i \in \mathbb{R}^q$

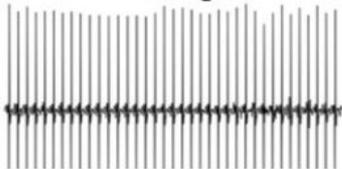
$$\|f(\mathbf{x}) - \mathbf{p}_i\|_2^2 = \rho_i$$

$$\begin{aligned} \mathcal{L}((f, g, h), X) = & E(h \circ f, X) + \lambda_R R(g \circ f, X) \\ & + \lambda_1 R_1(p_1, \dots, p_m, X) \\ & + \lambda_2 R_2(p_1, \dots, p_m, X) \end{aligned}$$

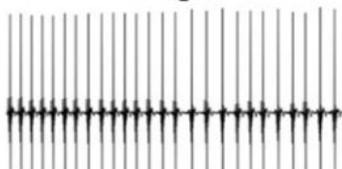
## Predicting Bradycardia from ECG signals



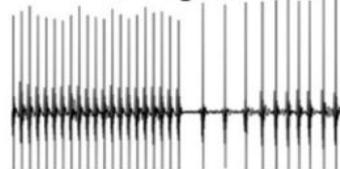
**Normal ECG**  
134 bpm



**Mild Bradycardia**  
86 bpm

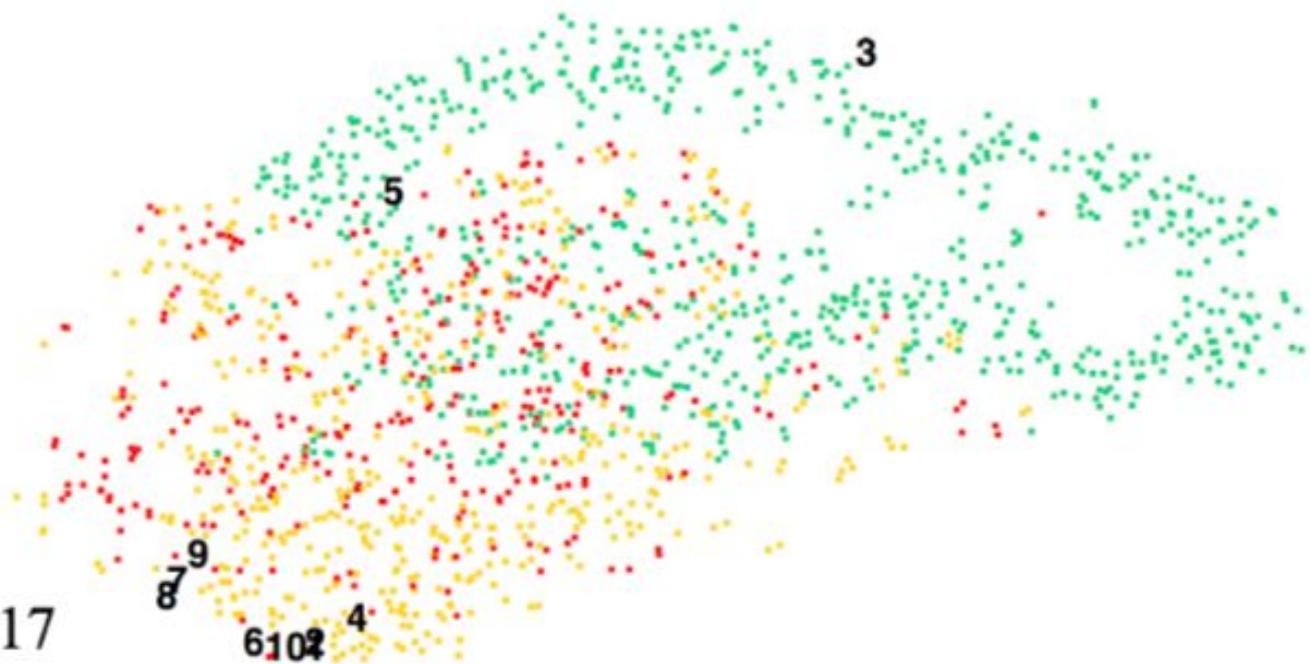


**Moderate/Severe**  
55 bpm



# Prior work

## Latent Space Representation for Bradycardia task



Loss from  
 Li *et al.* 2017

Prototype  
 Classifier  
 Network Updated

$$\begin{aligned}
 \mathcal{L}((f, g, h), X) = & E(h \circ f, X) + \lambda_R R(g \circ f, X) \\
 & + \lambda_1 R_1(p_1, \dots, p_m, X) \\
 & + \lambda_2 R_2(p_1, \dots, p_m, X) \\
 & + \lambda_{pd} PDL(p_1, \dots, p_m)
 \end{aligned} \tag{2}$$

