Modeling Interactions with Deep Learning

Jack Lanchantin | PhD Thesis Defense | July 20th 2021

University of Virginia Department of Computer Science

Committee: Vicente Ordoñez (chair), Yanjun Qi (advisor), Yangfeng Ji, Clint Miller, Casey Greene

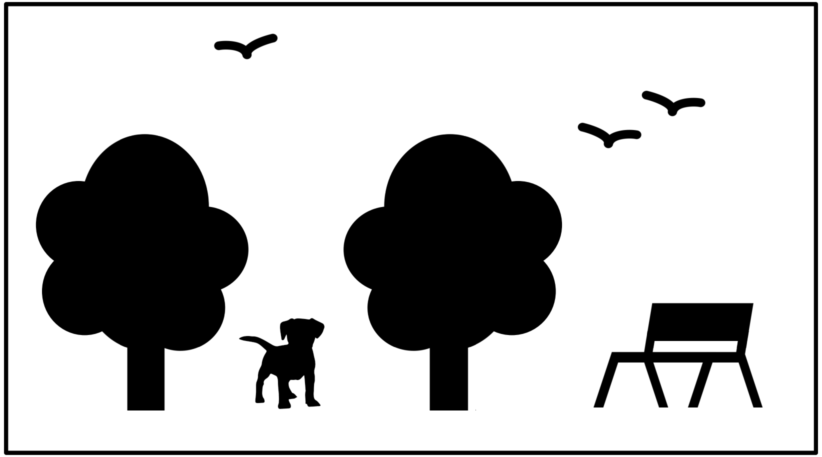
UNIVERSITY of VIRGINIA

tree

bird

bench

dog

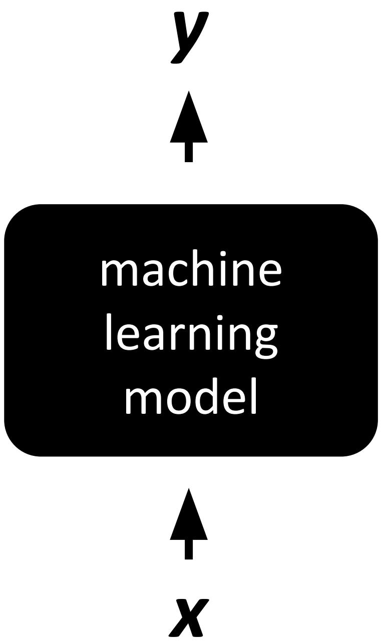


the cat sat on the small mat.

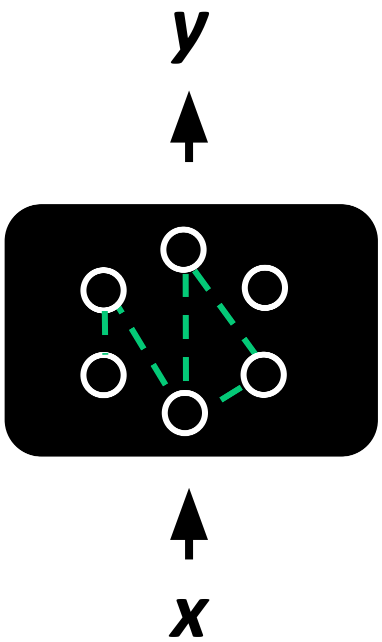
ATCGATCGATGCCGTTACGATGATCGTACGAAT


Protein A
Protein B

Machine learning models



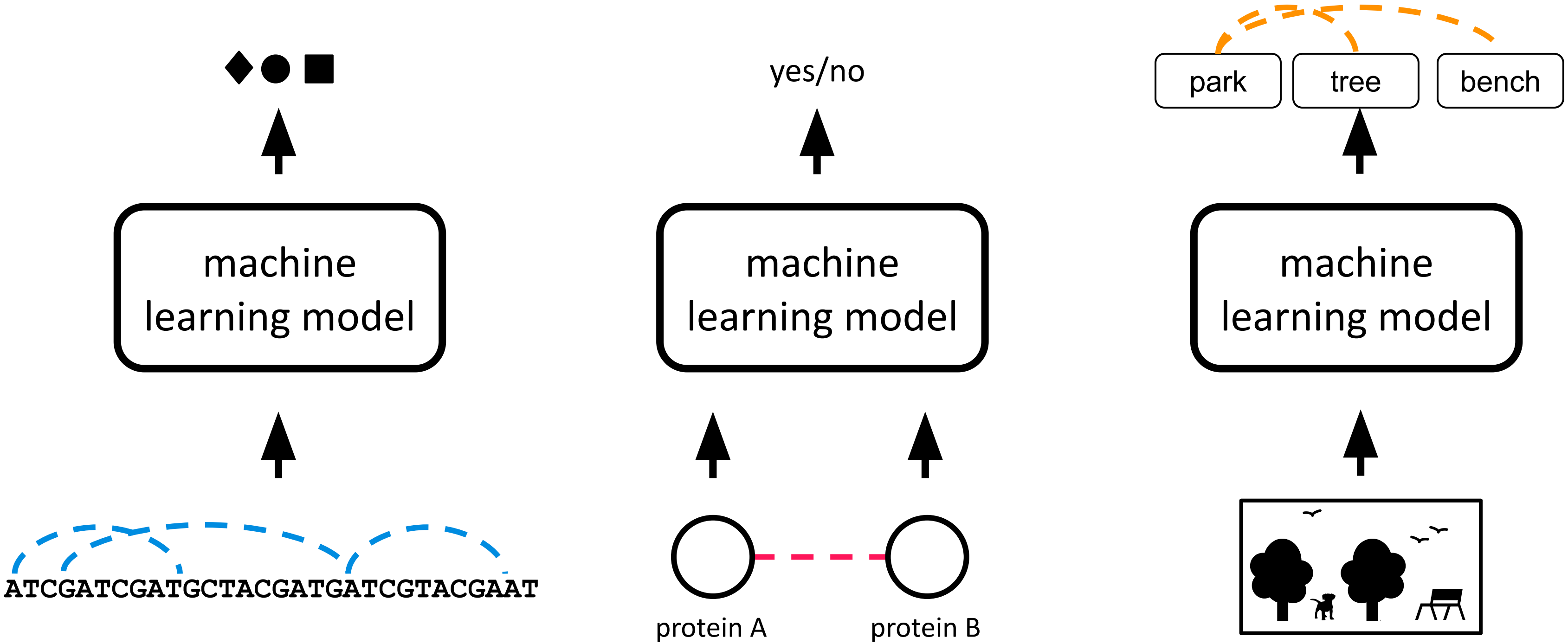
Machine learning models with relational biases



Thesis hypothesis

Deep learning with relational biases can be used to understand and improve tasks that involve complex interactions.

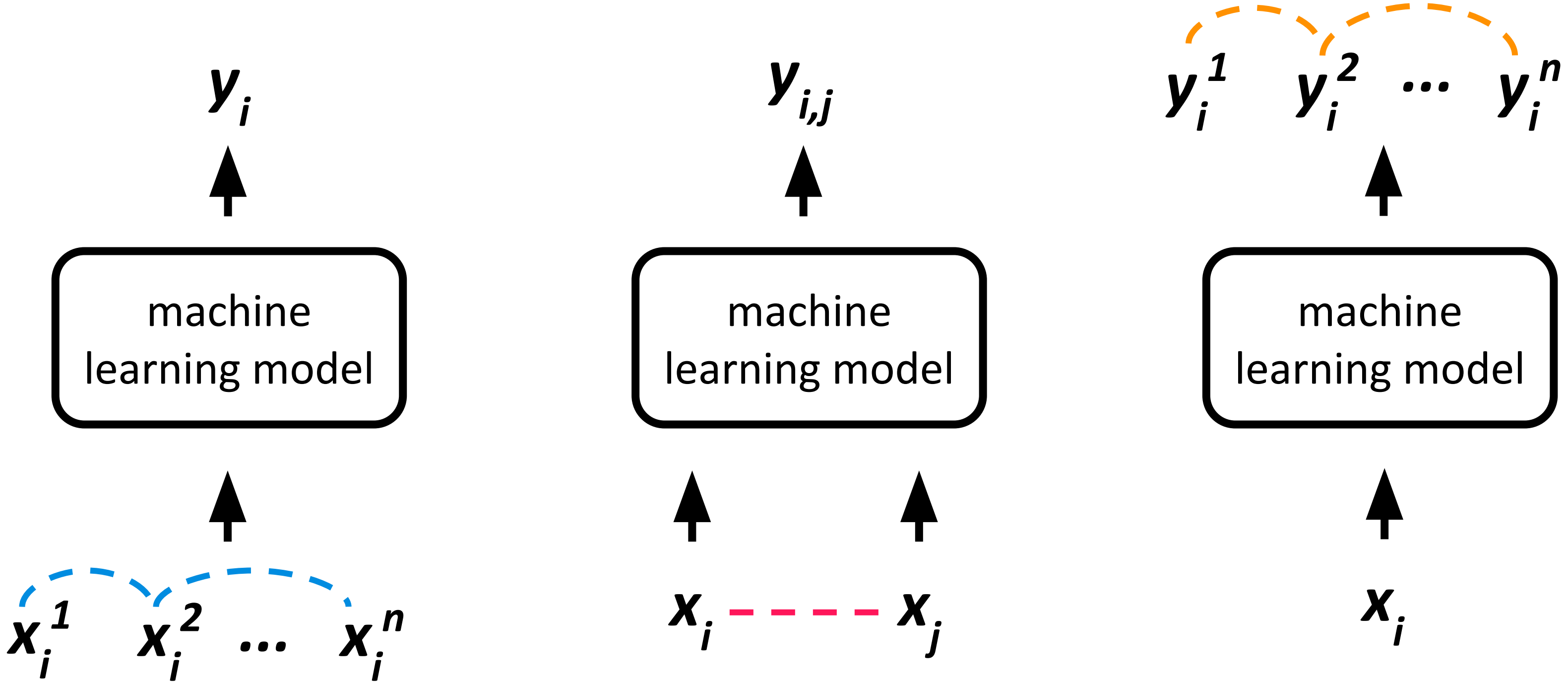
Using Deep Learning to Model Interactions



interactions between **input features**

interactions between **input samples**

interactions between **output labels**



Genomic Sequences

ChromeGCN
Lanchantin et al.
ECCB 2020

Deep Motif Dashboard
Lanchantin et al.
PSB 2017

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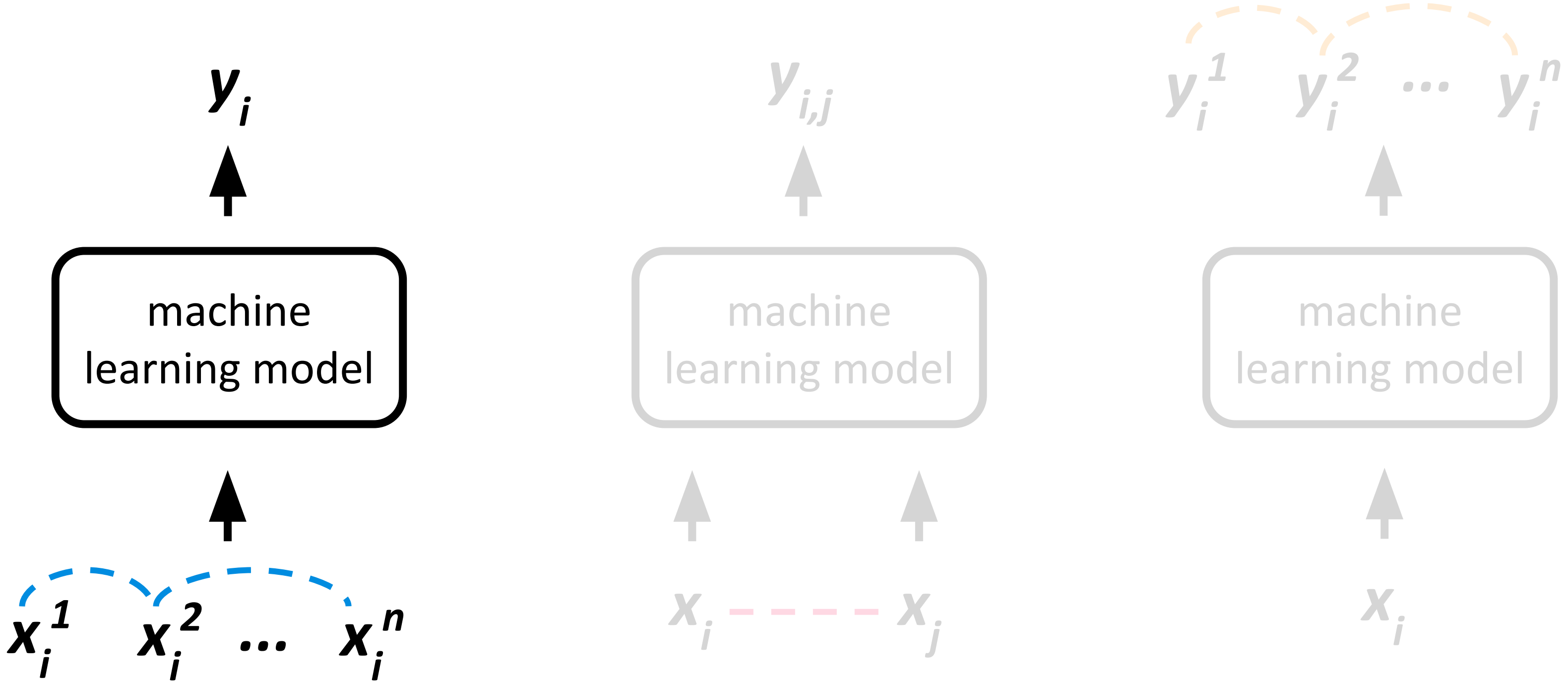
Modeling Genomic Sequence Interactions with ChromeGCN

interactions between **input features**

interactions between **input samples**

interactions between **output labels**



What is DNA?

phosphate backbone

nucleotide molecules

sequence with alphabet of characters A, C, G, T

What is DNA?

ATGCTCGATGCTAATACGACTGAGATTACTGAGACTGAGACTCTAGAT

What is DNA?

ACTGCTACCTATGACGTGATGCATCGTAGCTA

← 250M chars →

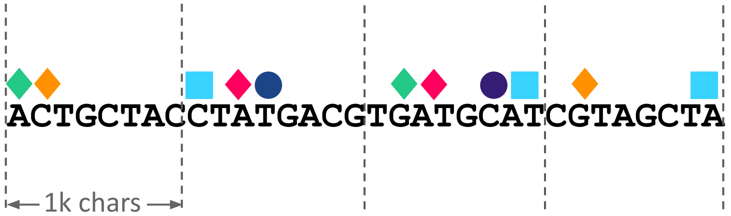
chromosome 1

Chromatin Profile

Chromatin profile signals: elements that control gene expression

(transcription factors, histone modifications, DNA accessibility)

