

# 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]
```



→

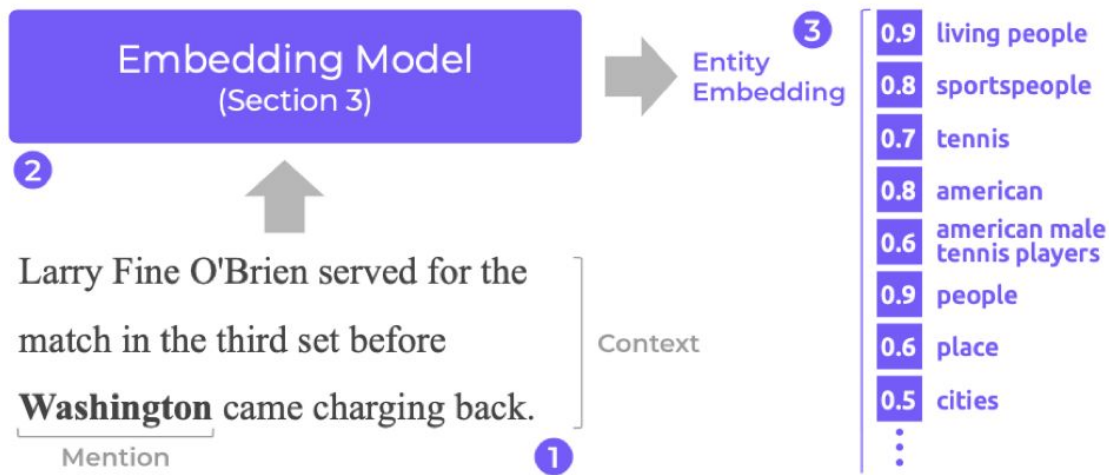
```
>>> word_embedding_for_sad
[0.656, 0.407, 0.568, -0.035, -0.842, -0.257, 0.202, -0.31, 0.886, 0.386,
34, -0.823, -0.929, -0.068, -0.238, 0.236, -0.463, 0.56, -0.687, -0.521,
88, 0.54, 0.047, -0.434, -0.009, 0.59, 0.971, 0.798, 0.202, 0.225, 0.131,
88, 0.44, -0.835, -0.032, -0.935, 0.318, 0.72, -0.23, -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

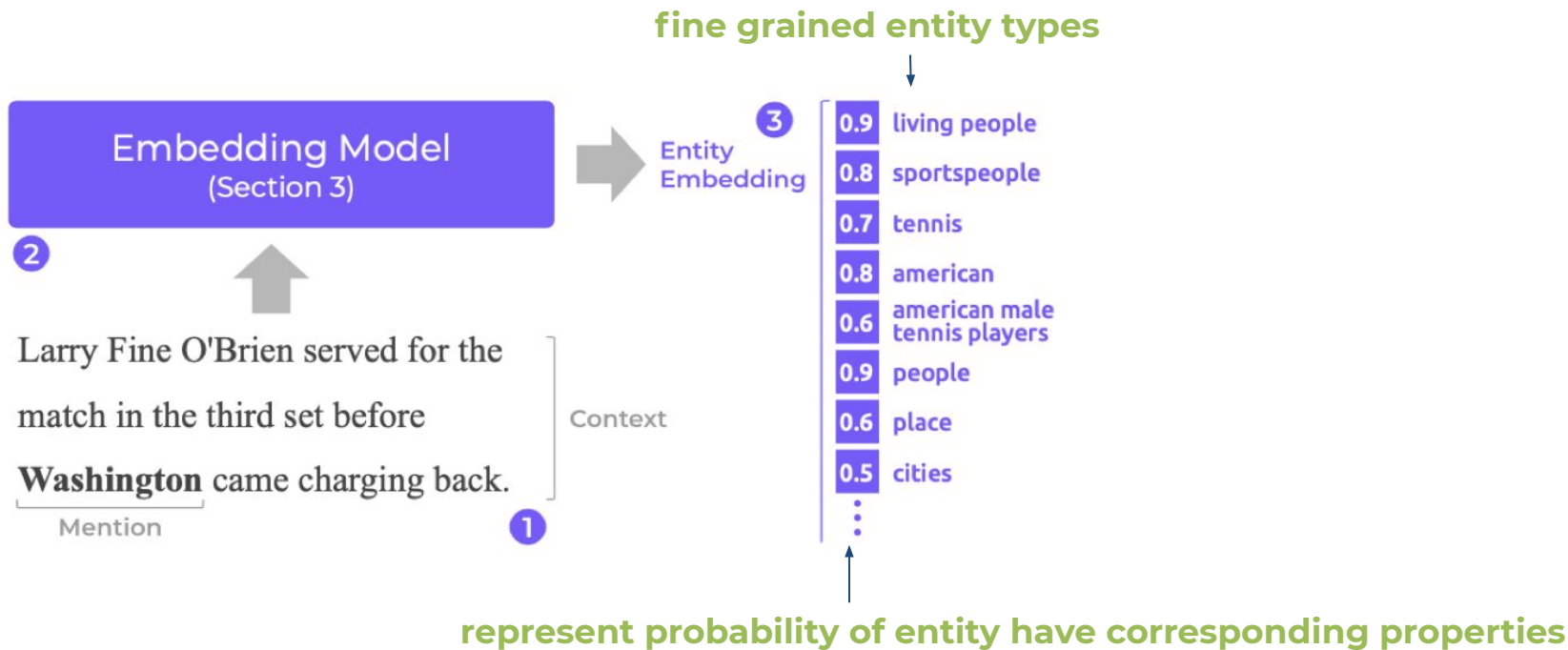
= Give good performance for entity-related tasks,  
but using them in those tasks  
requires additional processing in neural models.