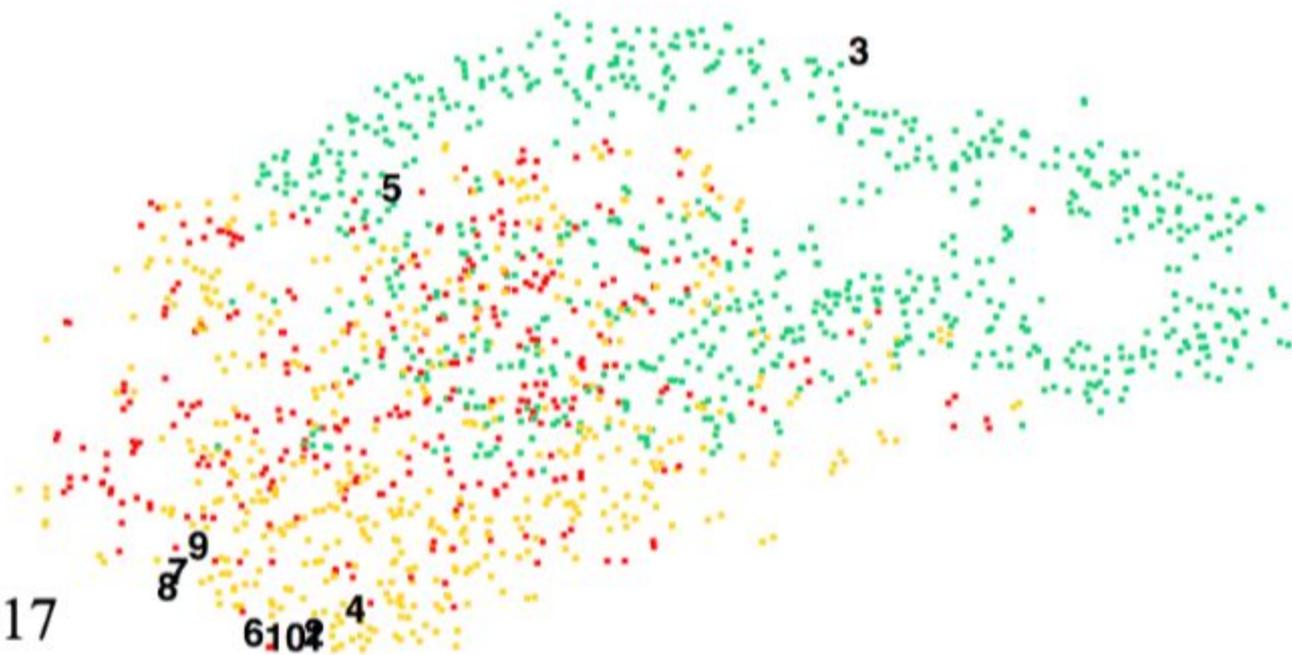
Prototype Diversity Loss

$$\lambda_{pd} PDL(p_1, \dots, p_m) = \frac{1}{\log\left(\frac{1}{m} \sum_{j=1}^m \min_{i>j \in [1, m]} \|p_i - p_j\|_2^2\right) + \epsilon} \tag{1}$$

$$R_1(p_1, \dots, p_m, X) = \frac{1}{m} \sum_{j=1}^m \min_{i \in [1, n]} \|p_j - f(x_i)\|_2^2, \tag{3}$$

$$R_2(p_1, \dots, p_m, X) = \frac{1}{n} \sum_{i=1}^n \min_{j \in [1, m]} \|f(x_i) - p_j\|_2^2 \tag{4}$$

## Prior work: Latent Space Representation for Bradycardia task

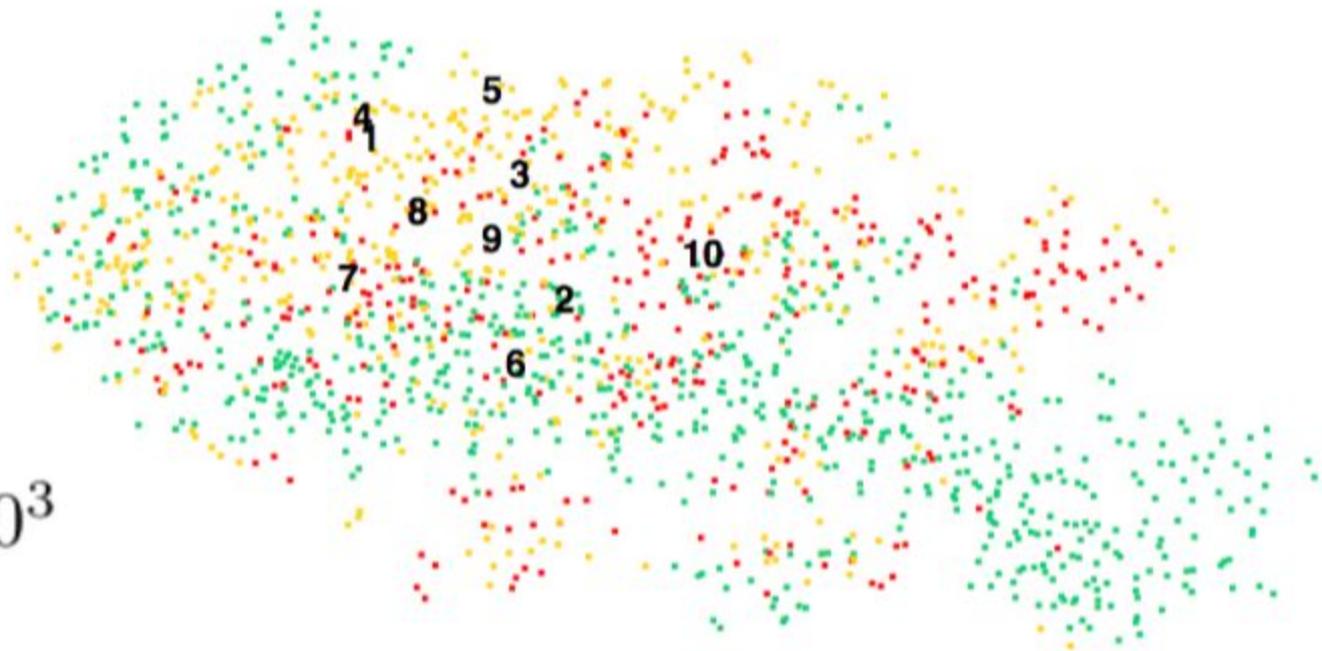


Loss from  
 Li *et al.* 2017

$$(\lambda_{pd} = 0)$$

## Our work: Latent Space Representation for Bradycardia task

$$\lambda_{pd} = 10^3$$



ECG: Bradycardia			
$\lambda_{pd}$	Accu.	$\Psi_N$	$\Psi_C$
0	$92.1 \pm 0.1\%$	$0.83 \pm 0.04$	$0.78 \pm 0.19$
500	$92.7 \pm 1.0\%$	$0.86 \pm 0.07$	$0.89 \pm 0.19$
$1e3$	$92.4 \pm 1.3\%$	$0.87 \pm 0.11$	$0.89 \pm 0.19$
$2e3$	<b><math>93.1 \pm 0.4\%</math></b>	<b><math>0.90 \pm 0.04</math></b>	<b><math>1.00 \pm 0.00</math></b>