Local Sequence Chromatin Profile Prediction



Local Sequence Chromatin Profile Prediction

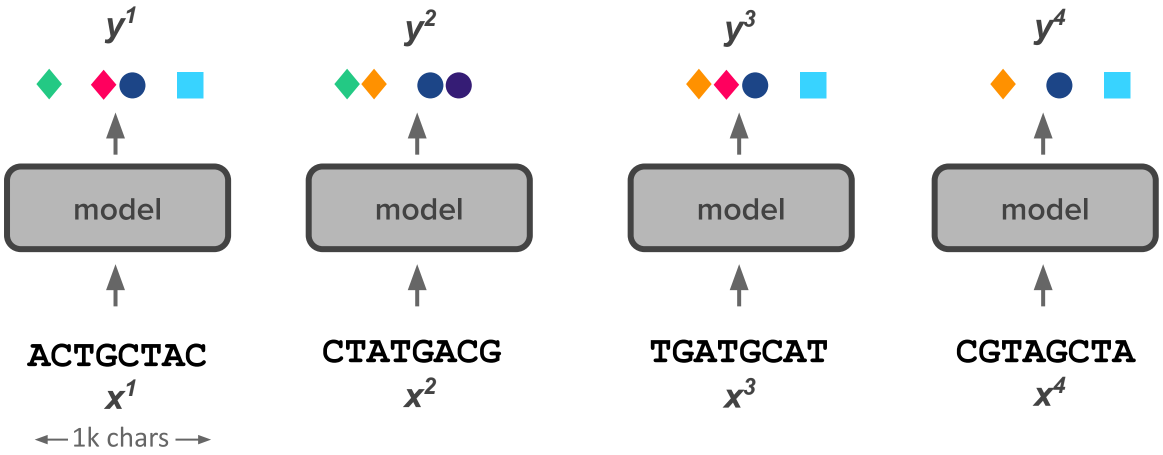
ACTGCTAC — x^1 — ← 1k chars →

CTATGACG — x^2

TGATGCAT — x^3

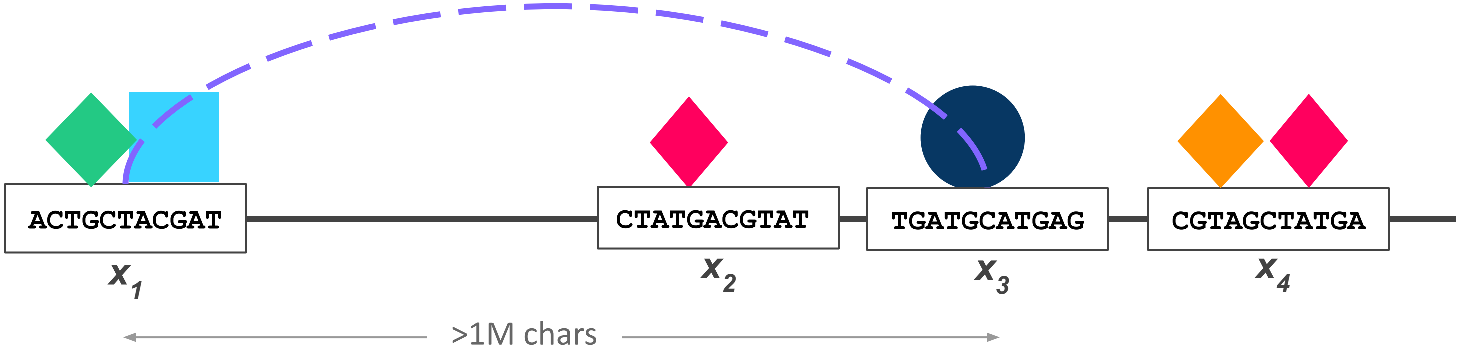
CGTAGCTA — x^4

Local Sequence Chromatin Profile Prediction

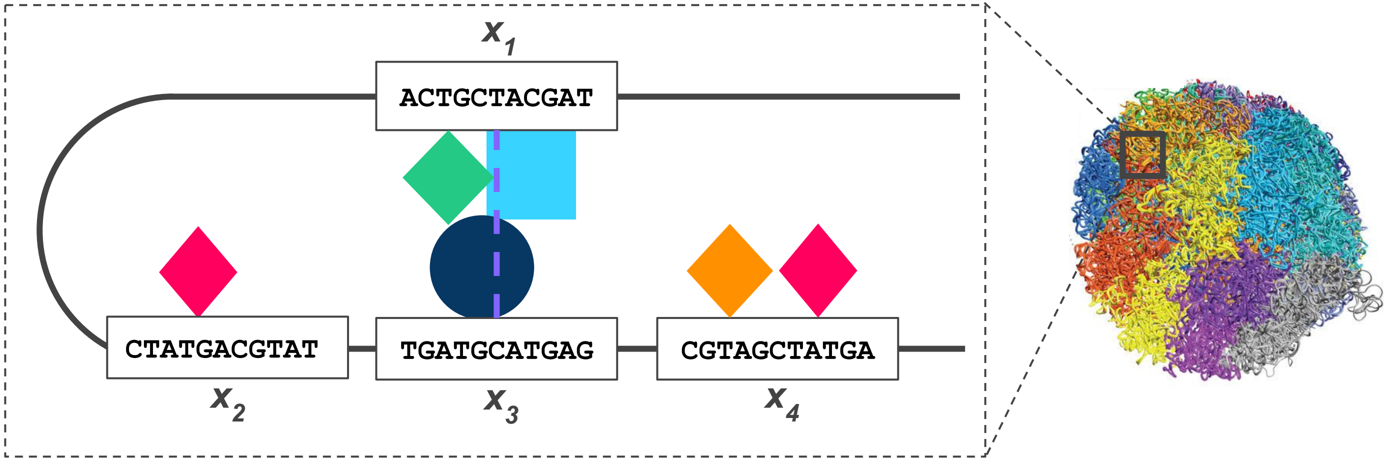


Zhou and Troyanskaya 2015, Alipanahi et al. 2015, Kelley et al. 2016

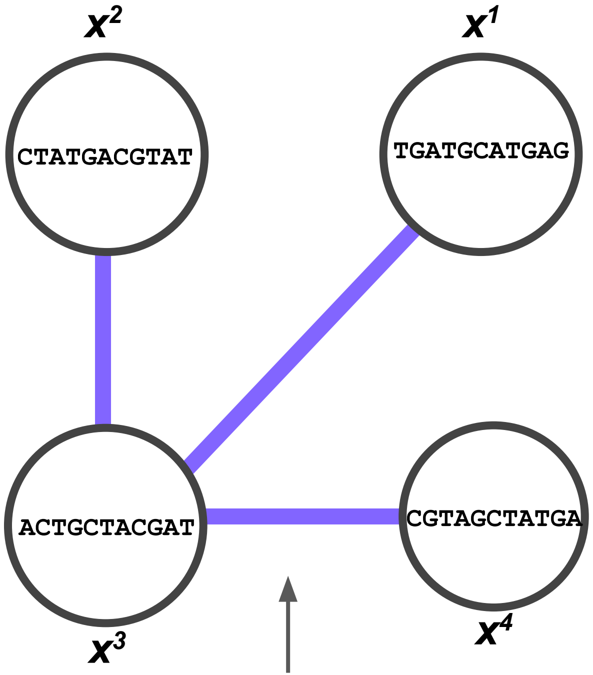
Influence of Long-Range Interactions on Chromatin Profile



Influence of Long-Range Interactions on Chromatin Profile

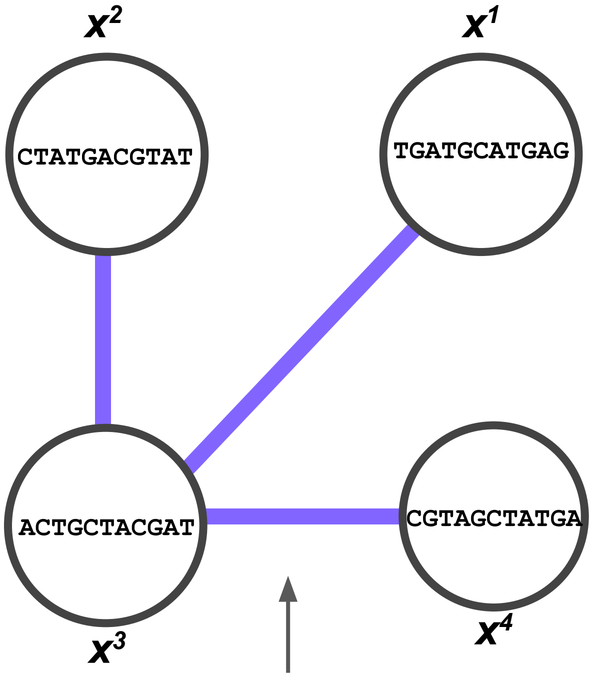


Genome: Locally a Sequence, Globally a Graph

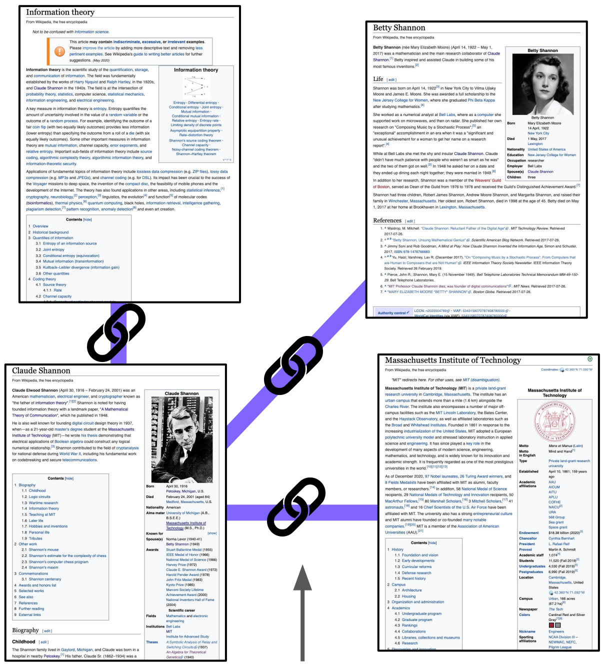


"Hi-C" interaction data

Genome: Locally a Sequence, Globally a Graph



↔



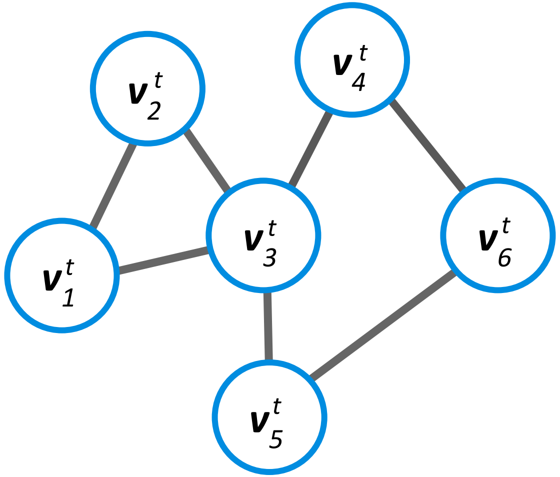
"Hi-C" interaction data

Hyperlinks

Research Question 1

Can we model both local sequence features and long range interactions for chromatin profile prediction?

Graph Neural Networks (GNNs)



$G = (V,E)$

$\boldsymbol{v}_i^t \in \mathbb{R}^d$

Scarselli et al. 2008, Li et al. 2015, Kipf et al. 2016, Gilmer et al. 2017, Bronstein et al. 2017, Battaglia et al. 2018

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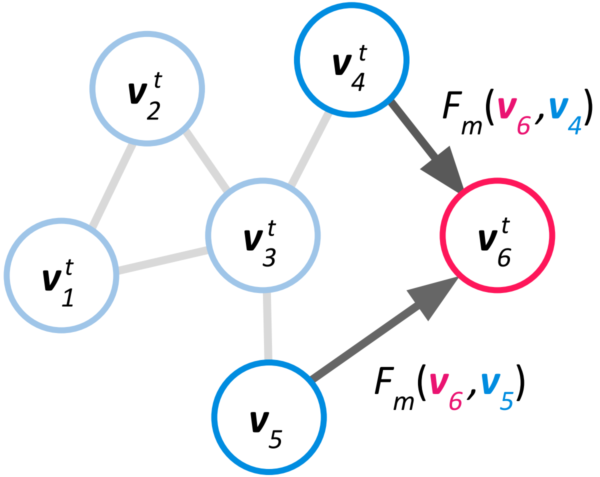

$G = (V,E)$

$\boldsymbol{v}_i^t \in \mathbb{R}^d$

message function F_m $\quad \boldsymbol{m}_i^t = \sum_{j \in \mathcal{N}(i)} F_m(\boldsymbol{v}_i^t, \boldsymbol{v}_j^t),$

node update function F_u $\quad \boldsymbol{v}_i^{t+1} = F_u(\boldsymbol{m}_i^t)$

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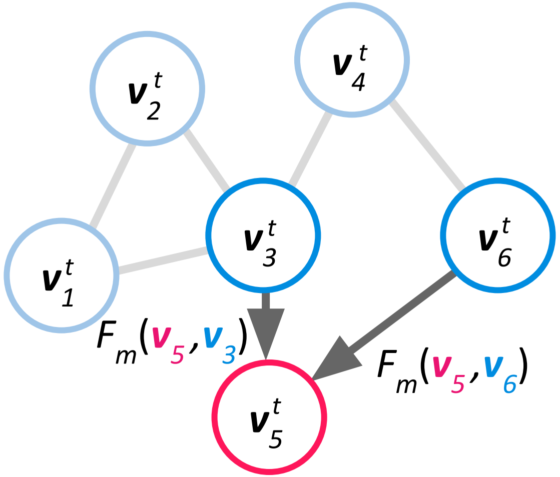

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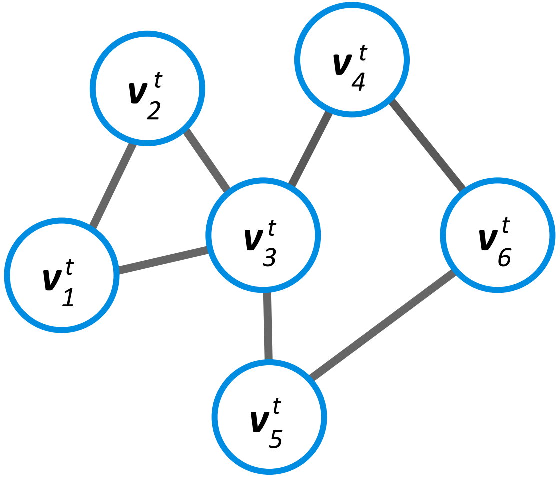
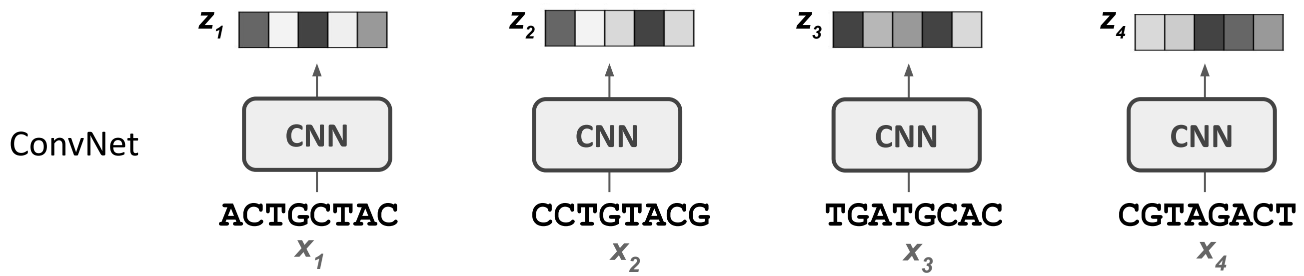
Graph Neural Networks (GNNs)



Graph neural networks are good at modeling ***interactions.***

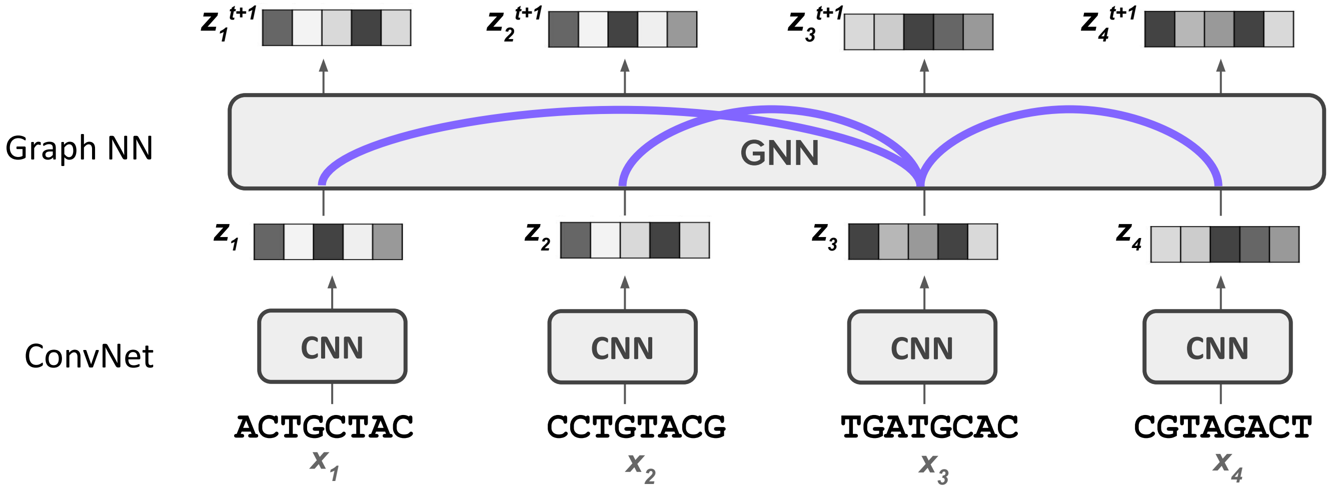
ChromeGCN: Combining Local Sequence and Long Range Interactions for Chromatin Profile Prediction

ChromeGCN



z_1
z_2
z_3
z_4
ConvNet
CNN
CNN
CNN
CNN
ACTGCTAC
CCTGTACG
TGATGCAC
CGTAGACT
x_1
x_2
x_3
x_4

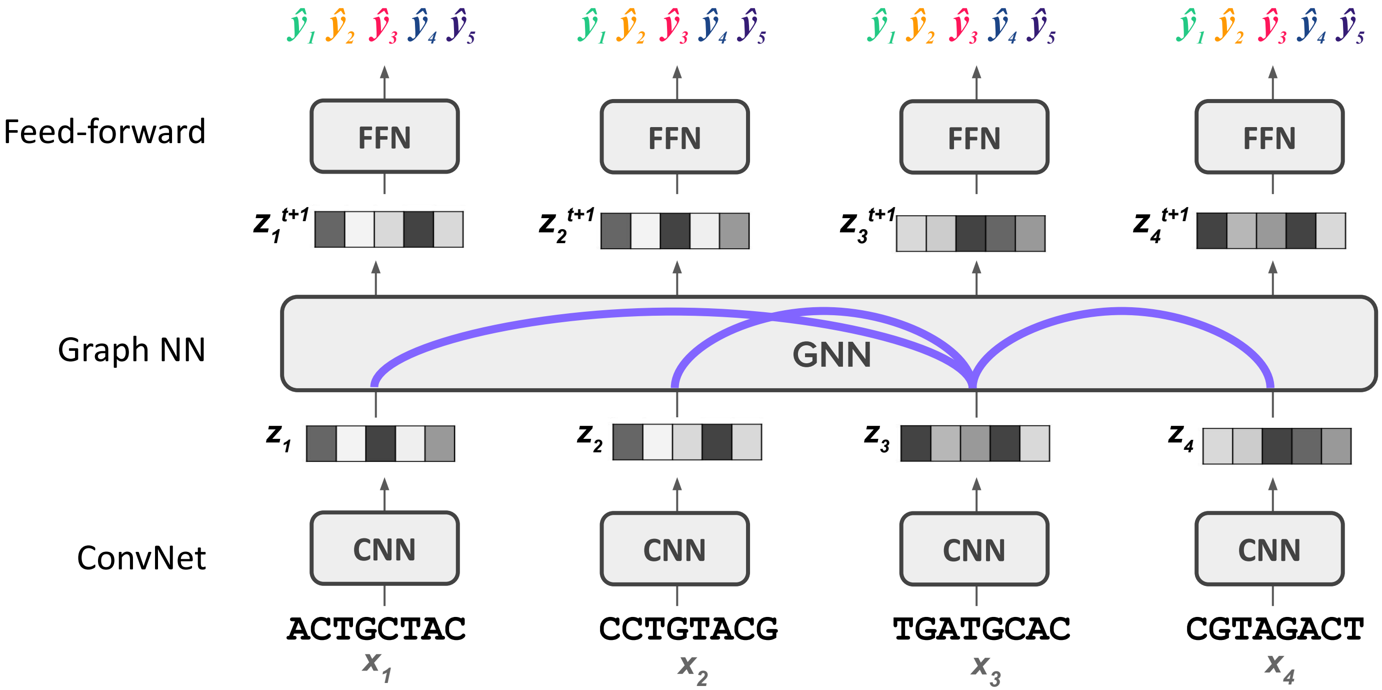
ChromeGCN



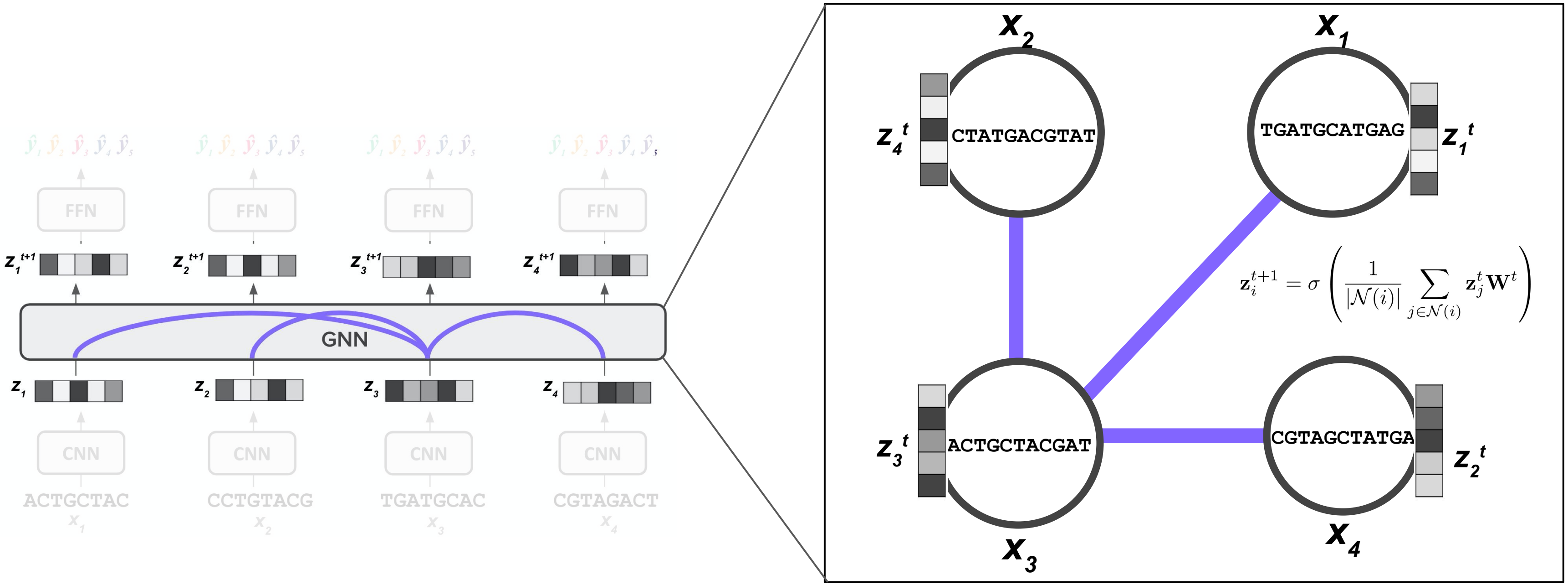
z_1^{t+1}
z_2^{t+1}
z_3^{t+1}
z_4^{t+1}
Graph NN
GNN
z_1
z_2
z_3
z_4
ConvNet
CNN
CNN
CNN
CNN
ACTGCTAC
CCTGTACG
TGATGCAC
CGTAGACT
x_1
x_2
x_3
x_4