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”)



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

# 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

Most probable  
entity types for  
mention/context



of 60k wiki  
entity types

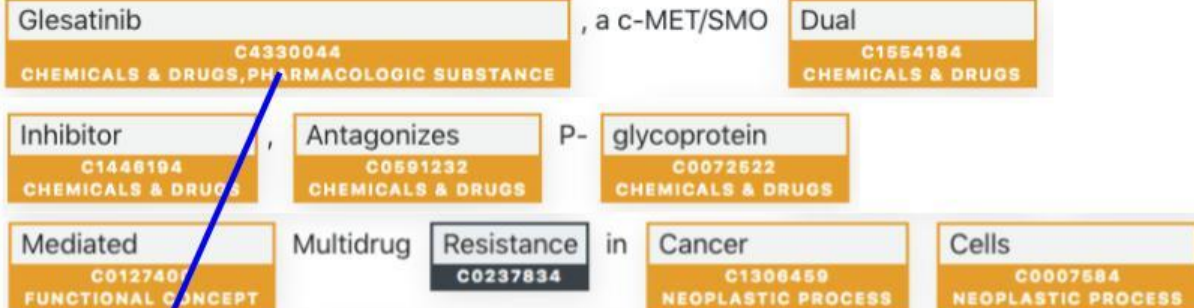
# BIOMEDICAL ENTITY TYPE SYSTEM & TRAINING DATA CONSTRUCTION

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

PubMed  
Abstracts  
( 460k )



NAMED  
ENTITY  
TAGGER



UMLS  
CUIDs  
( Concept Unique  
Identifiers )