  
 Prototype neighbor  
 diversity  $\Psi_N$

  
 Prototype class  
 diversity  $\Psi_C$

## Class. Task 1: Speaker

— person

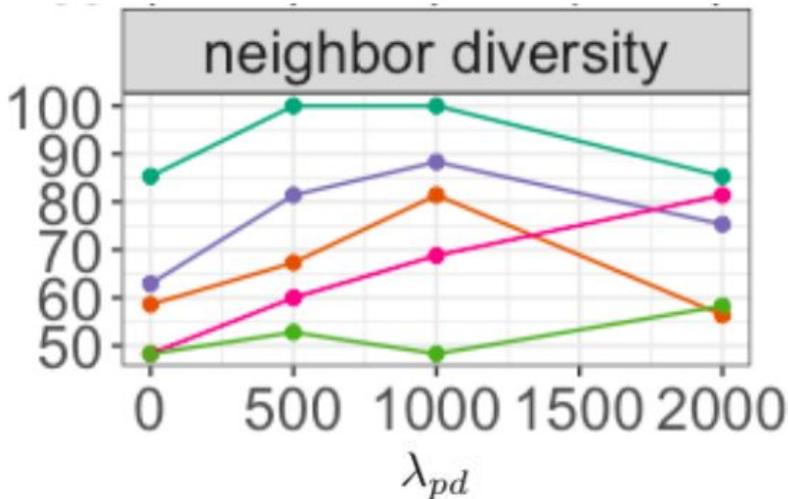
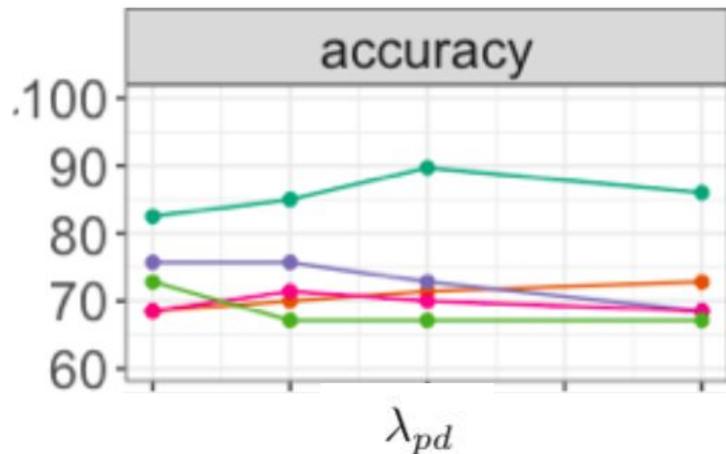
## Class. Task 2: Digits