ChromeGCN

$$\mathcal{L} = \frac{1}{L}\sum_{i=1}^{L} -(y_i \log(\hat{y}_i) + (1-y_i)\log(1-\hat{y}_i))$$



ChromeGCN

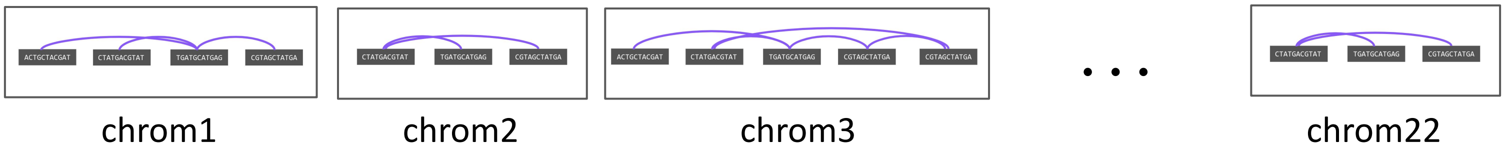


FFN
GNN
CNN
ACTGCTAC
CCTGTACG
TGATGCAC
CGTAGACT
CTATGACGTAT
TGATGCATGAG
ACTGCTACGAT
CGTAGCTATGA
$$\mathbf{z}_i^{t+1} = \sigma\left(\frac{1}{|\mathcal{N}(i)|}\sum_{j\in\mathcal{N}(i)} \mathbf{z}_j^t \mathbf{W}^t\right)$$

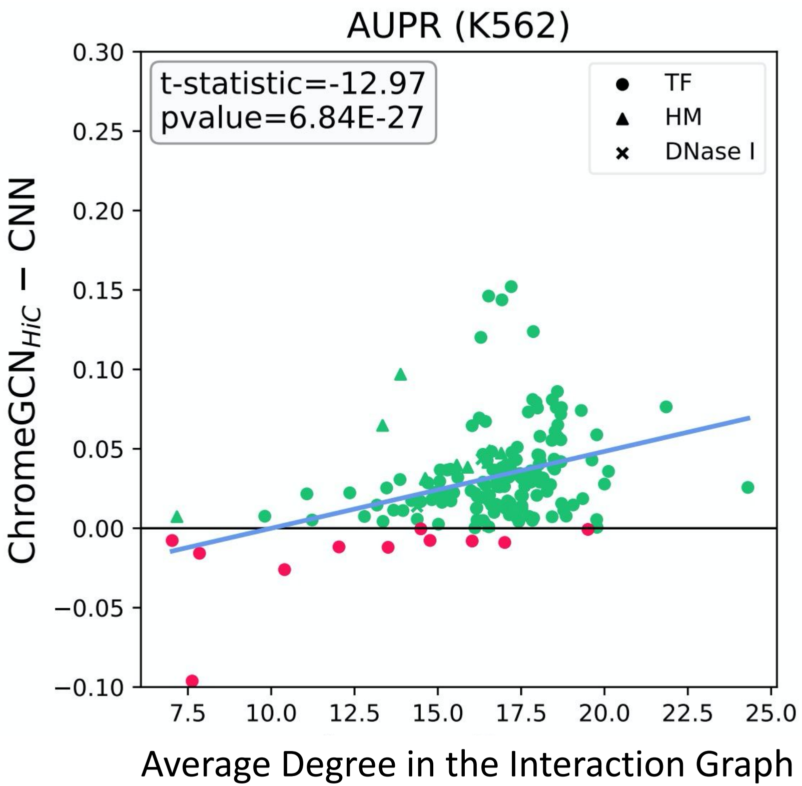
Chromatin Profile Prediction: Experimental Setup

Chromatin profile labels and interaction graph data: transcription factor, histone modification, DNA accessibility, Hi-C, for two cell lines (GM12878, K562)

Data splits: 16 training chromosomes, 3 validation, 3 testing



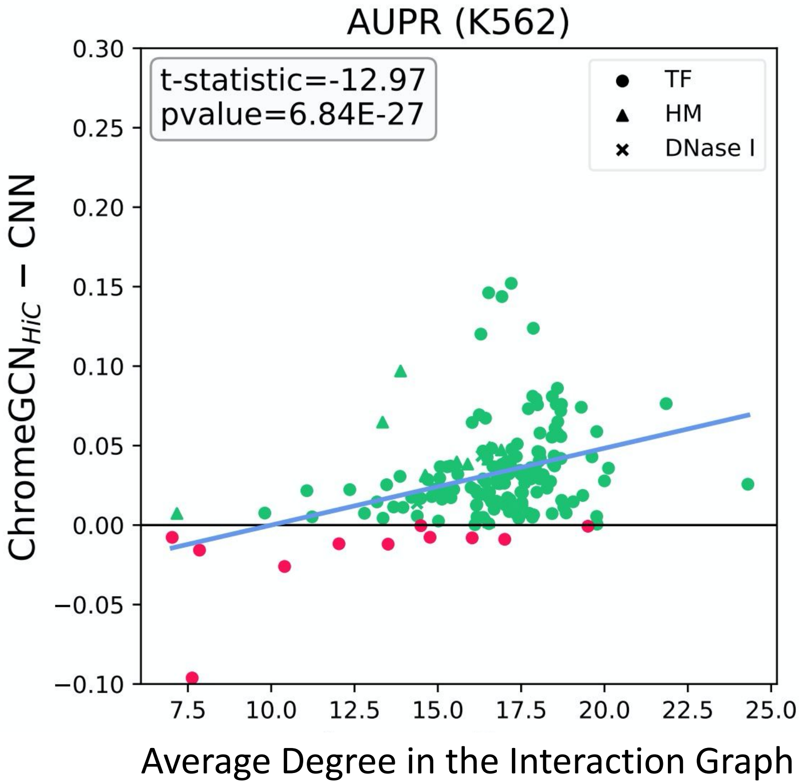
Chromatin Profile Prediction: Results



ChromeGCN is better

CNN is better

Chromatin Profile Prediction: Results



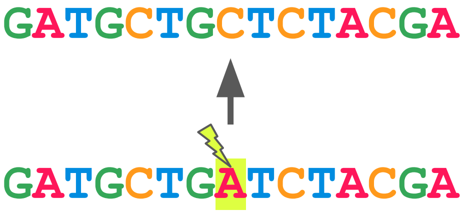
modeling long range interactions is important for signals with many interactions (high degree)

ChromeGCN is better

CNN is better

Implications of Predictive Genomic Sequence Models

1. Mutation Analysis



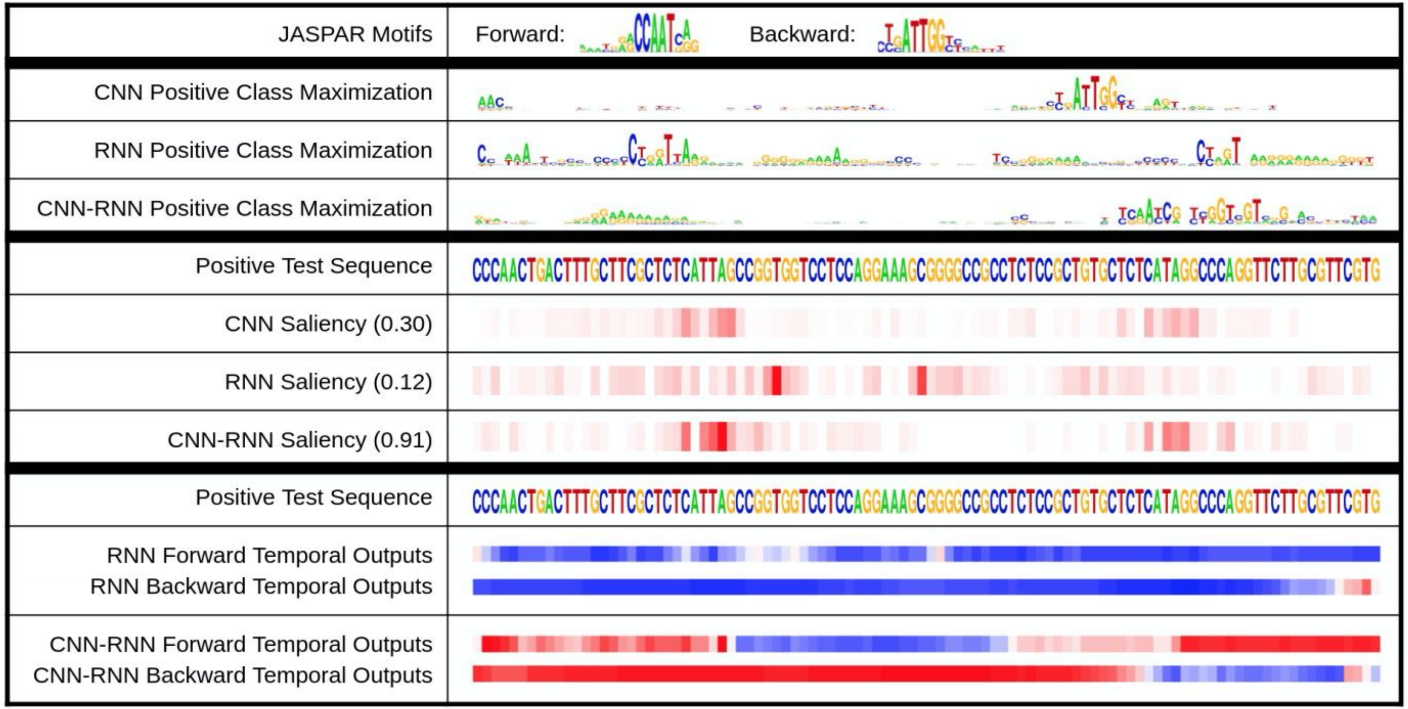
2. Feature Attribution

Implications of Predictive Genomic Sequence Models

1. Mutation Analysis

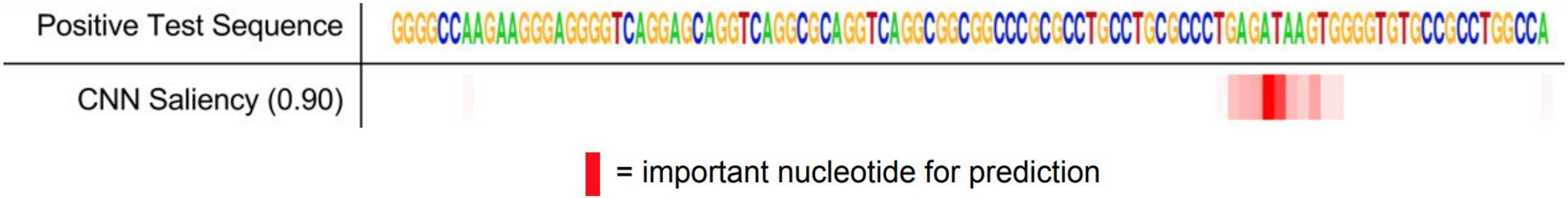
2. Feature Attribution

Deep Motif Dashboard: Visualizing Genomic Sequence Syntax



Lanchantin, Singh, Lin, Wang, Qi. ICLR Workshop Track 2016, PSB 2017

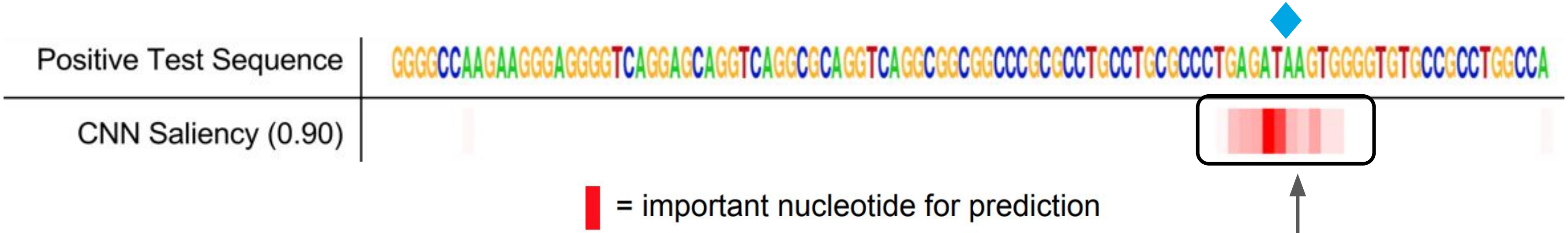
Sequence saliency maps: finding important sequence features



$$\hat{y}_+(X) \approx w^T X + b = \sum_{i=1}^{|X|} w_i x_i$$

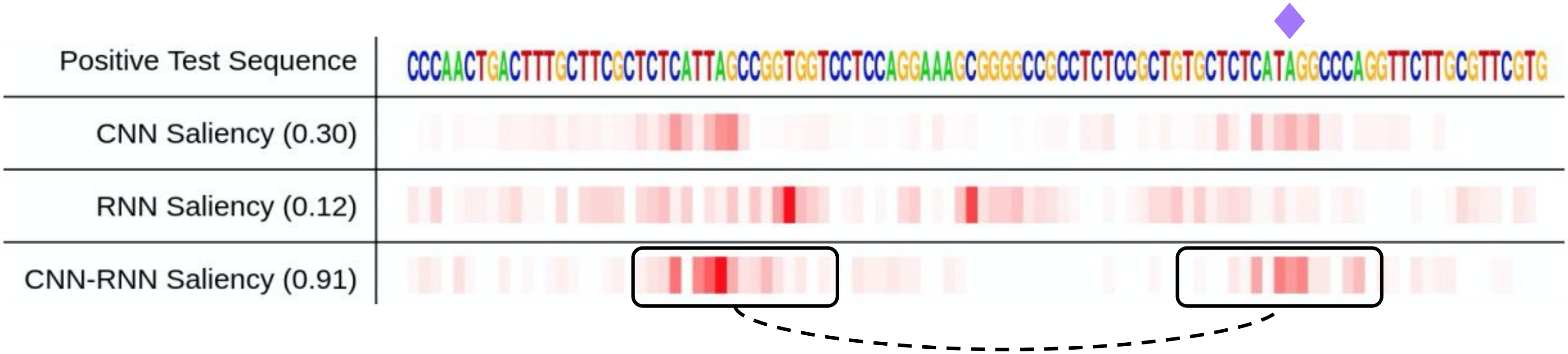
$$w = \left.\frac{\partial \hat{y}_+}{\partial X}\right|_{X_0}$$ = "sequence saliency map"

Sequence saliency maps: finding important sequence features



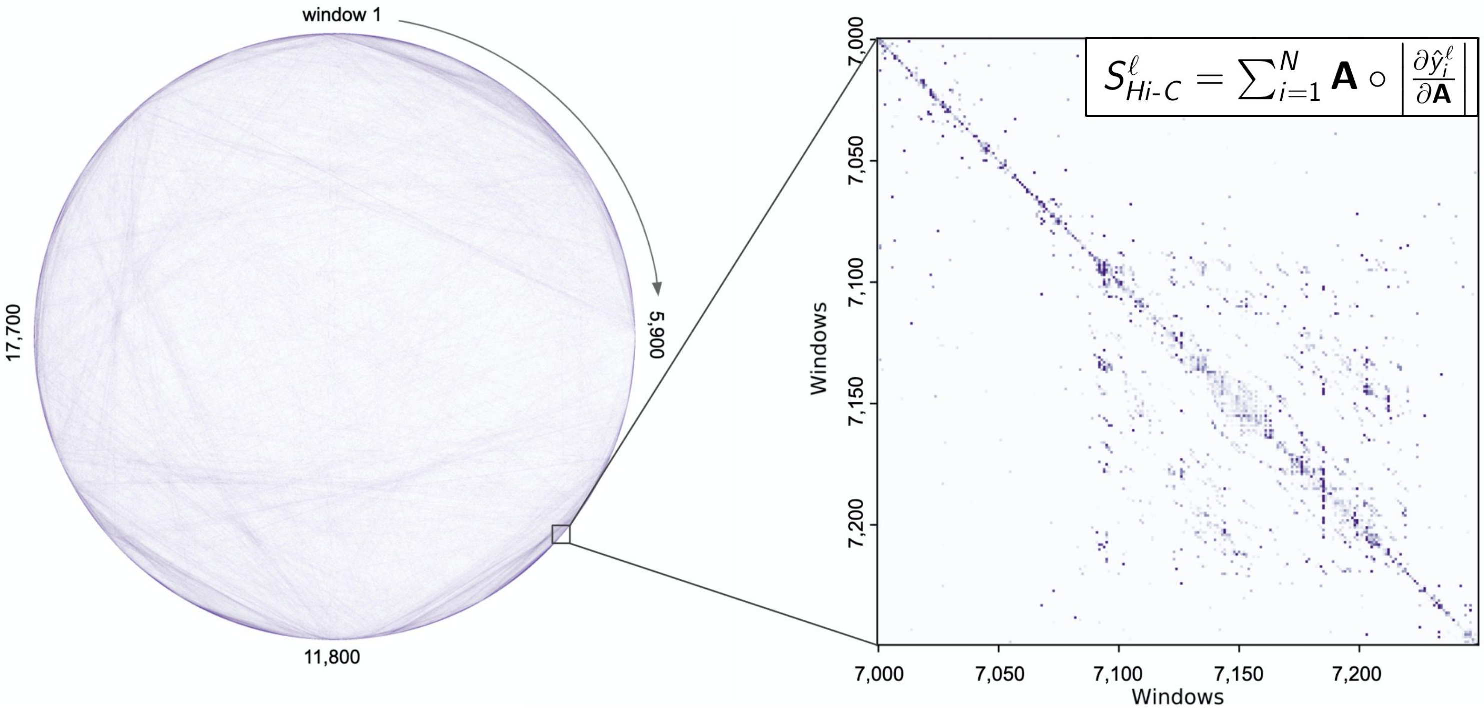
DNA sequence "motifs":
short local patterns

Sequence saliency maps: finding important sequence features



Local motif interactions are important!