CUID to  
DBPedia  
mapper

SLING

WIKI  
PEDIA

## Glesatinib

From Wikipedia, the free encyclopedia

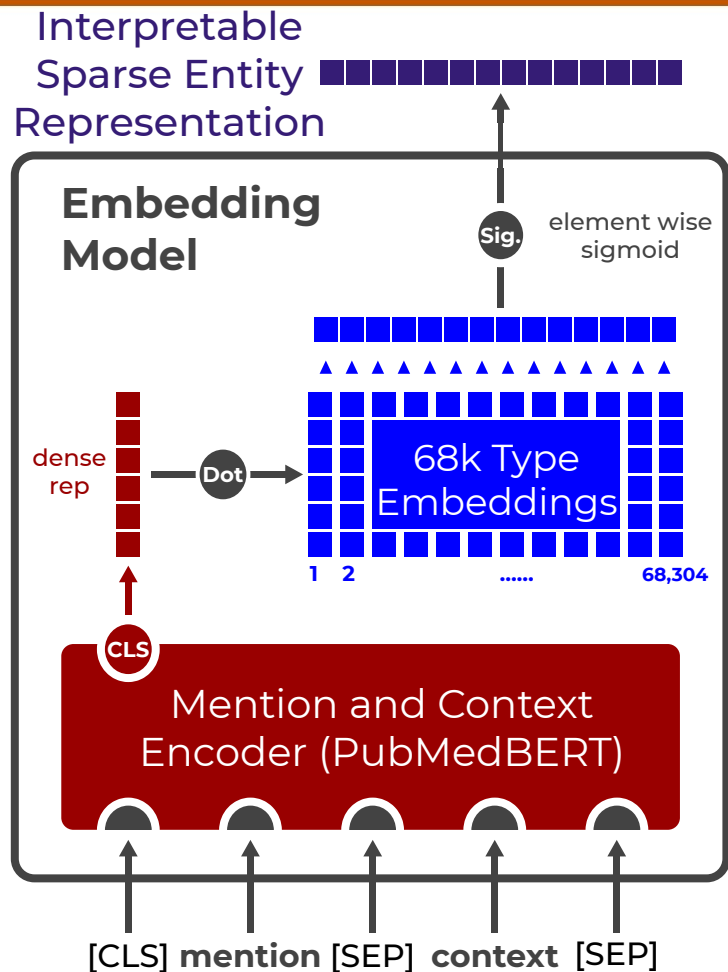
**Glesatinib** (MGCD265) is an experimental anti-cancer drug.<sup>[1]</sup>

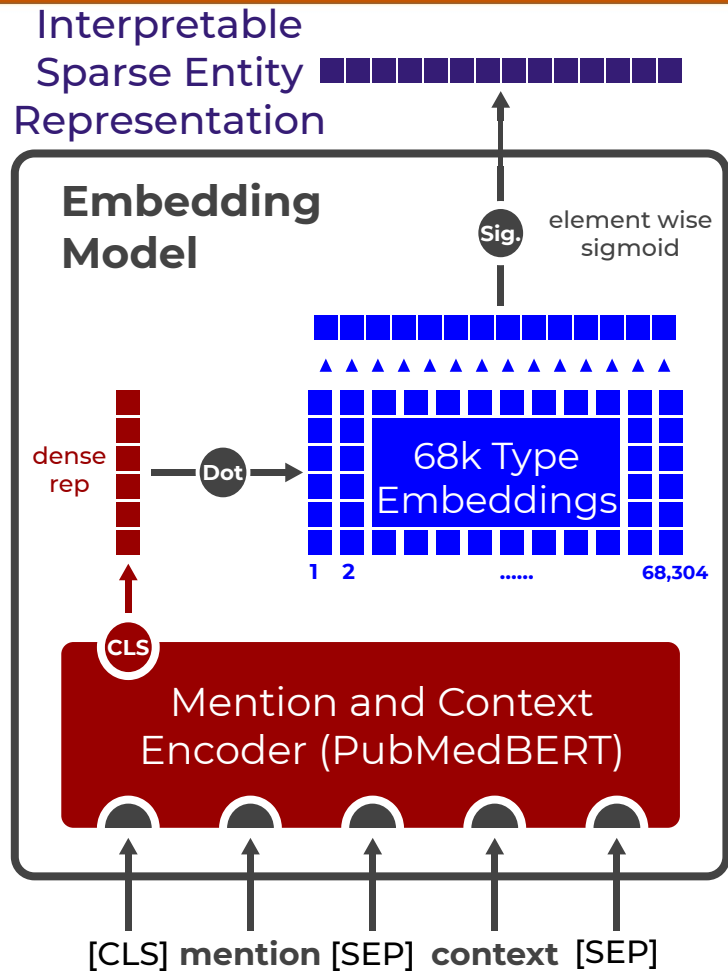
Categories: Drugs not assigned an ATC code  
Tyrosine kinase inhibitors | Acetamides | Thiourea  
Fluoroarenes | Experimental cancer drugs  
Antineoplastic and immunomodulating drug stubs