— jackson

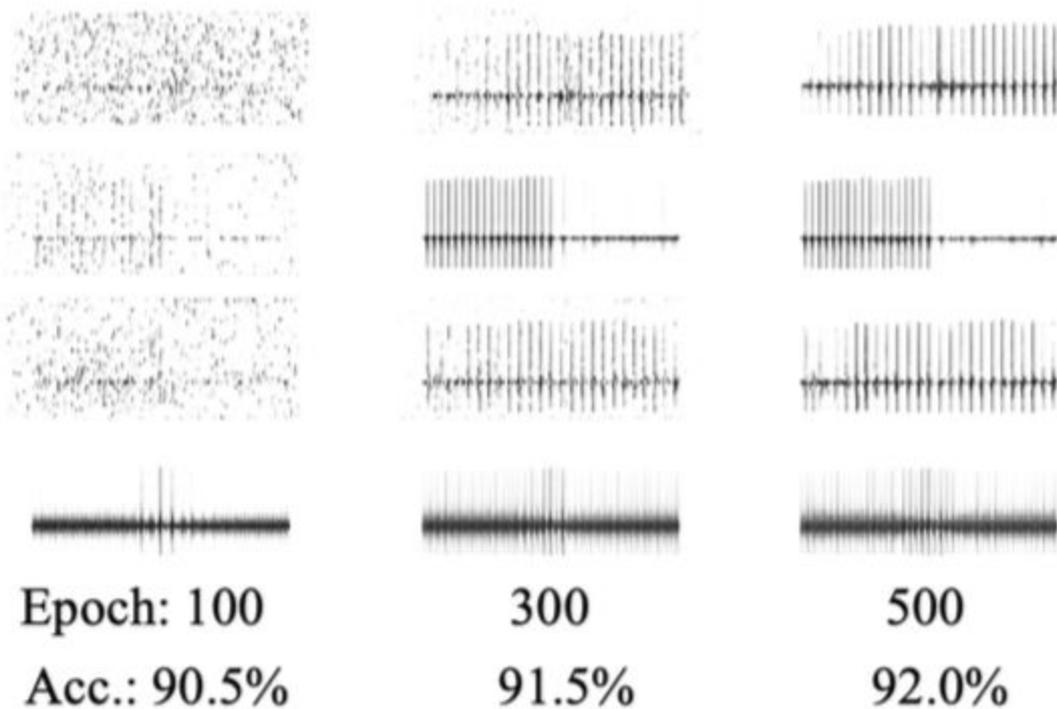
— theo

— nicolas

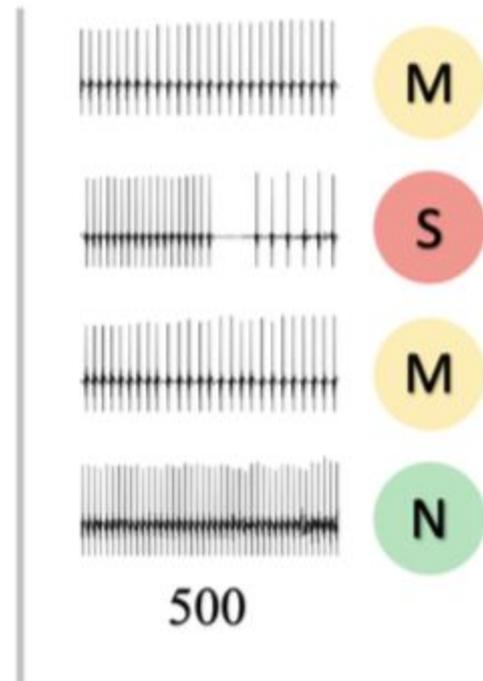
— yweweler



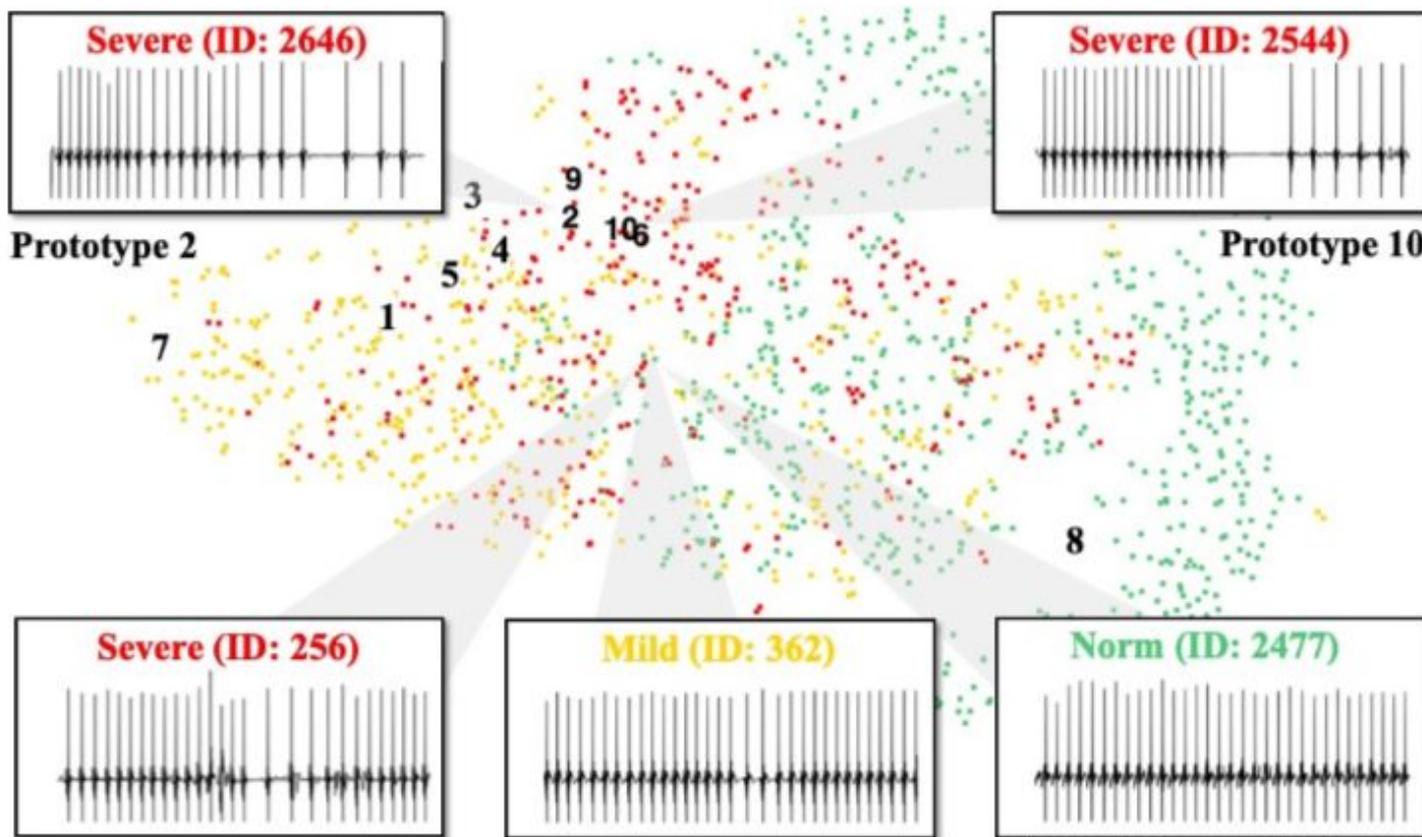
## Maturation of Learned Prototypes



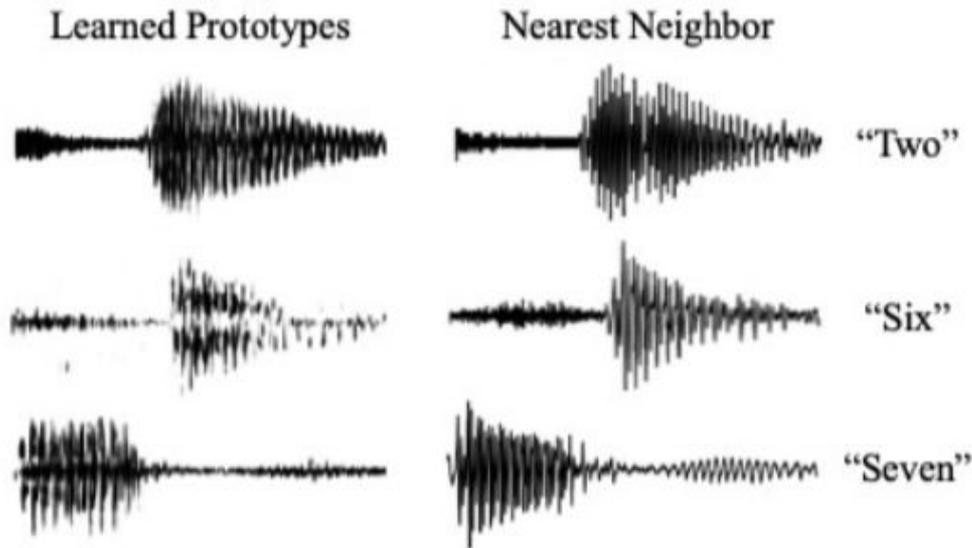
## Nearest Neighbor



## Decoded Representations of Prototypes



## Spoken Digit Global Explainability



## Instance Explainability

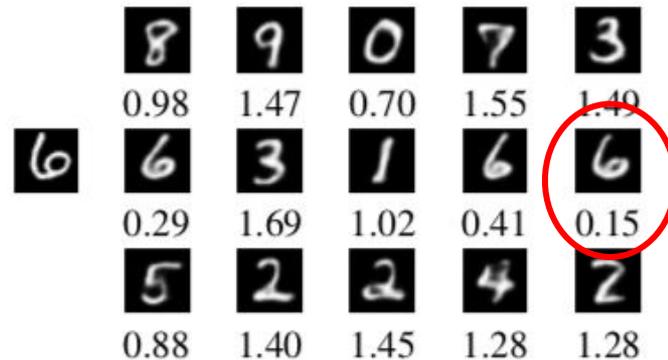


Figure 8: Learned prototypes from audio waveforms of spoken digits by Nicolas from the FSDD ( $\lambda_{pd} = 500$ ).