Hi-C saliency maps: identifying important long range interactions



YY1 Hi-C saliency map for all 500k edges in Hi-C graph

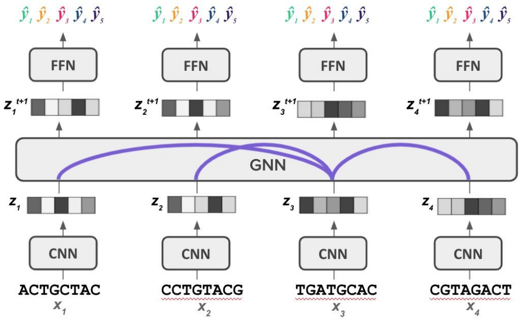
■ = important interaction for prediction

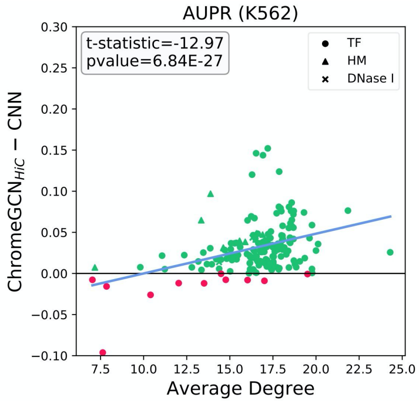
Contributions

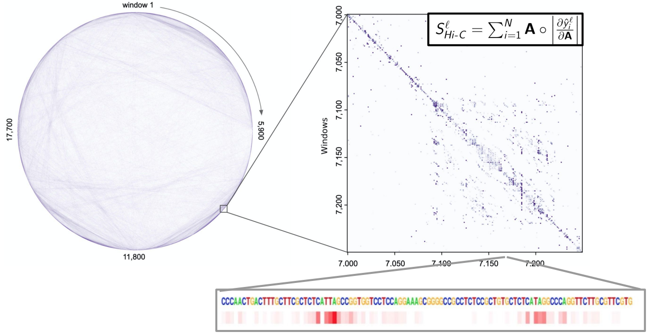
1. Cohesive framework: we **fuse local sequence features and long range interactions** for chromatin profile prediction

2. Accurate: incorporating **long range interactions outperforms** the baselines

3. Interpretable: we introduce **deep motif dashboard** to interpret local features and **Hi-C saliency maps** to find important interactions







Graph neural network models can effectively exploit and discover important interactions in DNA for functional genomics

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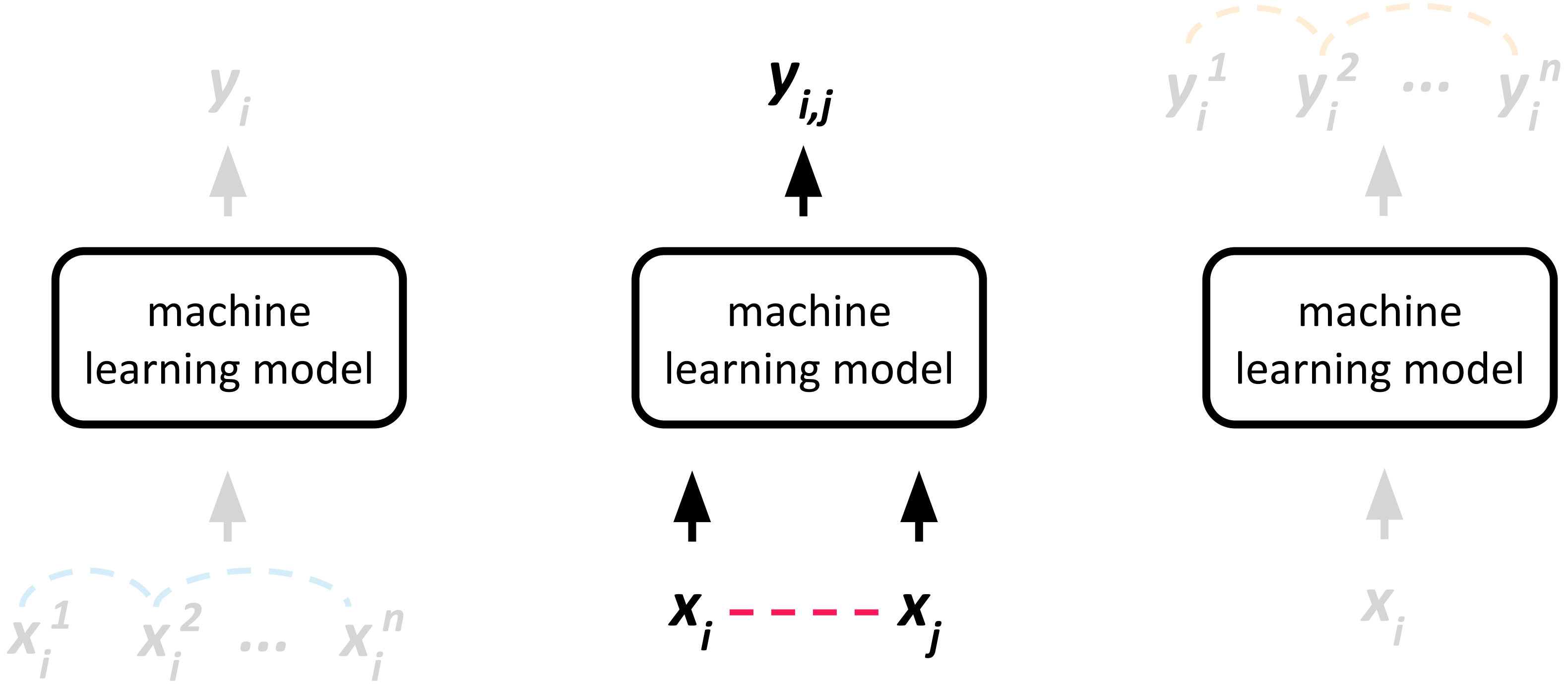
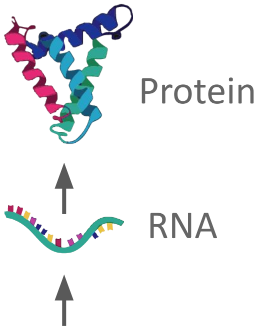
Modeling Host-Virus Protein-Protein Interactions with DeepVHPPI

interactions between **input features**

interactions between **input samples**

interactions between **output labels**

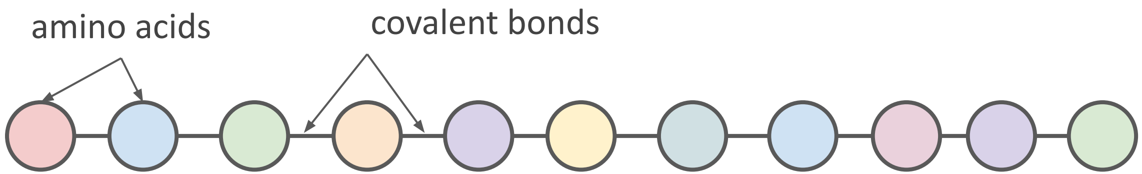




ATGCTCGATGCTAATACGACTGAGATTACTGAGACTGAGACTCTAGAT

Gene

What is a protein?



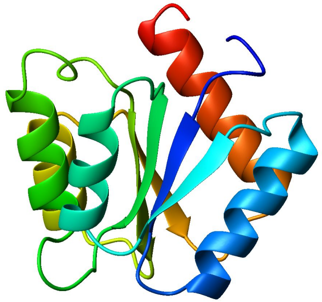
sequences with alphabet of 20 characters

What is a protein?

MQGHFTETKHE

sequences with alphabet of 20 characters

What is a protein?



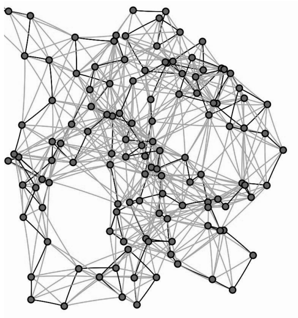
3D Structure

↑

MHFTEDKATILWGKVNVEGETLGRVYPWQ

Primary Sequence

What is a protein?



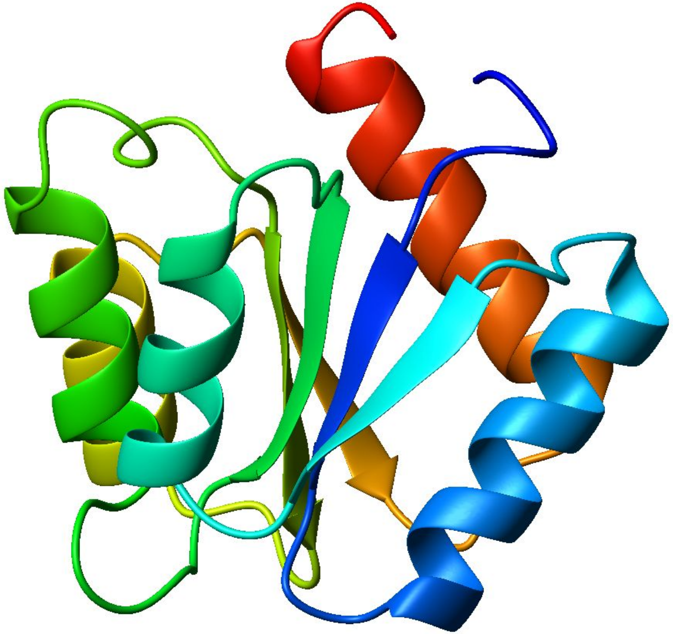
3D Structure

↑

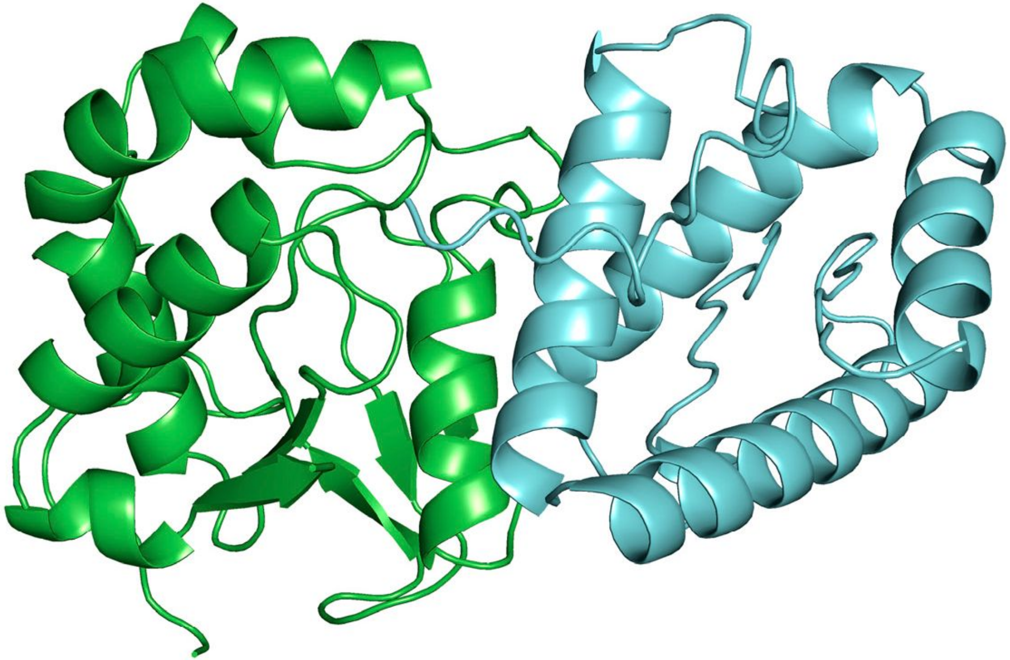
MHFTEDKATILWGKVNVEGETLGRVYPWQ

Primary Sequence

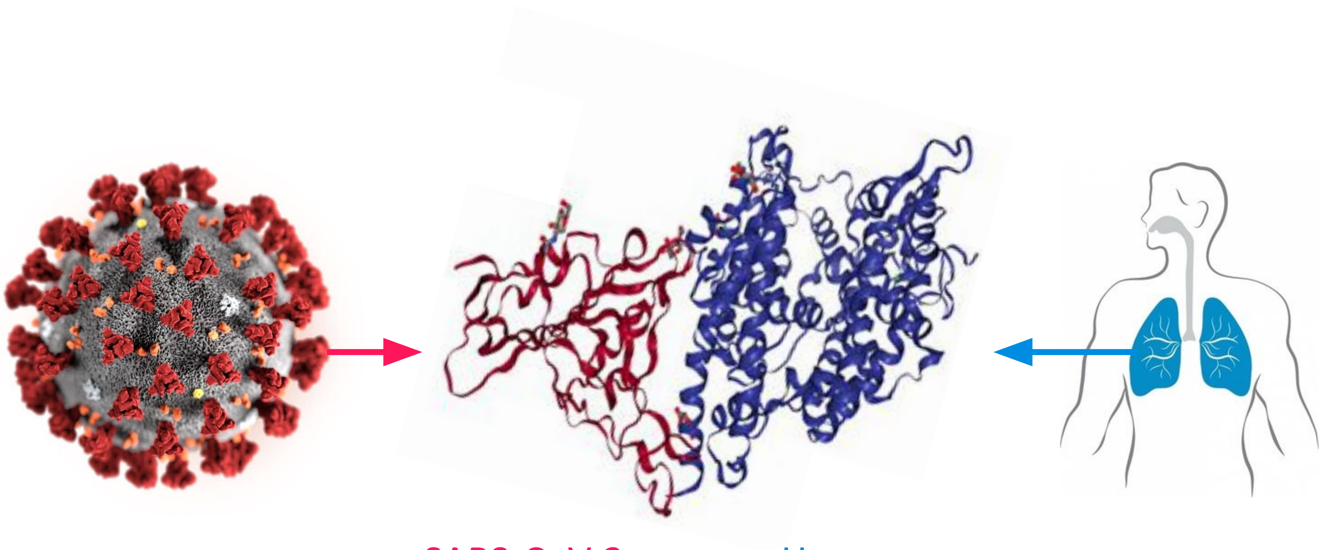
Structure Determines Function



Protein-Protein Interactions (PPIs)



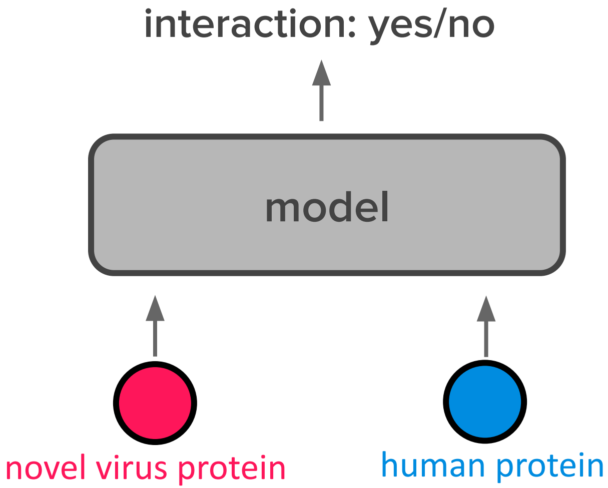
Virus-Host Protein-Protein Interactions



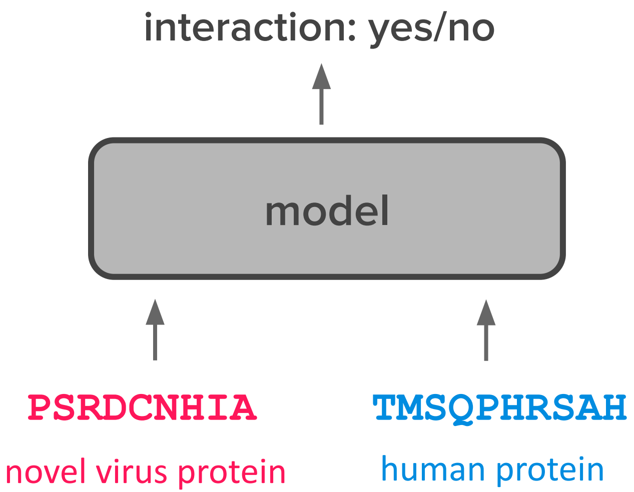
SARS-CoV-2
Spike Protein

Human
ACE2 Protein

Novel Virus-Human Protein Interaction Prediction from Sequence

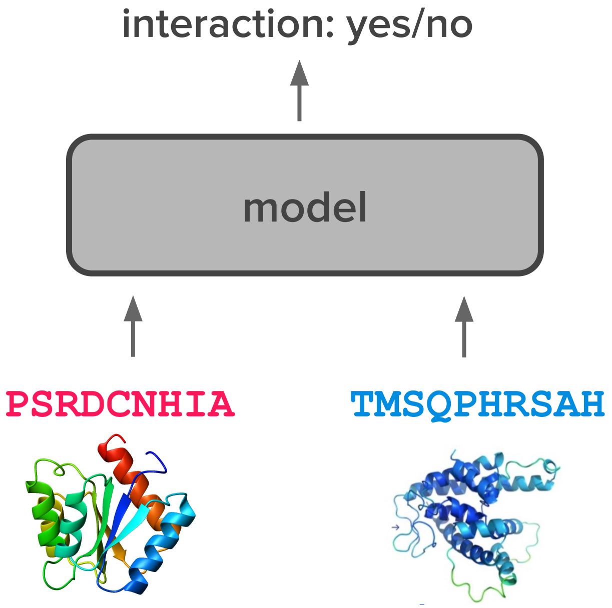


Novel Virus-Human Protein Interaction Prediction from Sequence



Gomez et al. 2003, Ben-Hur and Noble 2005, Qi et al. 2010, Eid et al. 2015, Yang et al. 2020

Novel Virus-Human Protein Interaction Prediction from Sequence

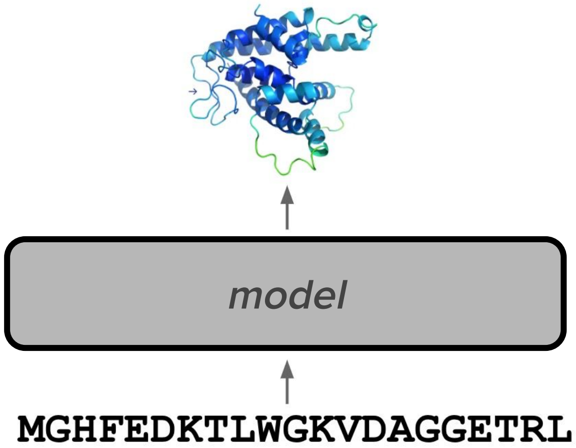


structure (3D shape) is important, but hard to obtain

Research Question 2

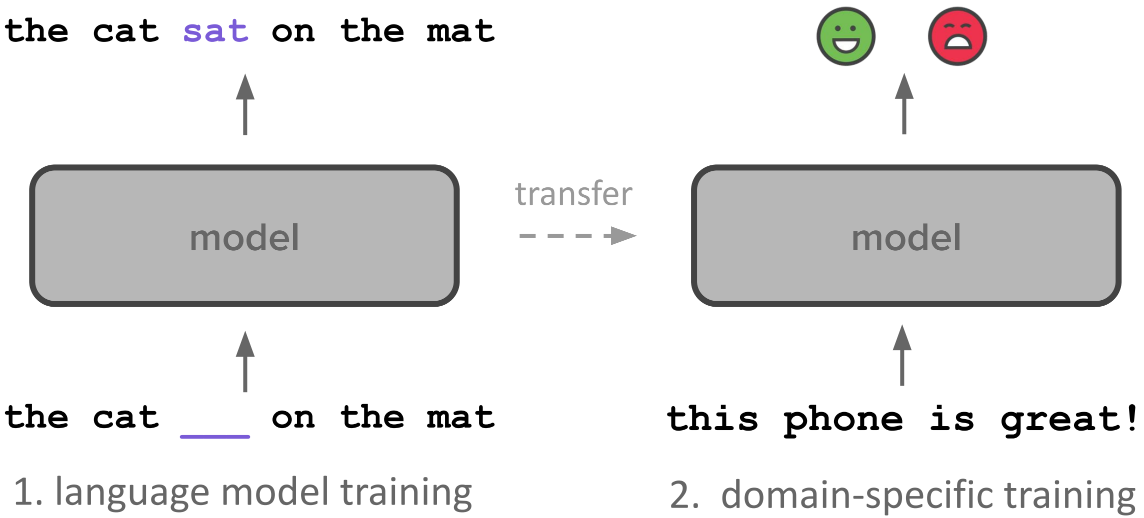
Can we incorporate individual protein structure into a sequence based protein-protein interaction prediction model?