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

68K unique entity types total







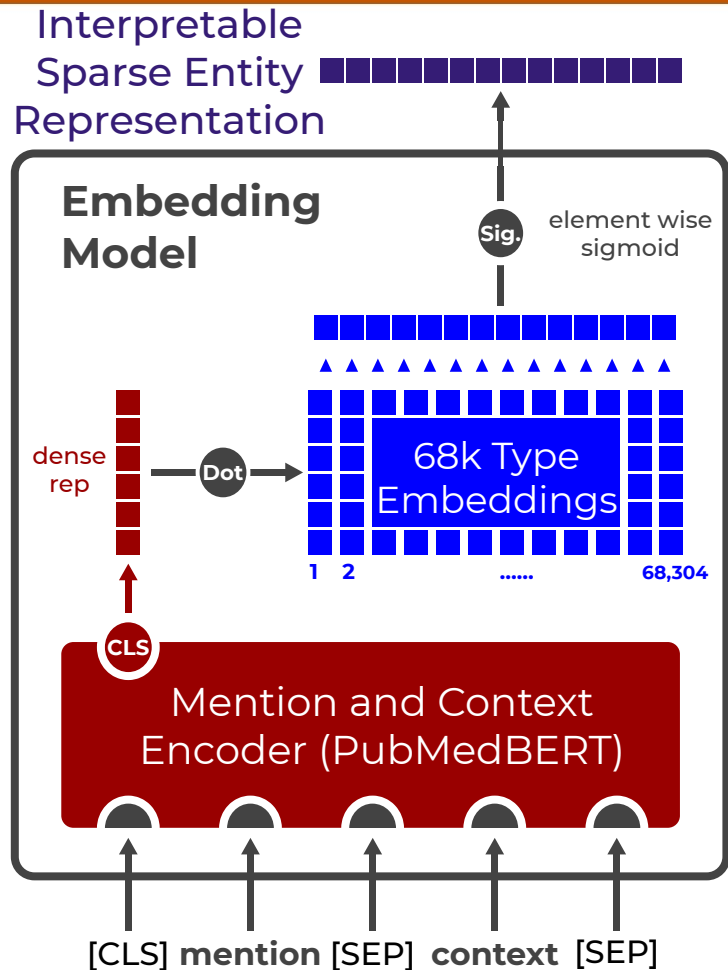
## Training loss:

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

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

true types for training instance  $i$

predicted types



**Inference** via simple cosine similarity  
between Biomedical IERs  
without fine-tuning on task data !

# (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.

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	-

Prior work

Fine tuned approaches

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
Onoe and Durrett (2020)	63.9	55.1	60.0	59.9
PubMedBERT	77.3	-	69.3	-
SciBERT	74.4	-	75.2	-
BioBERT	67.6	-	59.6	-

Prior work

Fine tuned approaches

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.

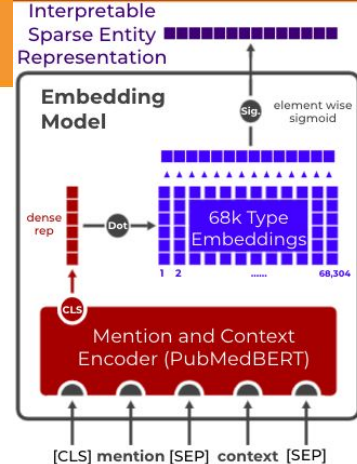
## (2) Entity label Classification for Cancer Genetics



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.

# Debugging with BIERs



**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.



# Thank you!

## Code and data available:

[https://github.com/diegoolano/biomedical\\_interpretable\\_entity\\_representations](https://github.com/diegoolano/biomedical_interpretable_entity_representations)



IBM  
Research

Science for Social Good



TEXAS  
The University of Texas at Austin



Northeastern  
University