# Biomedical Interpretable Entity Representations

Garcia-Olano, D., Onoe, Y., Baldini, I., Ghosh, J., Wallace, B., Varshey, K. "Biomedical Interpretable Entity Representations". Findings of the Association for Computational Linguistics (ACL-IJCNLP 2021)

Entities over text = typically embedded in dense vector spaces  
with pre-trained language models ([BERT](#), etc).

```
[0.519, 0.917, -0.935, 0.891, 0.396, 0.711, 0.479, 0.417, 0.744, -0.254,  
-0.174, 0.233, -0.315, 0.497, -0.516, 0.22, -0.679, 0.389, -0.683, 0.909,  
23, 0.528, 0.116, 0.334, 0.717, 0.857, -0.262, 0.624, -0.178, -0.045, -0.  
-0.952, 0.4, 0.356, 0.091, 0.976, -0.337, -0.002, 0.054, 0.512, -0.312,  
.278, -0.409, -0.655, -0.294, -0.453, 0.735, 0.461, 0.282, -0.43, -0.838,  
3, -0.736, -0.001, 0.889, -0.228, 0.645, 0.883, 0.805]
```

```
[0.656, 0.407, 0.568, -0.035, -0.842, -0.257, 0.202, -0.31, 0.886, 0.386,  
34, -0.823, -0.929, -0.068, -0.238, 0.236, -0.463, 0.56, -0.687, -0.521,  
88, 0.54, 0.047, -0.434, -0.009, 0.59, 0.971, 0.798, 0.202, 0.225, 0.131,  
88, 0.44, -0.835, -0.032, -0.935, 0.318, 0.72, -0.23, -0.903, 0.912, -0.8  
0.981, -0.23, 0.797, -0.785, -0.583, 0.055, -0.511, 0.413, -0.757, 0.914,  
943, -0.62, -0.78, 0.888, 0.288, 0.807, -0.207, -0.284]
```

Entities over text = typically embedded in dense vector spaces with pre-trained language models (BERT, etc.).

```
>>> word_embedding_for_happy
[0.519, 0.917, -0.935, 0.891, 0.396, 0.711, 0.479, 0.417, 0.744, -0.254,
-0.174, 0.233, -0.315, 0.497, -0.516, 0.22, -0.679, 0.389, -0.683, 0.909, ←
23, 0.528, 0.116, 0.334, 0.717, 0.857, -0.262, 0.624, -0.178, -0.045, -0.
-0.952, 0.4, 0.356, 0.091, 0.976, -0.337, -0.002, 0.054, 0.512, -0.312,
.278, -0.409, -0.655, -0.294, -0.453, 0.735, 0.461, 0.282, -0.43, -0.838,
3, -0.736, -0.001, 0.889, -0.228, 0.645, 0.883, 0.805]
```



→

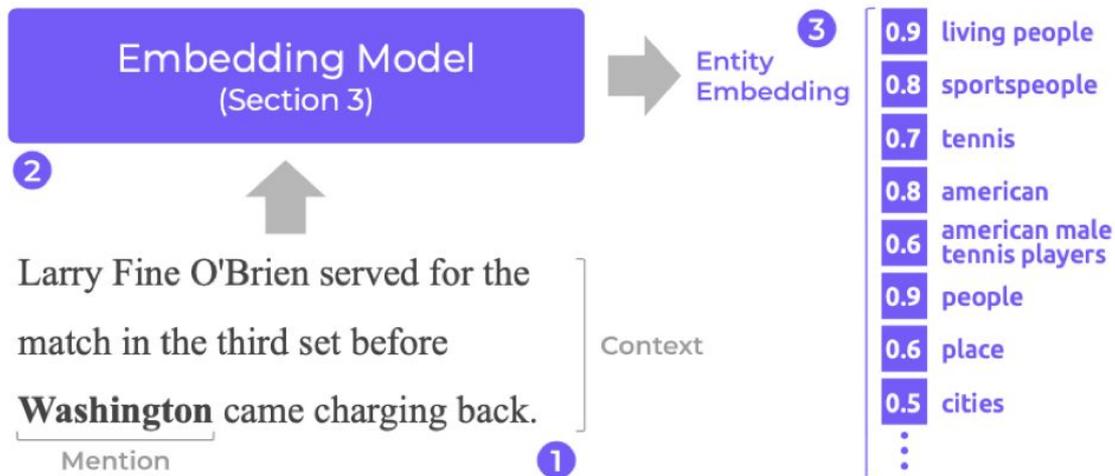
```
>>> word_embedding_for_sad
[0.656, 0.407, 0.568, -0.035, -0.842, -0.257, 0.202, -0.31, 0.886, 0.386,
34, -0.823, -0.929, -0.068, -0.238, 0.236, -0.463, 0.56, -0.687, -0.521,
88, 0.54, 0.047, -0.434, -0.009, 0.59, 0.971, 0.798, 0.202, 0.225, 0.131,
88, 0.44, -0.835, -0.032, -0.935, 0.318, 0.72, -0.23, -0.903, 0.912, -0.8
0.981, -0.23, 0.797, -0.785, -0.583, 0.055, -0.511, 0.413, -0.757, 0.914,
943, 0.62, -0.78, 0.888, 0.288, 0.807, -0.207, -0.284]
```

Not immediately interpretable.

Dense Entity  
Embeddings

= Give good performance for entity-related tasks,  
but using them in those tasks  
requires additional processing in neural models.