Structure Prediction from Sequence



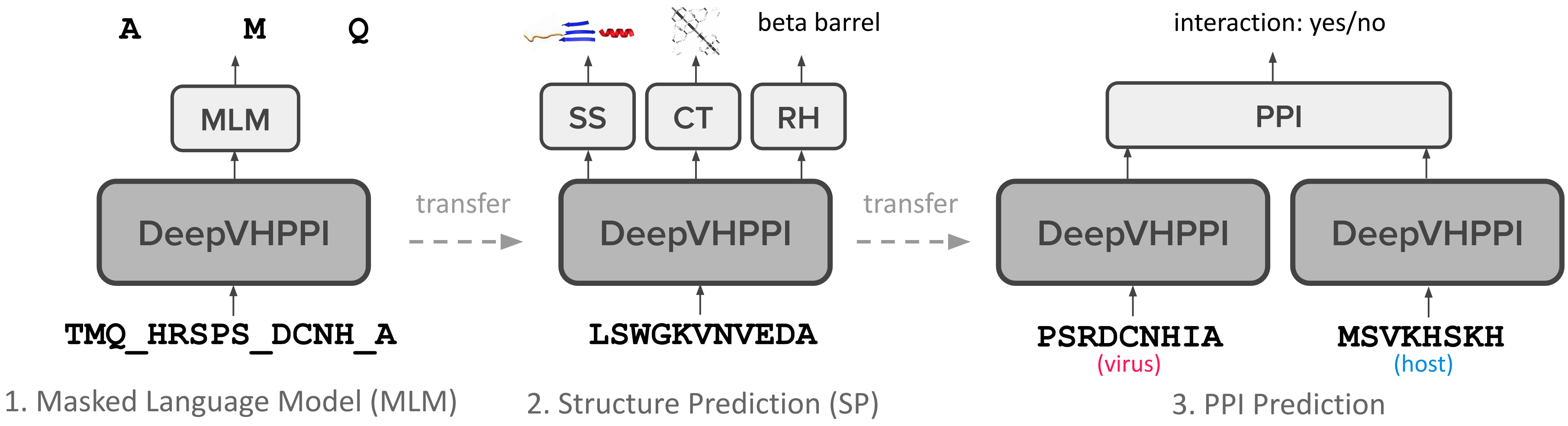
*Lin, **Lanchantin**, Qi 2016, Rives et al. 2019, Rao et al. 2020, Jumper et al. 2020*

Transfer Learning

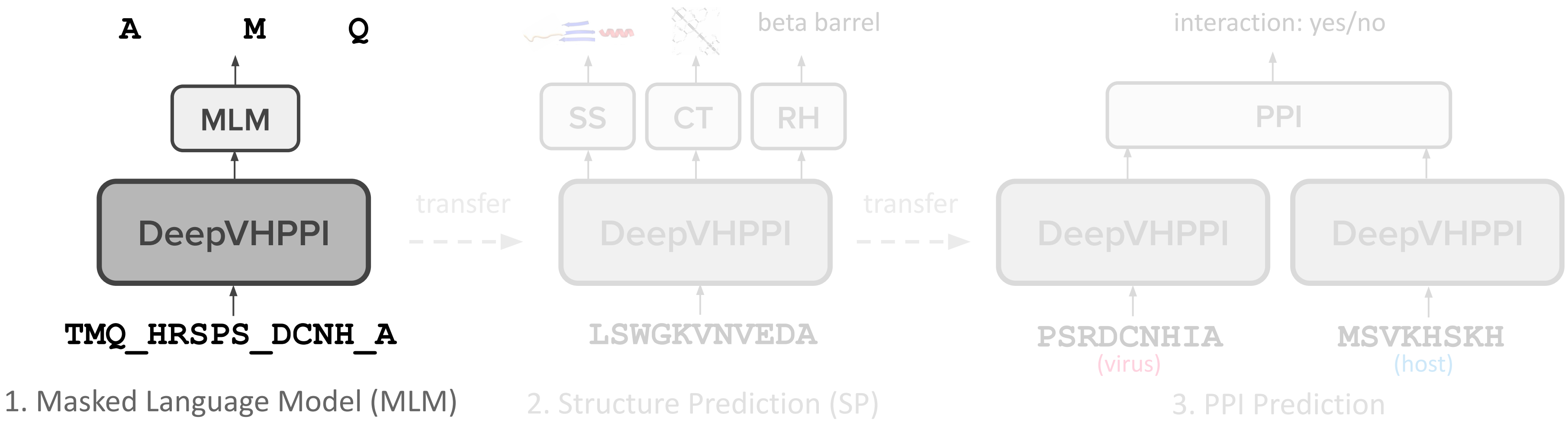


Glorot et al. 2011, Devlin et al. 2018

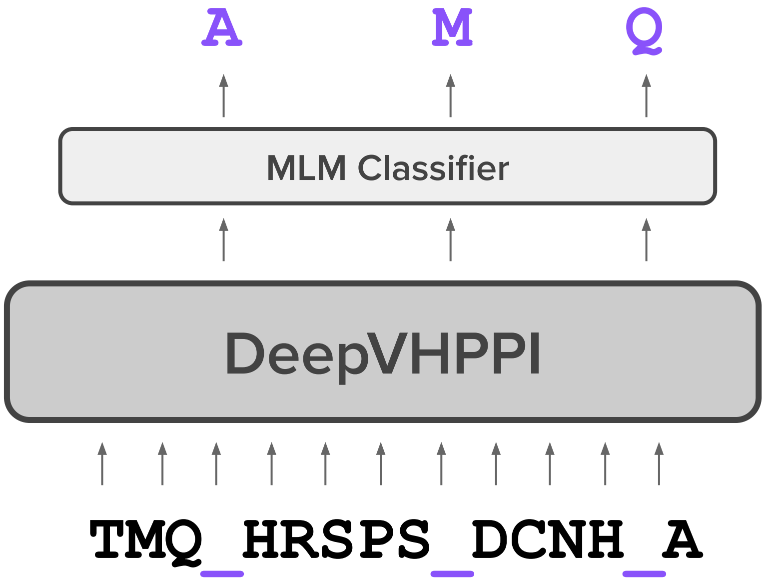
Transfer Learning for Sequence-Based Interaction Prediction



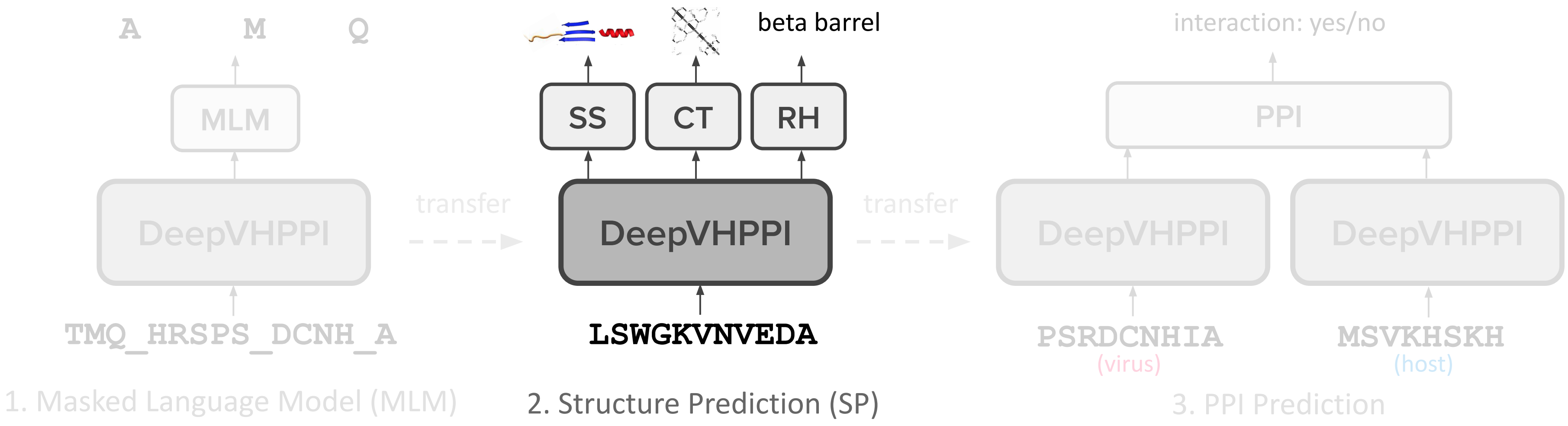
Transfer Learning for Sequence-Based Interaction Prediction



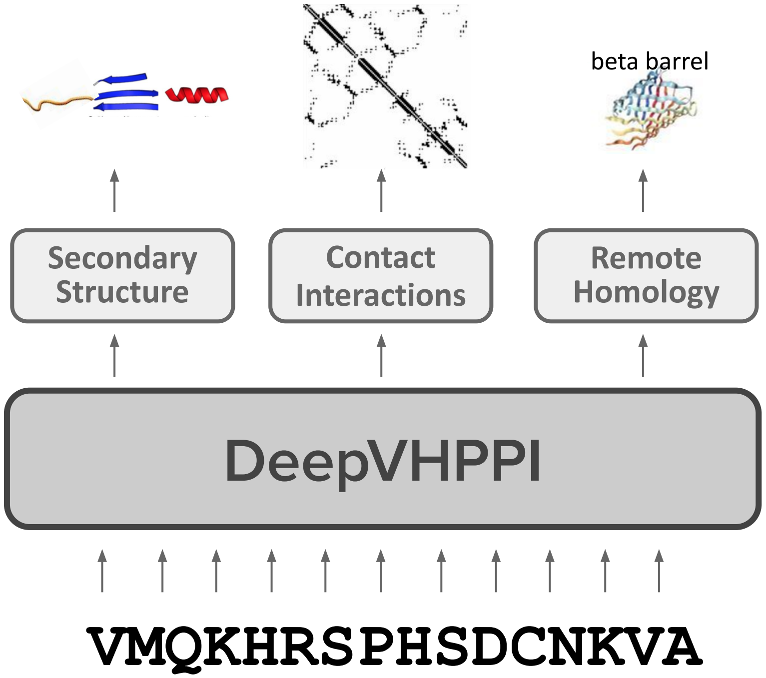
Masked Language Model (MLM) Pretraining



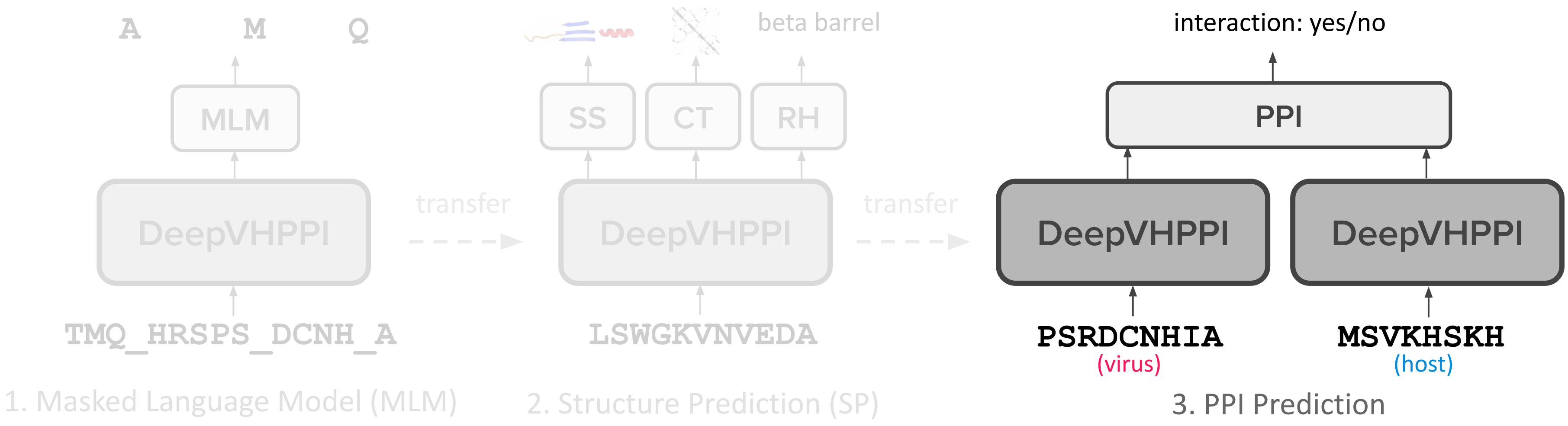
Transfer Learning for Sequence-Based Interaction Prediction