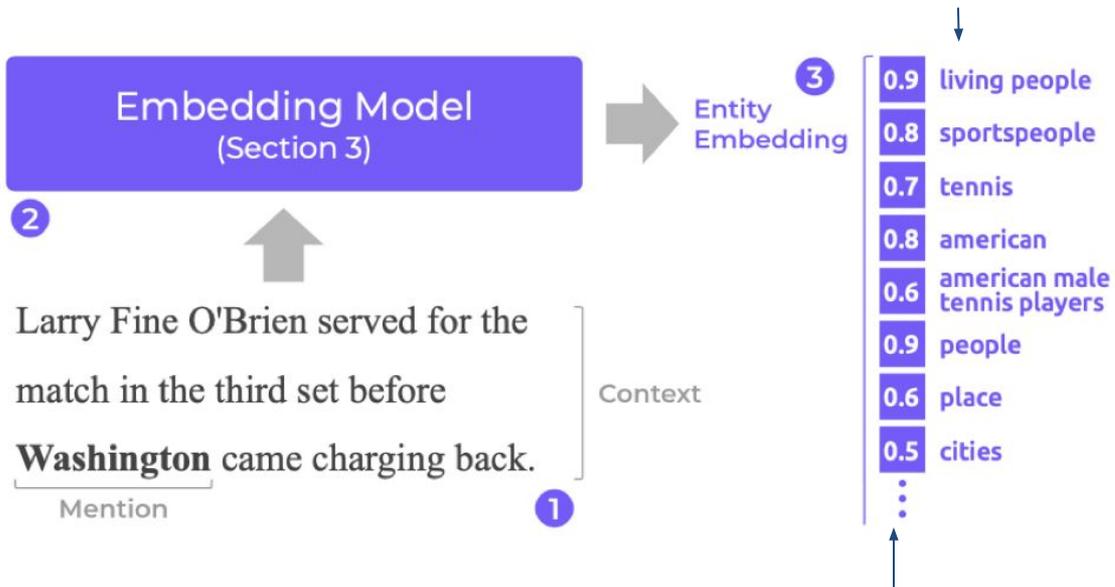
Onoe et al\* learn **human readable interpretable entity representations** that achieve high performance without additional learning (“out of the box”)



“Interpretable Entity Representations Through Large Scale Typing”  
 Yasumasa Onoe & Greg Durrett . Findings of EMNLP 2020

Onoe et al\* learn **human readable interpretable entity representations** that achieve high performance without additional learning (“out of the box”)

## fine grained entity types



represent probability of entity have corresponding properties

experiments using Ultra Fine Entity Type system (10k)  
and Wikipedia Categories Type System (60k)

## Problem setup: Interpretable Entity Representations

**s** = a sequence of **context words**,

**m** = an **entity mention span in s**.

**t**  $\in [0, 1]^T$  binary vector of **entity types** over types in  $T$

**Goal:** Learn **parameters  $\theta$**  of a **function  $f$**  that

**maps the mention  $m$  and its context  $s$**

**$\Rightarrow$  to a **vector  $t$****

that captures salient features of the entity mention in its context

High dimensional Multi-label classification task over entity types

# Can we adapt IERs for the **Biomedical Domain**?

\*[ **Glesatinib** ]\* is a dual inhibitor of c-Met and SMO  
that is under phase II clinical trial for non-small cell lung cancer.

## Can we adapt IERs for the **Biomedical Domain**?

\*[ Glesatinib ]\* is a dual inhibitor of c-Met and SMO that is under phase II clinical trial for non-small cell lung cancer.

```

world health organization essential medicines : 0.4941
      pyridines : 0.4073
      diols : 0.3539
      cancer treatments : 0.3260
      carboxylate esters : 0.2376
      chloroarenes : 0.1984
      rtt : 0.1879
hormonal antineoplastic drugs : 0.1768
  antineoplastic drugs : 0.1037
    alcohols : 0.0771
    prodrugs : 0.0315
    peptides : 0.0300
    methyl esters : 0.0223
      merck : 0.0191
transgender and medicine : 0.0135
  teratogens : 0.0130
world anti-doping agency prohibited substances : 0.0124
  peripherally selective drugs : 0.0103
    human proteins : 0.0099
      ureas : 0.0090
    withdrawn drugs : 0.0089
  iarc group 2a carcinogens : 0.0073
    prostate cancer : 0.0066
      mechanisms : 0.0066
    chemotherapy : 0.0058
  aromatase inhibitors : 0.0057

```



of 60k wiki  
entity types

Most probable  
entity types for  
mention/context



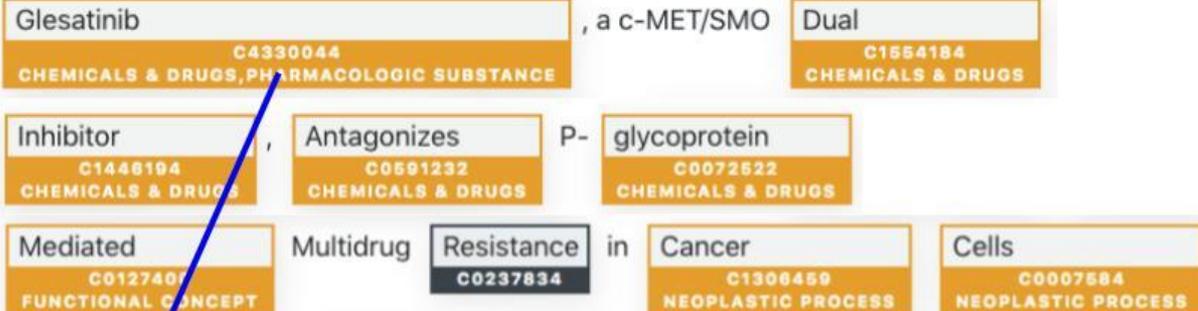
# BIOMEDICAL ENTITY TYPE SYSTEM & TRAINING DATA CONSTRUCTION

PubMed  
Abstracts  
( 460k )



NAMED  
ENTITY  
TAGGER

Distant Supervision  
to **construct**  
**Entity Type System**  
and **Training Data**.



UMLS  
CUIDs  
( Concept Unique  
Identifiers )

CUID to  
DBPedia  
mapper

SLING

WIKI  
PEDIA

## Glesatinib

From Wikipedia, the free encyclopedia

**Glesatinib** (MGCD265) is an experimental anti-cancer drug.<sup>[1]</sup>

Categories: [Drugs not assigned an ATC code](#) | [Tyrosine kinase inhibitors](#) | [Acetamides](#) | [Thiourea](#) | [Fluoroarenes](#) | [Experimental cancer drugs](#) | [Antineoplastic and immunomodulating drug stubs](#)

**37 million triples of the form**  
( mention, context, [types] )

**68K unique entity types total**

Interpretable  
 Sparse Entity  
 Representation



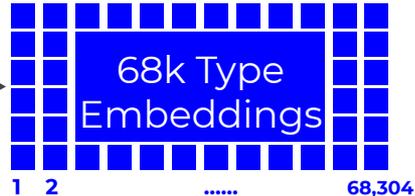
element wise  
 sigmoid

**Embedding  
 Model**

dense  
 rep



Dot



1 2 ..... 68,304

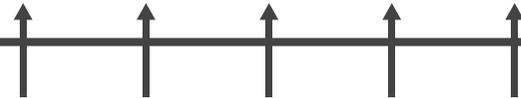


CLS

Mention and Context  
 Encoder (PubMedBERT)



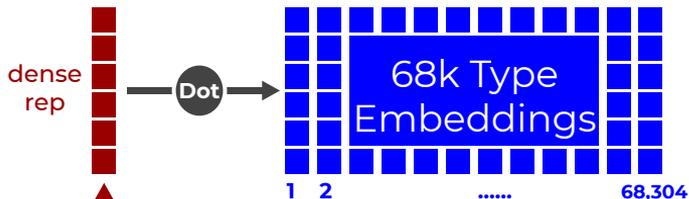
[CLS] mention [SEP] context [SEP]



Interpretable  
Sparse Entity  
Representation



**Embedding Model**



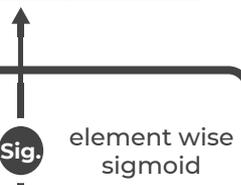
[CLS] mention [SEP] context [SEP]

## Training loss:

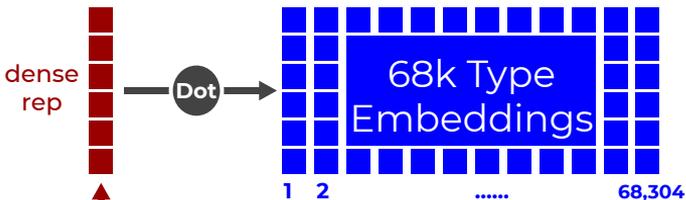
Independent sum of binary cross entropy losses over all entity types  $T$  over all training examples  $D$ .

$$-\sum_i^D \sum_j^T t_{ij}^* \cdot \log(t_{ij}) + (1 - t_{ij}^*) \cdot \log(1 - t_{ij}),$$

Interpretable  
Sparse Entity  
Representation



**Embedding Model**



[CLS] mention [SEP] context [SEP]

## Training loss:

Independent sum of binary cross entropy losses over all all entity types  $T$  over all training examples  $D$ .

$$- \sum_i^D \sum_j^T t_{ij}^* \cdot \log(t_{ij}) + (1 - t_{ij}^*) \cdot \log(1 - t_{ij}),$$

**Inference** via distance metric (cosine sim, dot prod) between Biomedical IERs **without fine-tuning** (leverages quantized based efficient similarity search)

(1) **Named Entity Disambiguation** (NED) on Clinical Entities.

Given a entity mention, context & set of candidate entities,  
identify which of the candidates is the true one linked to the mention.

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Given a entity mention, context & set of candidate entities identify which of the candidates is the true one linked to the mention.

Model	Test Acc.	
	Dot Prod	Cosine Sim
BIER-PubMedBERT (ours)	80.1	<b>84.0</b>
BIER-SciBERT (ours)	76.4	77.3
BIER-BioBERT (ours)	71.9	75.9
Onoe and Durrett (2020)	63.6	69.8
Popular Prior	73.9	-
PubMedBERT (Gu et al., 2020)	77.6	-
SciBERT (Beltagy et al., 2019)	77.4	-
BioBERT (Lee et al., 2019)	77.9	-



Table 2: BIER zero shot test results vs Logistic Regression Baselines trained on task data for NED task

## (2) Entity label Classification for Cancer Genetics

Model	Test Acc.			
	L2 Dist		Dot Prod	
	Dense	Sparse	Dense	Sparse
BIER-PubMedBERT	85.5	86.8	<b>88.2</b>	<b>87.5</b>
BIER-SciBERT	70.8	77.0	72.8	76.8
BIER-BioBERT	83.4	85.9	85.6	86.8
<i>Onoe and Durrett (2020)</i>	63.9	55.1	60.0	59.9
PubMedBERT	77.3	-	69.3	-
SciBERT	74.4	-	75.2	-
BioBERT	67.6	-	59.6	-

Table 3: Test accuracy on Cancer Genetics data using a nearest neighbor classifier ( $k=1$ ) without fine-tuning based on sparse output or intermediate dense embeddings using L2 or Dot Product distance metrics.

## (2) Entity label Classification for Cancer Genetics

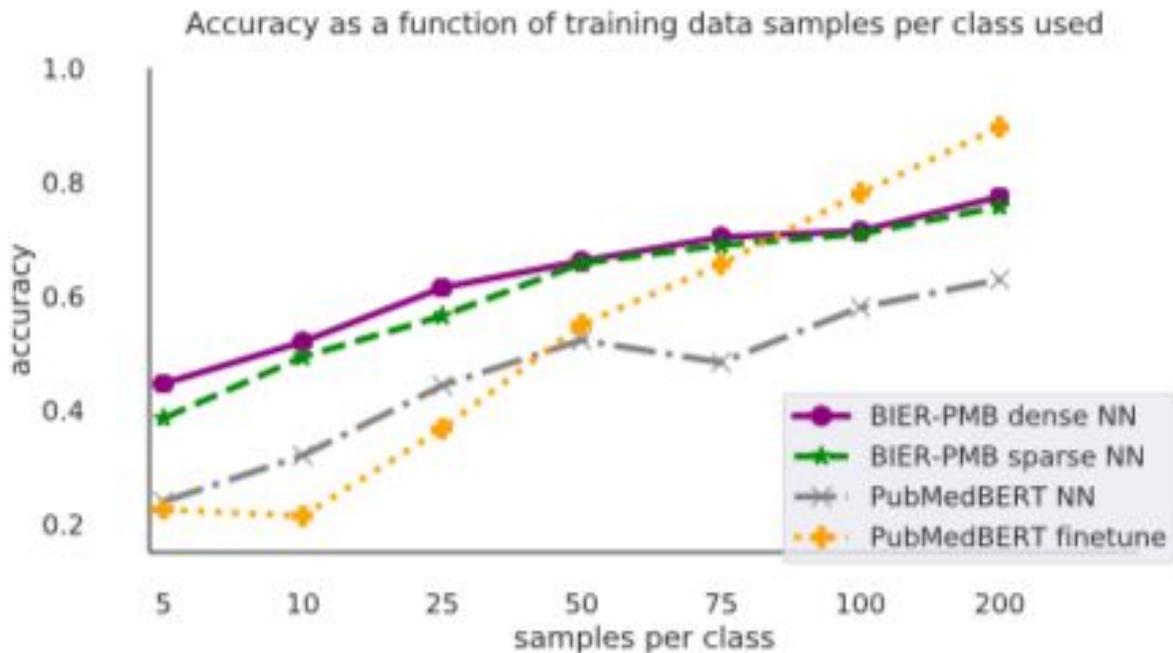
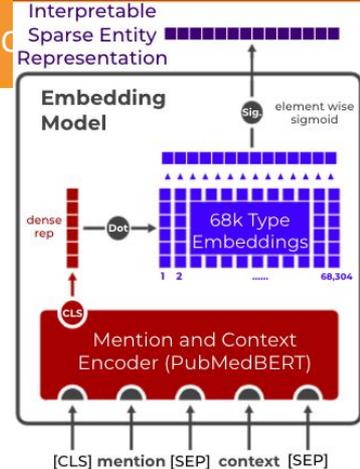


Figure 3: Results for the entity label classification task under varying amounts of supervision.