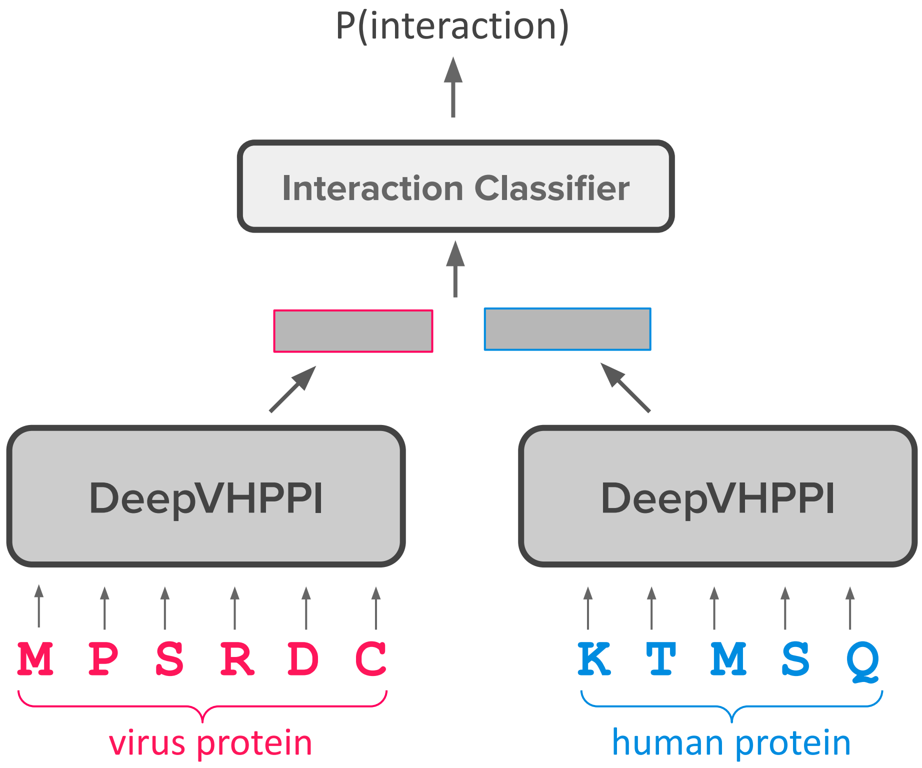
Structure Prediction (SP) Pretraining



Transfer Learning for Sequence-Based Interaction Prediction

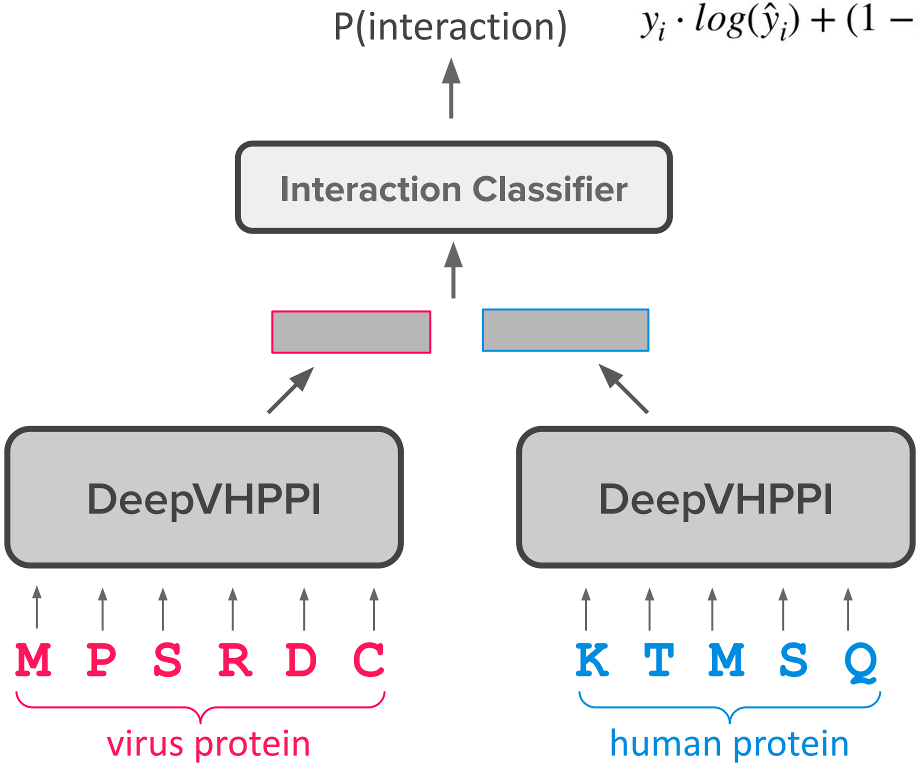


Interaction Prediction

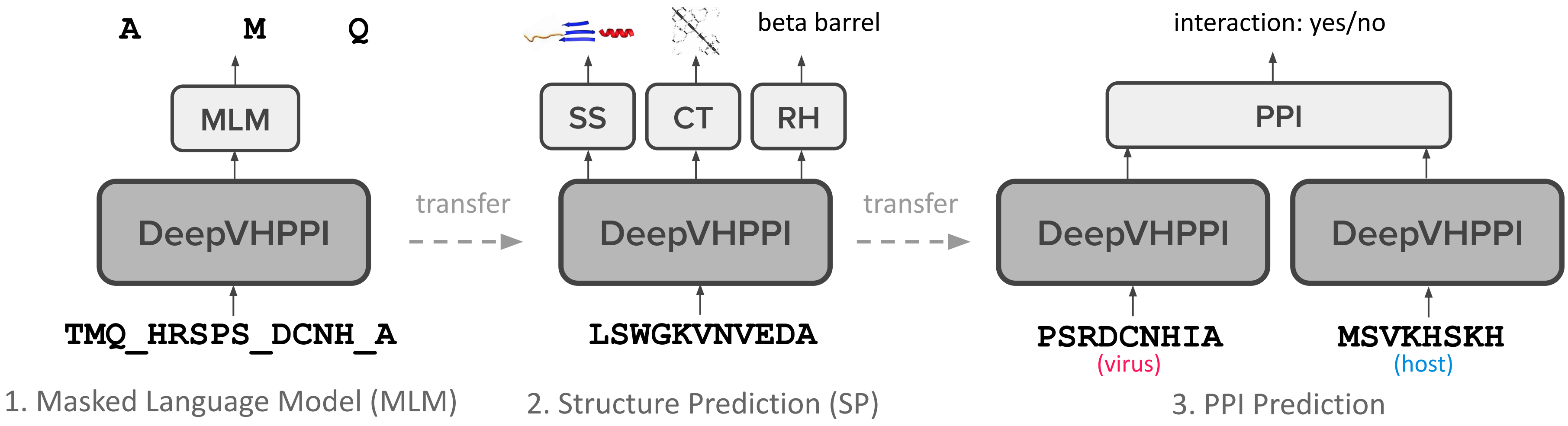


Interaction Prediction

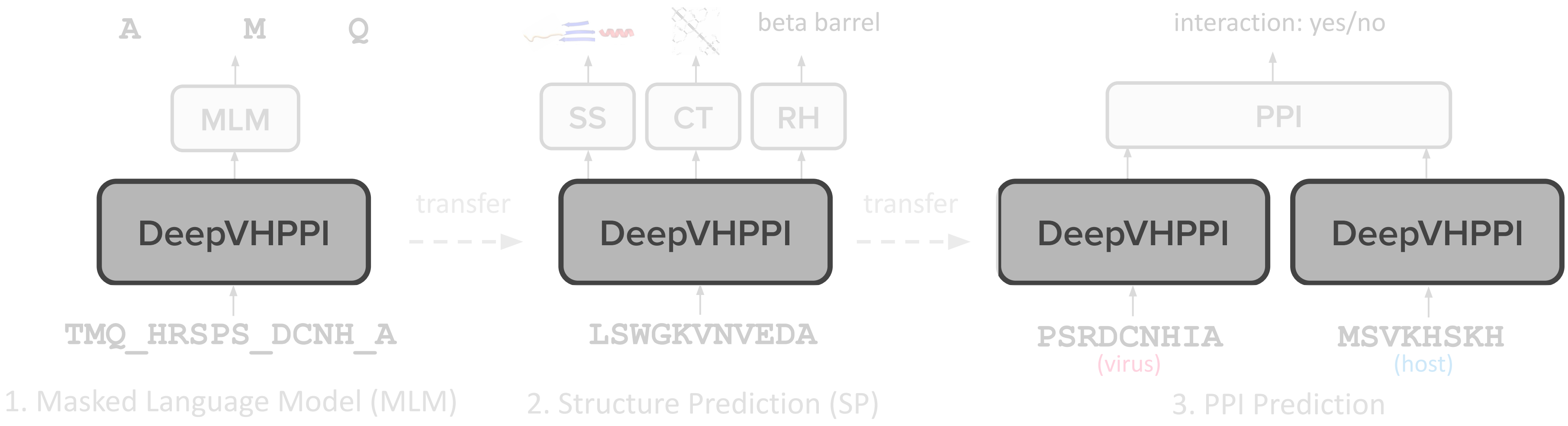
$$y_i \cdot log(\hat{y}_i) + (1 - y_i) \cdot log(1 - \hat{y}_i)$$



Transfer Learning for Sequence-Based Interaction Prediction

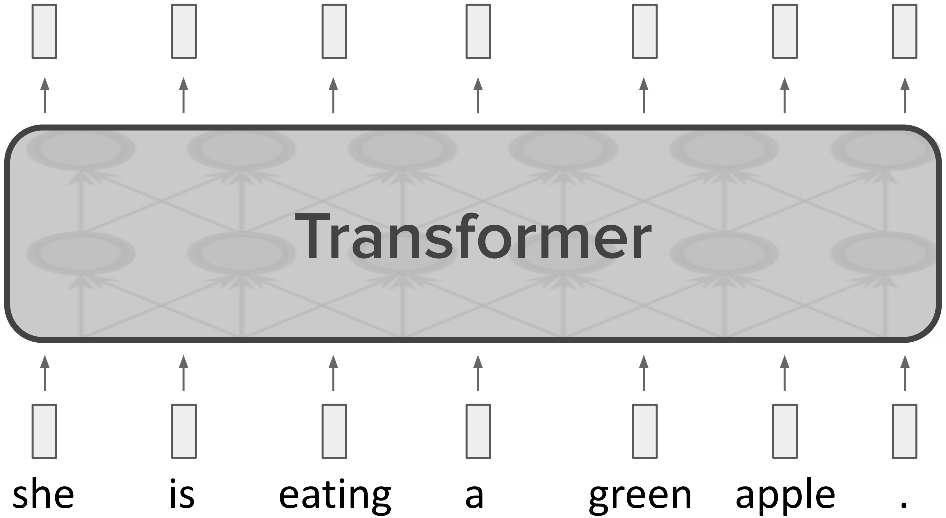


Transfer Learning for Sequence-Based Interaction Prediction



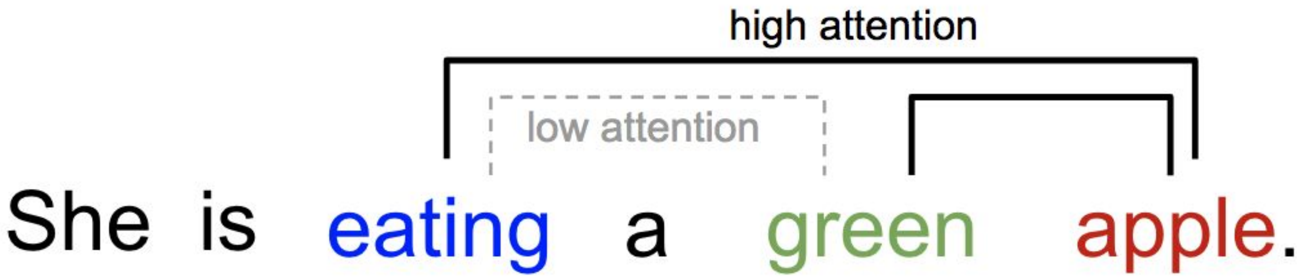
Transformers

Word relationships are learned via neural attention



Vaswani et al. 2017, Devlin et al. 2018

Neural Attention



Attention coefficient e_{ij}^t for pair of nodes $(\boldsymbol{v}_i^t, \boldsymbol{v}_j^t)$

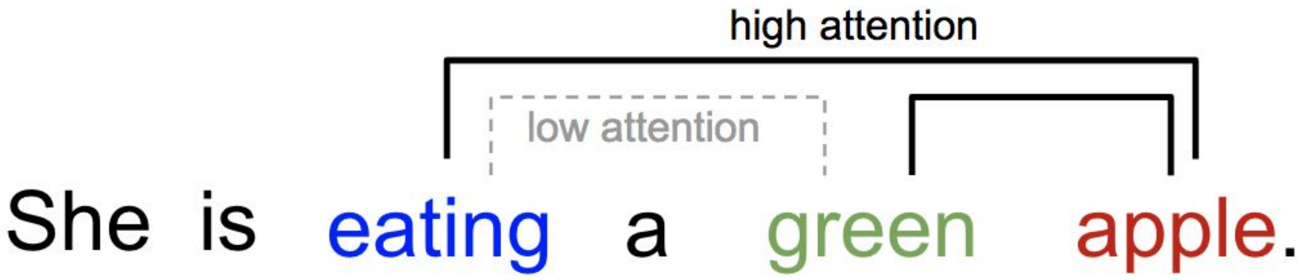
$$e_{ij}^t = (\mathbf{W}^q \boldsymbol{v}_i^t)^\top (\mathbf{W}^u \boldsymbol{v}_j^t)$$

Attention weight α_{ij}^t produced by normalizing over neighboring nodes

$$\alpha_{ij}^t = \mathrm{softmax}_j(e_{ij}^t) = \frac{\exp(e_{ij}^t)}{\sum_{k \in \mathcal{N}(i)} \exp(e_{ik}^t)}.$$

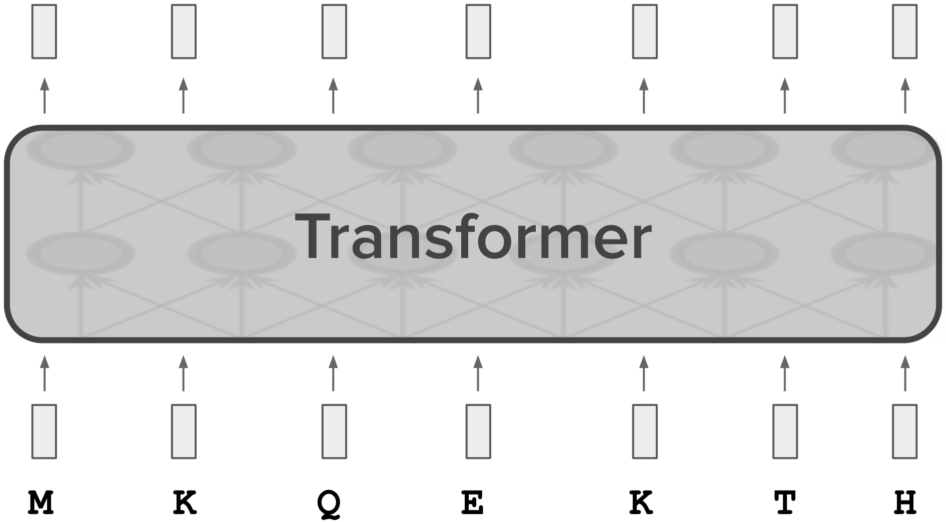
Bahdanau et al. 2013, Vaswani et al. 2017

Neural Attention

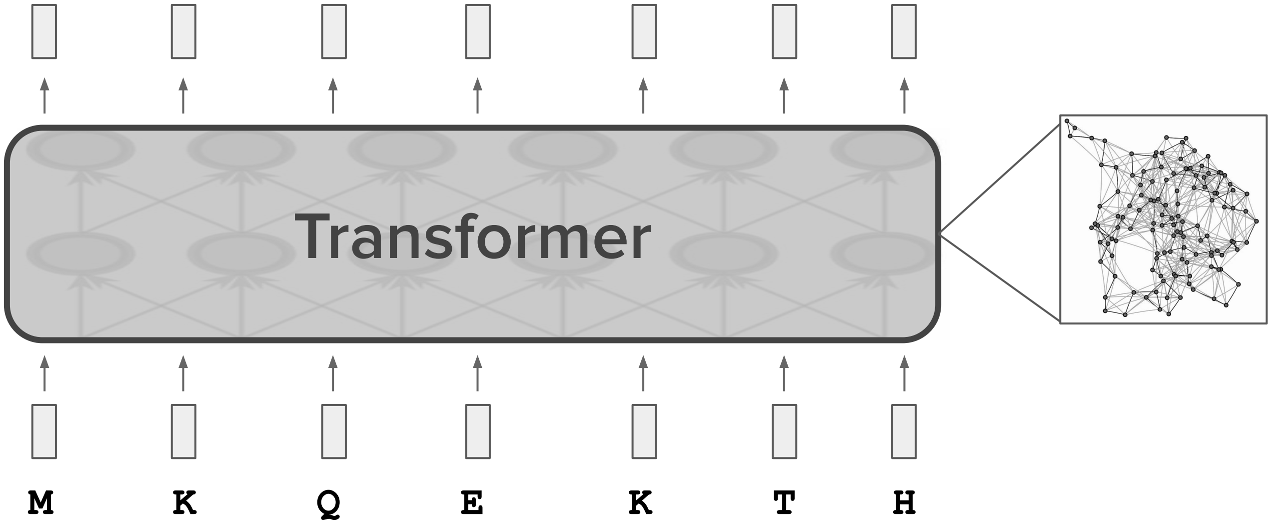


Attention allows us to learns interaction importance when it is not known or predefined

Transformers for Protein Sequences

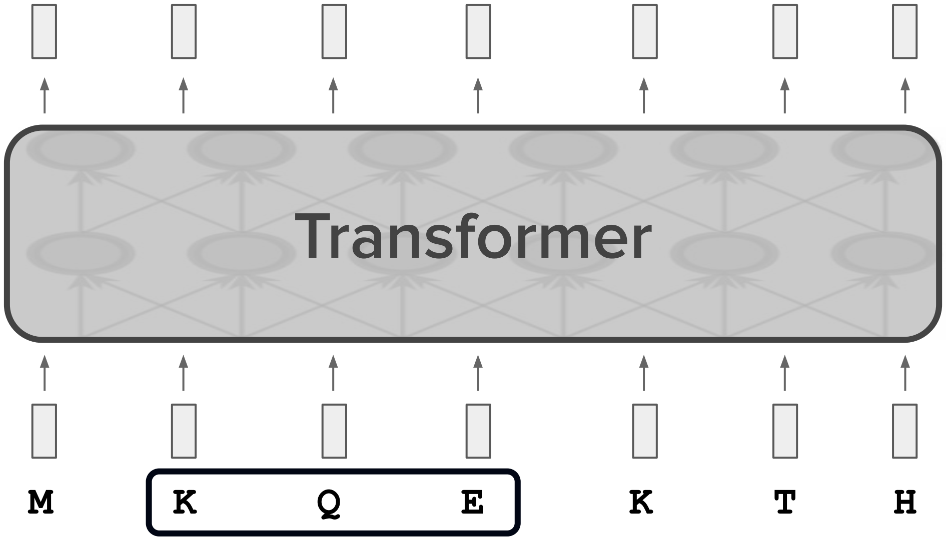


Transformers for Protein Sequences



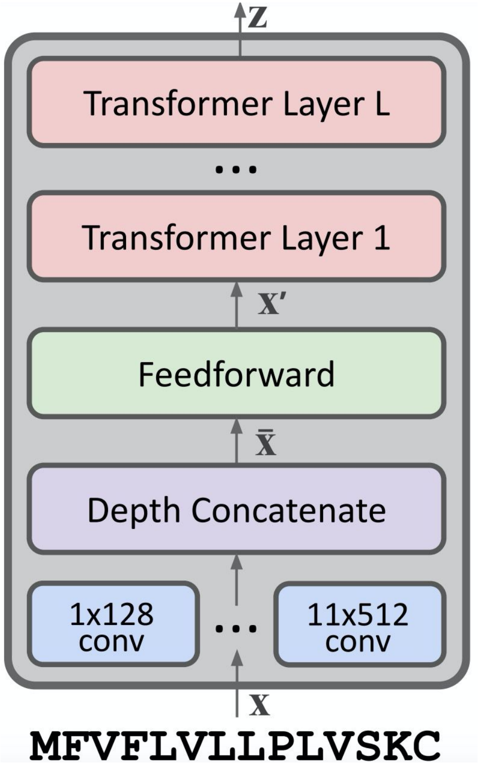
Rives et al. 2019, Rao et al. 2020

Transformers for Protein Sequences

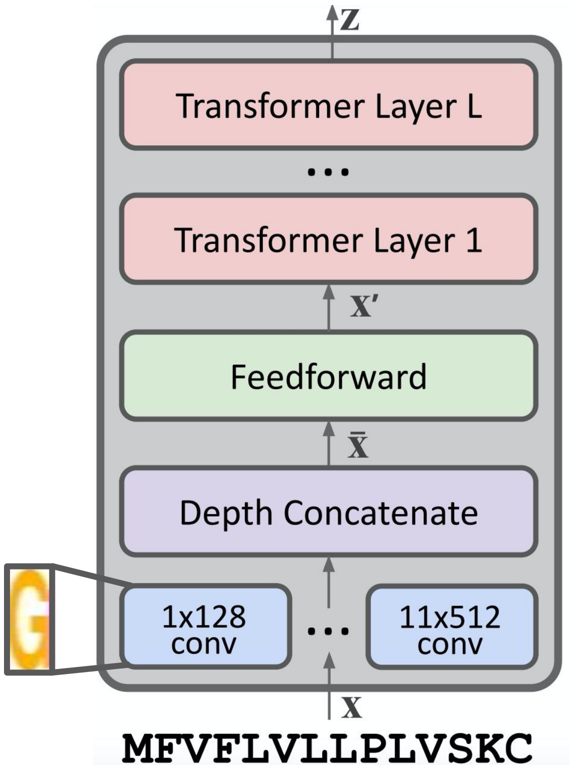


protein motifs (i.e. “words”) influence protein-protein interactions

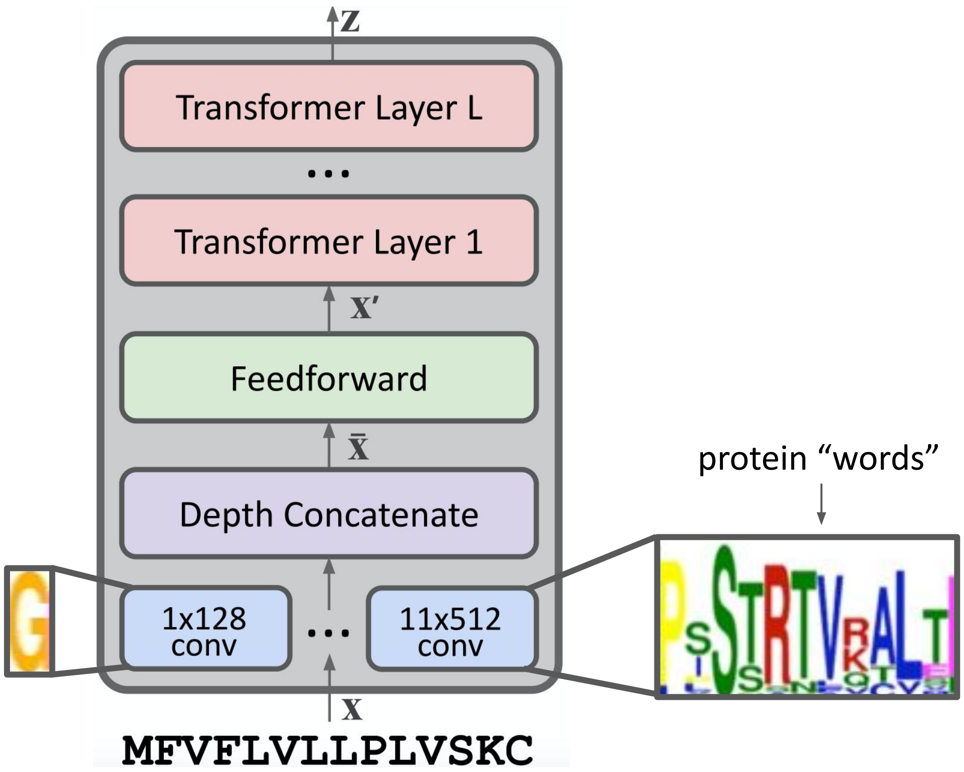
DeepVHPPI Transformer



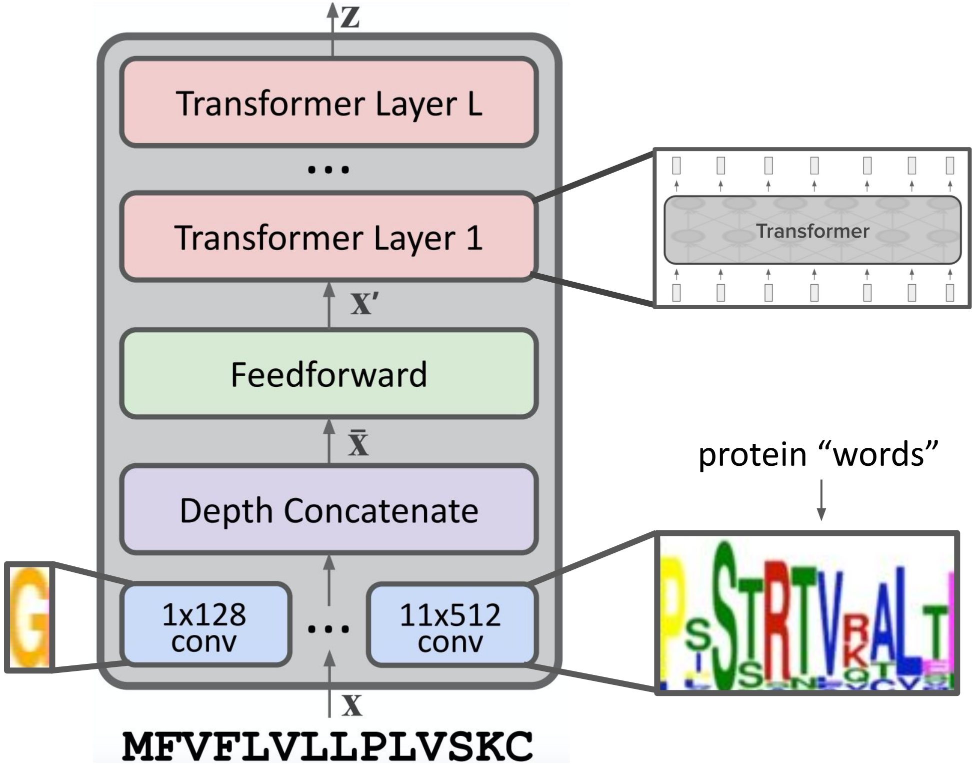
DeepVHPPI Transformer



DeepVHPPI Transformer

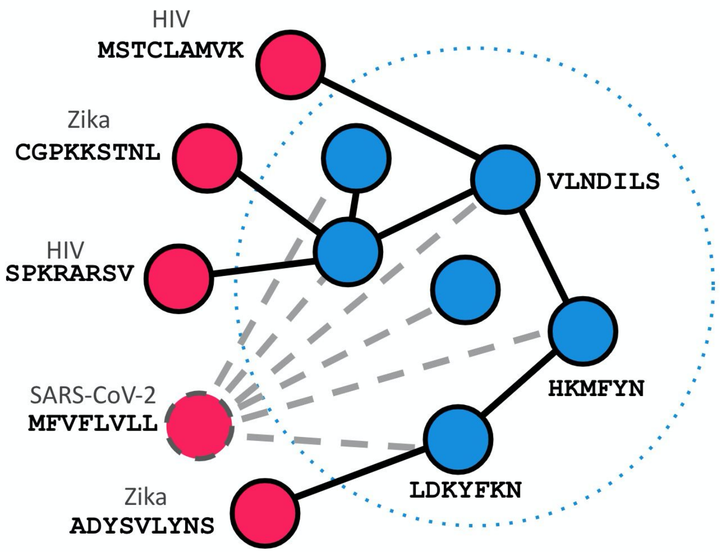


DeepVHPPI Transformer

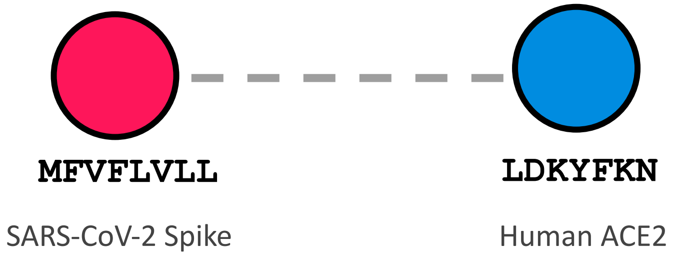


Use Cases of Sequence Based Interaction Predictors

1. predict novel virus interactions



2. analyze how mutations affect interactions



Use Cases of Sequence Based Interaction Predictors

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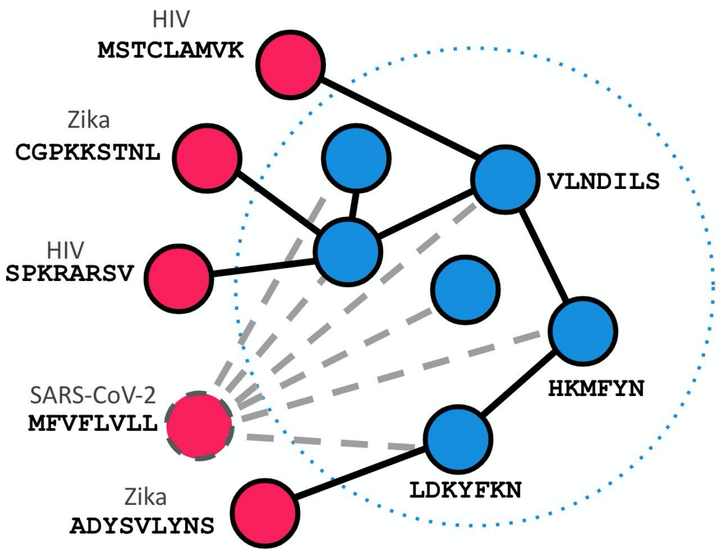


2. analyze how mutations affect interactions

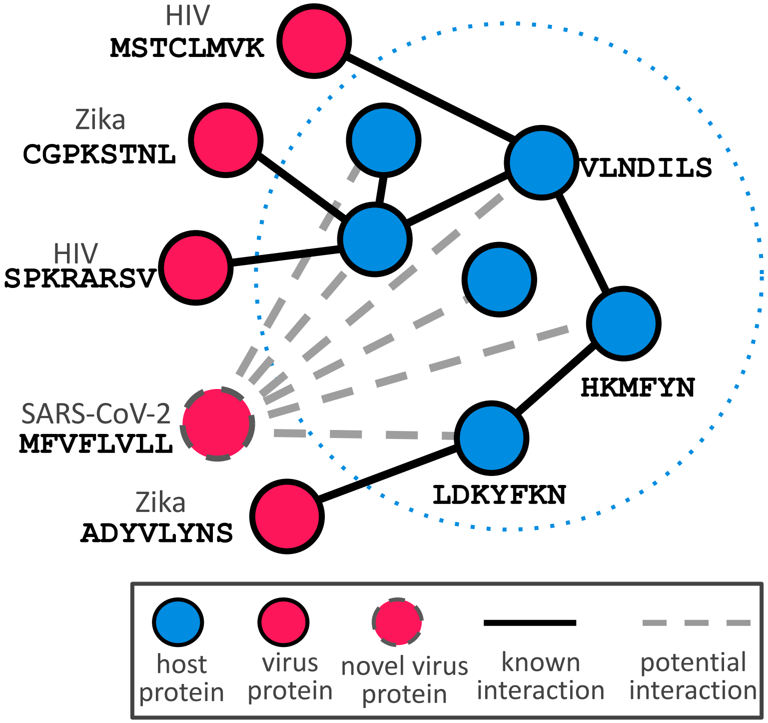
Protein-Protein Interaction Prediction: Experimental Setup

Training Data: HPIDB 3.0 Dataset

- 22,000 positive interactions, 226,000 negative interactions
- 1,100 virus proteins, 20,000 host (human) proteins

Testing Data:

- H1N1, Ebola, SARS-CoV-2 proteins



Protein-Protein Interaction Prediction: Results

	H1N1[1]		Ebola[1]		SARS-CoV-2[2]	
Method	AUROC	F1	AUROC	F1	AUROC	F1
SVM (Zhou et al.)	0.886	0.762	0.867	0.760	-	-
Embedding + RF (Yang et al)	-	-	-	-	0.748	**0.115**
DeepVHPPI	0.906	0.821	0.927	0.836	0.726	0.089
DeepVHPPI + MLM	0.920	0.804	0.943	0.867	0.735	0.095
DeepVHPPI + MLM + SP	**0.957**	**0.867**	**0.976**	**0.895**	**0.767**	0.105

[1]Even positive/negative testing split [2]Imbalanced positive/negative testing split

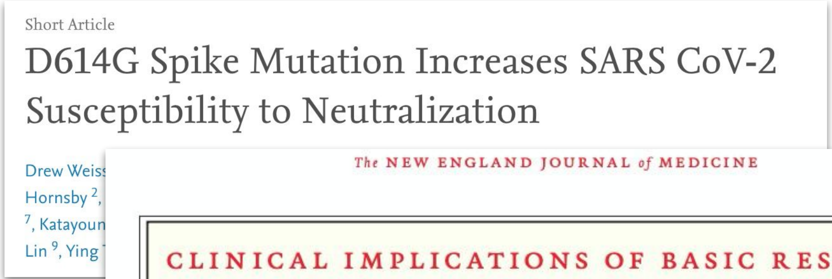
Transformers and transfer learning helps in all three testing datasets

Use Cases of Sequence Based Interaction Predictors

1. predict novel virus interactions

2. analyze how mutations affect interactions

Perturbation Analysis: Investigating Mutations


Short Article

D614G Spike Mutation Increases SARS CoV-2 Susceptibility to Neutralization

Drew Weiss
Hornsby [2],
[7], Katayoun
Lin [9], Ying


The NEW ENGLAND JOURNAL of MEDICINE

CLINICAL IMPLICATIONS OF BASIC RESEARCH

Elizabeth G. Phimister, Ph.D., *Editor*

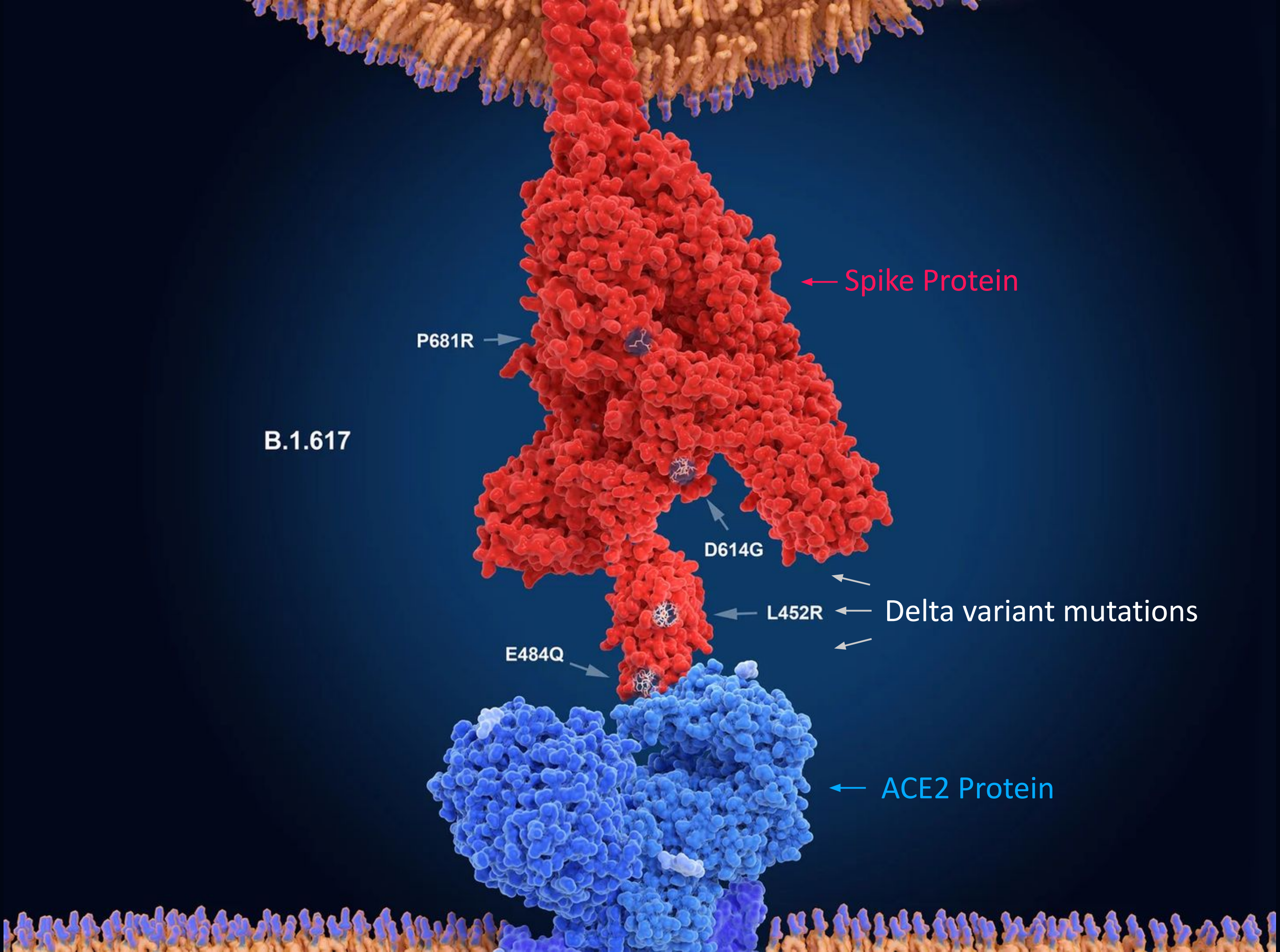
Emergence of a Highly Fit SARS-CoV-2 Variant


nature

https://doi.org/10.1038/s41586-021-03777-9

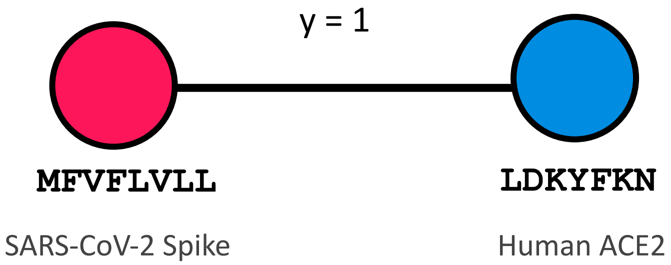
Accelerated Article Preview

Reduced sensitivity of SARS-CoV-2 variant Delta to antibody neutralization

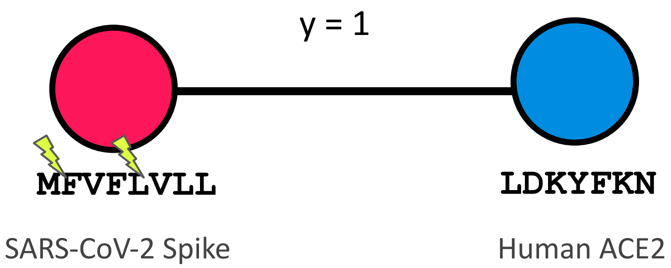


Spike Protein
P681R
B.1.617
D614G
L452R
Delta variant mutations
E484Q
ACE2 Protein
Juan Gaertner

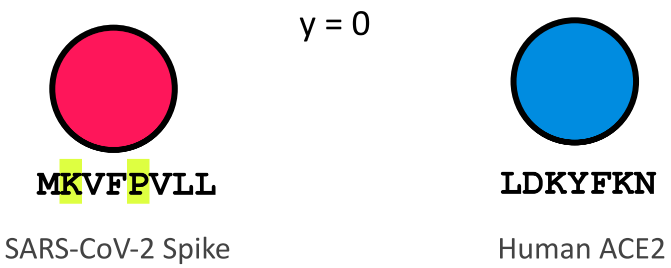
Perturbation Analysis: Investigating Mutations



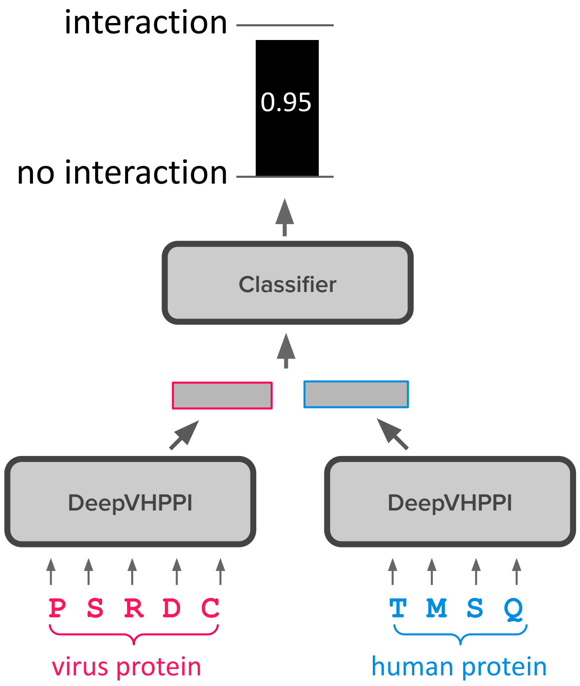
Perturbation Analysis: Investigating Mutations



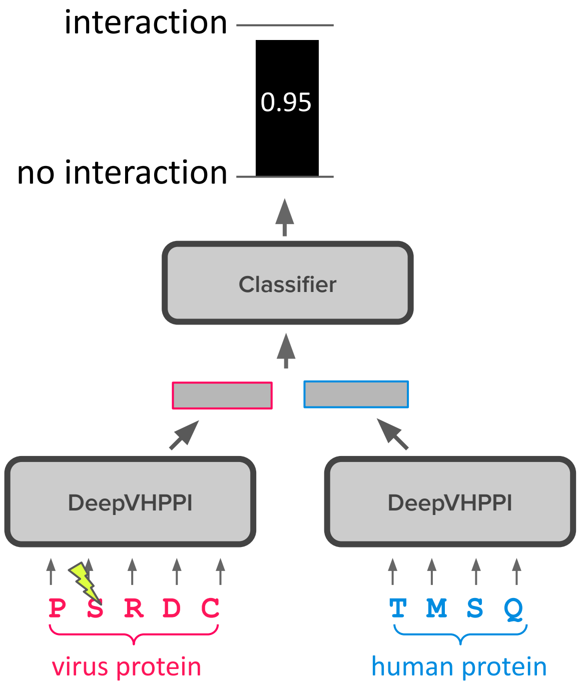
Perturbation Analysis: Investigating Mutations