**Allows for error analysis** at the component level to identify areas lacking in supervision and/or possible changes to the type system.



**Allows for error analysis** at the component level to identify areas lacking in supervision and/or possible changes to the type system.

**How well the model could have done** had it known to fallback to **using the intermediate dense embedding** in cases where the sparse representation led to an **incorrect prediction**

Motivation for **future work** on developing a dynamic approach to making predictions that is a function of model confidence.

Task	Test Acc.			$\Delta$
	Dense	Sparse	Combined	
NED	84.0	81.0	<b>91.7</b>	+7.7
ELC	87.5	88.2	<b>91.9</b>	+3.7

Table 5: Results for both tasks showing improvements that could have been achieved by combining intermediate dense and interpretable sparse output embeddings generated by the same BIER-PubMedBERT model.

context: The presence of activating TSH-R mutations has also been demonstrated in differentiated **thyroid carcinomas**.

## Error analysis using BIERS

At present, the percentage of such a modification is low, unless referred to selected series of tumors.

mention: **thyroid carcinomas**

label: **Cancer**

Sparse NN model pred	Dense NN model pred
<b>thyroid</b> <b>(label: Organ)</b>	<b>esophageal carcinomas</b> <b>(label: Cancer)</b>
<b>Types</b>	<b>Types</b>
('gland', 0.99965), (('thyroid', 0.99932), (('rtt', 0.999), (('head_and_neck_cancer', 0.99093), (('neck', 0.97243), (('head_and_neck_anatomy', 0.93763), (('head', 0.86131), (('squamous-cell_carcinoma', 0.0024), (('ingredient', 0.00078), (('thyroid disease', 0.00047), (('nitrous_oxide', 0.00034), (('thyroid cancer', 0.0003), (('endocrine diseases', 0.00019),	('thyroid cancer', 0.99994), (('squamous-cell_carcinoma', 0.9998), (('thyroid', 0.99925), (('cancer', 0.99133), (('gland', 0.99039), (('nitrous_oxide', 0.01965), (('pancreatic_cancer', 0.00152), (('neck', 0.00023), (('thyroid_neoplasm', 0.00019), (('rtt', 0.00014), (('endocrine diseases', 2e-05), (('head', 1e-05), (('malignancy', 1e-05),

# Completed Work

Learning Dense Representations for Entity Retrieval. (CoNLL 2019)

Constructed a **dual mention-entity encoder** that learns dense representations for efficient neural **Entity Retrieval** with an **in-process, iterative hard-negatives procedure** for **model learning and inference time inspection**.

Deep Classification of Time-Series Data with Learned Prototype Explanations. (ICML 19)

Adapted a **prototypical autoencoder** classifier to be compatible with **time series data**; allowing for **tunable prototype diversity** and improved accuracy and **global and instance level explanations**.

Biomedical Interpretable Entity Representations. (ACL-IJCNLP 2021)

Learned a distantly supervised entity type system and data set for use in training a **Biomedical Interpretable Entity model** whose representations exist in a **semantically meaningful vector space** & whose **predictions may be diagnosed** with an oracle method.

This proposal shows in-process diagnostic techniques are useful for sequential data tasks both in accuracy & interpretability.

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- Garcia-Olano, D., Onoe, Y., Baldini, I., Ghosh, J., Wallace, B., Varshey, K. “Biomedical Interpretable Entity Representations”. Findings of the Association for Computational Linguistics (ACL-IJCNLP), Bangkok, Thailand, 2021
- Gillick, D., Kulkarni, S., Lansing, L., Presta, A., Baldrige, J., Ie, Eugene., Garcia-Olano, D. “Learning Dense Representations for Entity Retrieval”. Proceedings of the 23rd Conference on Computational Natural Language Learning (CoNLL), Hong Kong, China, 2019.
- Garcia-Olano, D., Gee, A., Ghosh, J., Paydarfar, D. “Explaining Deep Classification of Time-Series Data with Learned Prototypes”. Proceedings of the 4th International Workshop on Knowledge Discovery in Healthcare Data co-located with International Joint Conference on Artificial Intelligence, ( IJCAI ) , Macao, China, 2019
- Garcia-Olano, D., Gee, A., Ghosh, J., Paydarfar, D. “Deep Classification of Time-Series Data with Learned Prototype Explanations”. Proceedings of the 36th International Conference on Machine Learning (ICML), Long Beach, California, PMLR 97, 2019
- Sankaran, K., Garcia-Olano, D., Javed, M., Alcalá-Durand, M., De Unánue, A., van der Boor, P., Potash, E., Avalos, R., Encinas, L., Ghani, R., “Applying Machine Learning Methods to Enhance the Distribution of Social Services in Mexico”. Presented at UChicago Data Science for Social Good. arXiv:1709.05551. 2017.
- Garcia-Olano, D. Arias, M, Larriba Pey, J. “Automated construction and analysis of political networks via open government and media sources”. European Conference on Machine Learning and Principles and Practice of Knowledge Discovery in Databases (ECML). Riva del Garda, Italy, 2016
- Paz-Ortiz, García-Olano, D., Gay-García, C. (2015. July) “Term-frequency Inverse Document Frequency for the Assessment of Similarity in Central and State Climate Change Programs: An Example for Mexico”. In Proceedings of the 5th International Conference on Simulation and Modeling Methodologies, Technologies and Applications (MSCCES-2015), Colmar, France 2015.

# Thank you!