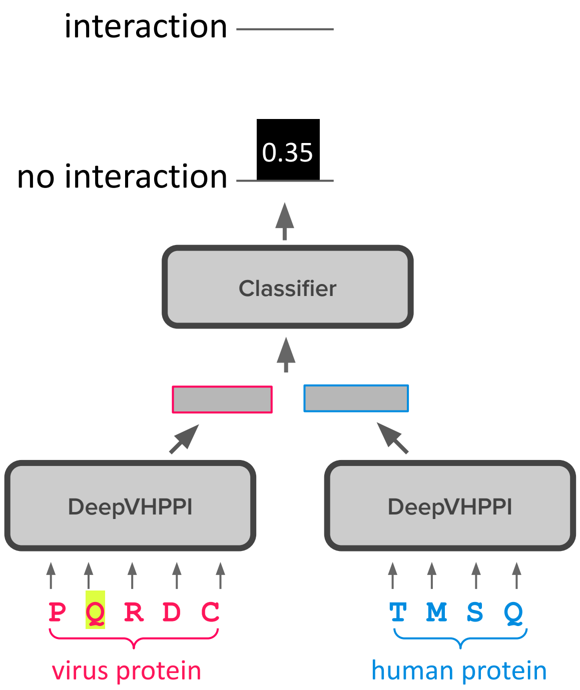
Perturbation Analysis



Perturbation Analysis

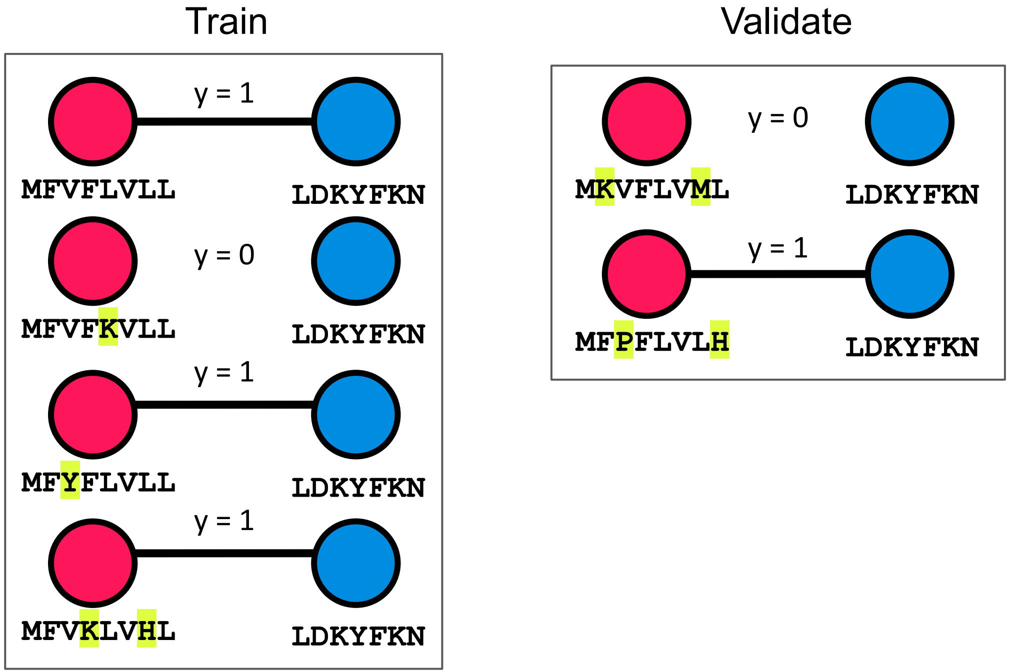


Perturbation Analysis



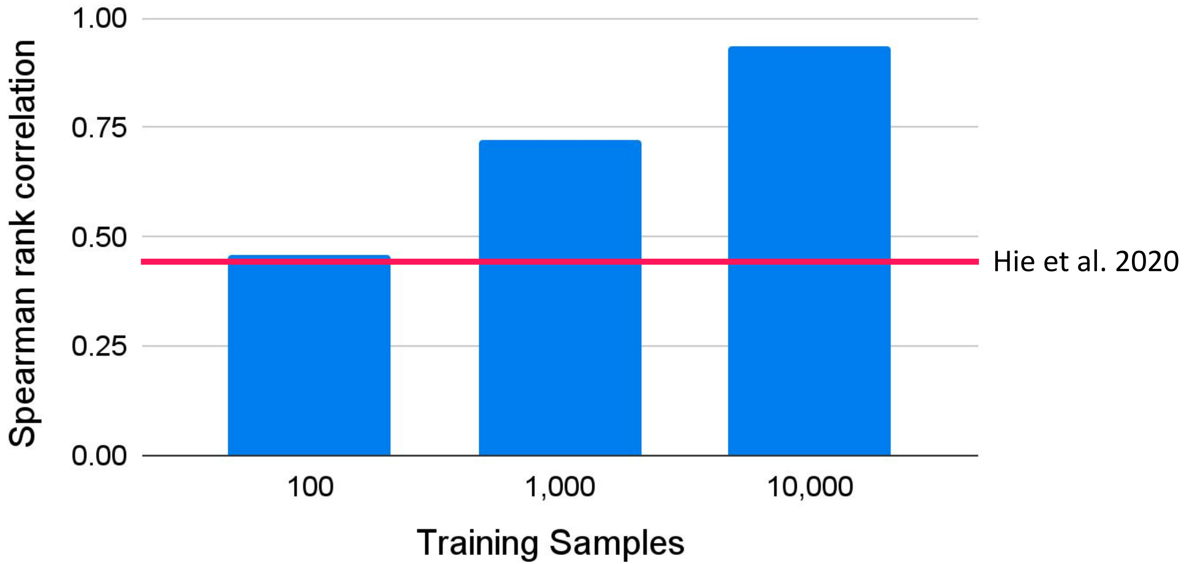
Experimental Setup

105,528 mutated Spike sequences and corresponding ACE2 binding affinities from Starr et al.



Perturbation Analysis: Mutated Spike and ACE2 Interactions

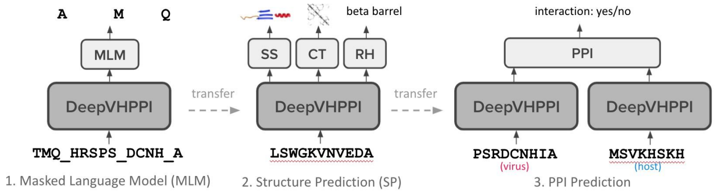
Correlation between DeepVHPPI binding prediction and dissociation constant



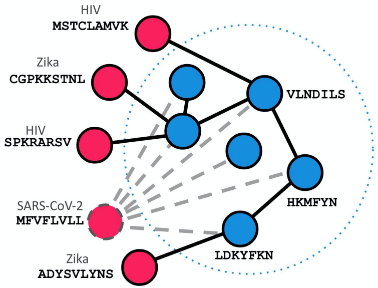
DeepVHPPI can be used to help understand the **effects of virus variants**

Contributions

1. Flexible transfer learning framework for protein-protein interaction prediction



2. Accurate novel virus interaction predictions



3. Interpretable and interactive mutation perturbation analysis

Transfer learning and Transformers can be used to accurately predict protein-protein interactions

Genomic Sequences

ChromeGCN
Lanchantin et al.
ECCB 2020

Deep Motif Dashboard
Lanchantin et al.
PSB 2017

Memory Matching Networks
Lanchantin et al.
ICLR Workshops 2017

DeepChrome
Singh et al.
ECCB 2016

AttentiveChrome
Singh et al.
NeurIPS 2017

Proteins

DeepVHPPI
Lanchantin et al.
ACM-BCB 2021

MUST-CNN
Lin et al.
AAAI 2016

Visual Objects & Natural Language

C-Tran
Lanchantin et al.
CVPR 2021

LaMP
Lanchantin et al.
ECML 2019

Re-evaluating Adversarial
Morris et al.
EMNLP Findings 2020

Deep WordBug
Gao et al.
DLS 2018

Modeling Image Label Interactions with C-Tran

interactions between **input features**

interactions between **input samples**

interactions between **output labels**

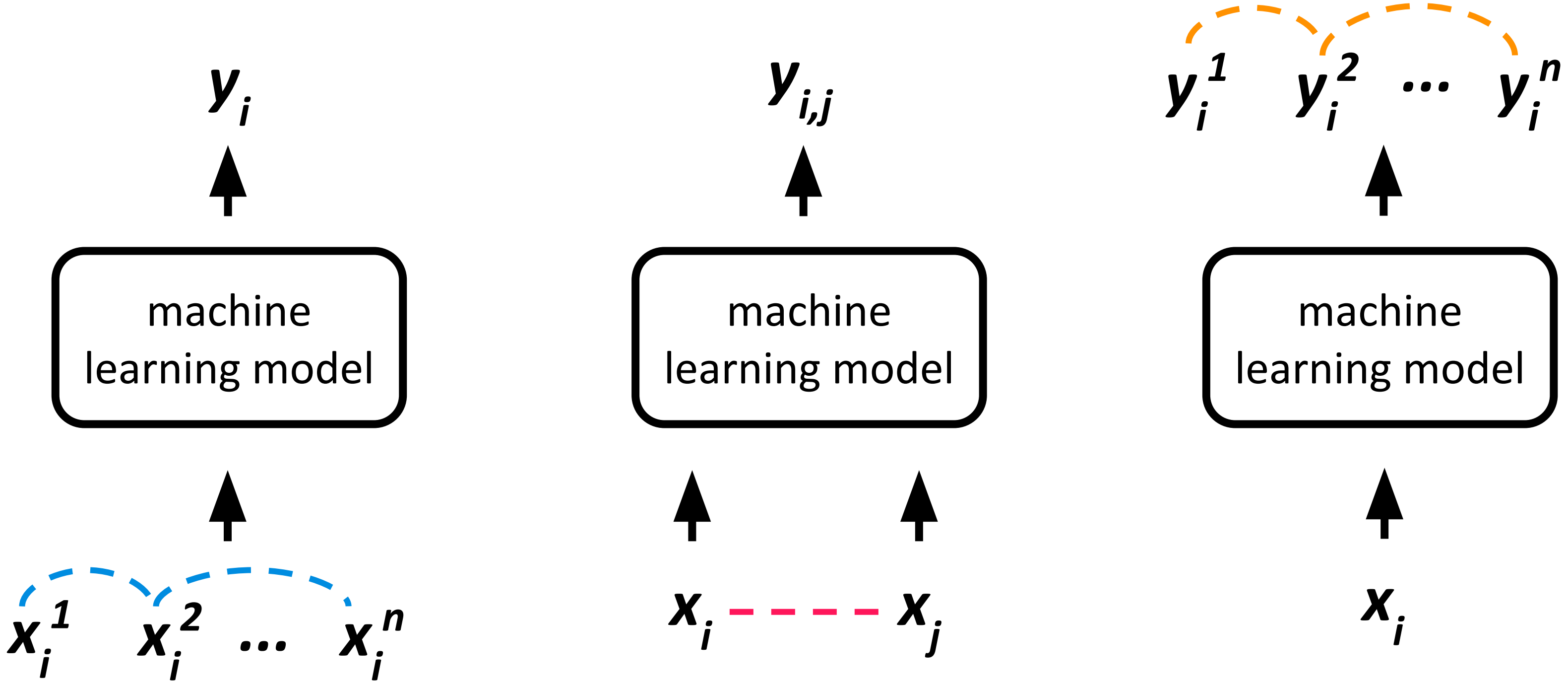
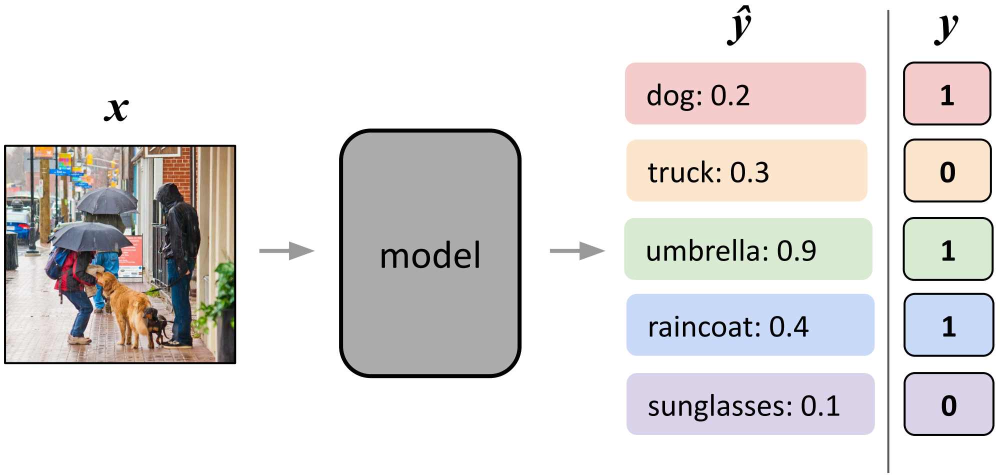


Image Scene Understanding

Multi-label Classification

Given input ***x***, predict the ***set*** of target labels $\{y_1, y_2, \ldots, y_L\}$, $y_i \in \{0,1\}$



Multi-label Classification

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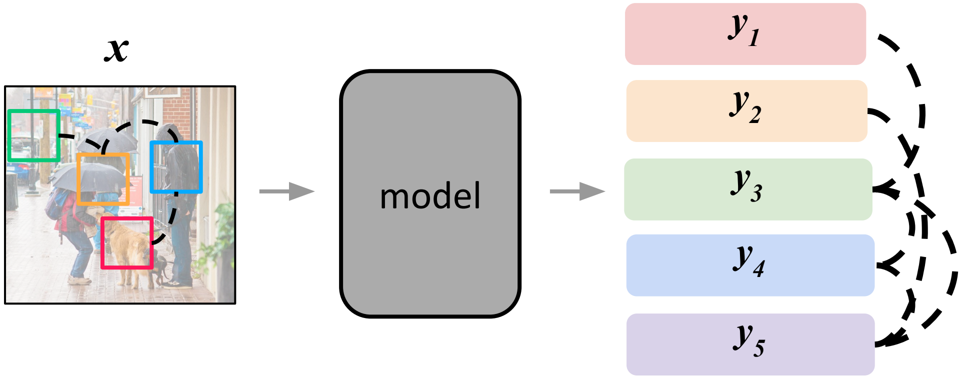


Regular inference

$\boldsymbol{x}$

model

$\hat{\boldsymbol{y}}$

dog: 0.2

truck: 0.3

umbrella: 0.9

raincoat: 0.4

sunglasses: 0.1

$p(\mathbf{y}|\mathbf{x})$

Inference with partial knowledge

Information (e.g. certain labels) can be known **prior to** performing any **visual recognition**

$\boldsymbol{x}$

raincoat = 1

Inference with partial knowledge

Information (e.g. certain labels) can be known **prior to** performing any **visual recognition**

$\boldsymbol{x}$

raincoat = 1

model

$\hat{\boldsymbol{y}}$

dog: 0.2

truck: 0.2

umbrella: 0.9

raincoat = 1

sunglasses: 0.1

unknown known

$$p(\mathbf{y}_u | \mathbf{x}, \mathbf{y}_k)$$

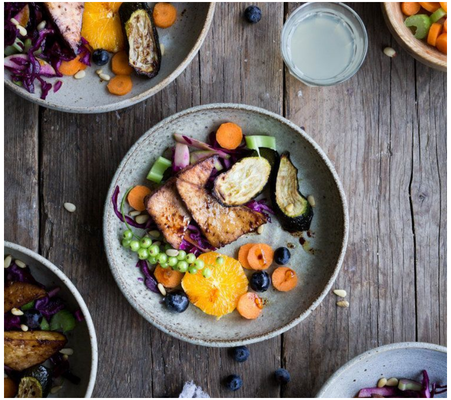
Inference with context-specific information: a realistic setting

Geo-Location Tags

Lake George, NY

lake

Social Media Tags



#avocado #bowl

avocado

bowl

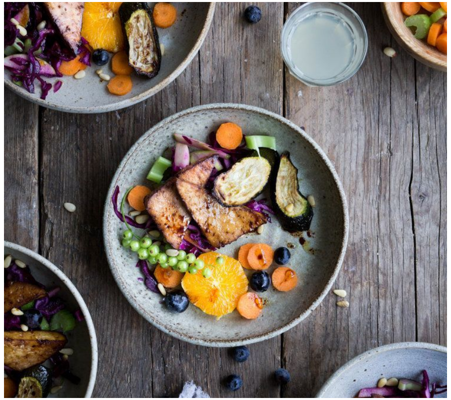
News Captions

Mt. Sinabung sent smoke over western Indonesia Wednesday.

mountain

smoke

Inference with context-specific information: a realistic setting



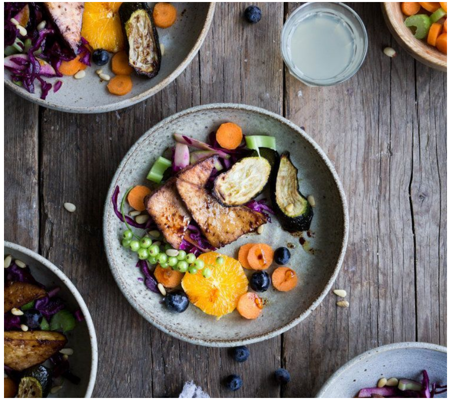
#avocado #bowl

avocado

bowl

problem: for each test image, known labels can be different

Inference with context-specific information: a realistic setting



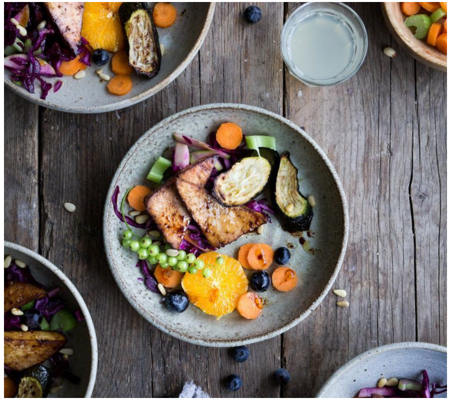
#cup #table

cup

table

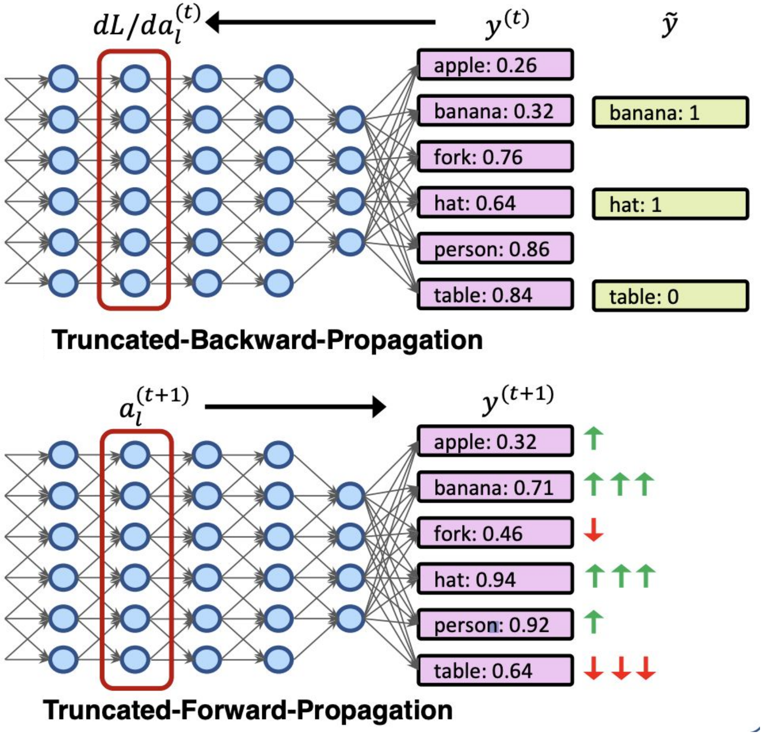
problem: for each test image, known labels can be <u>different</u>

Inference with context-specific information: a realistic setting



problem: for each test image, known labels can be <u>different</u>

Previous Work: Feedbackprop

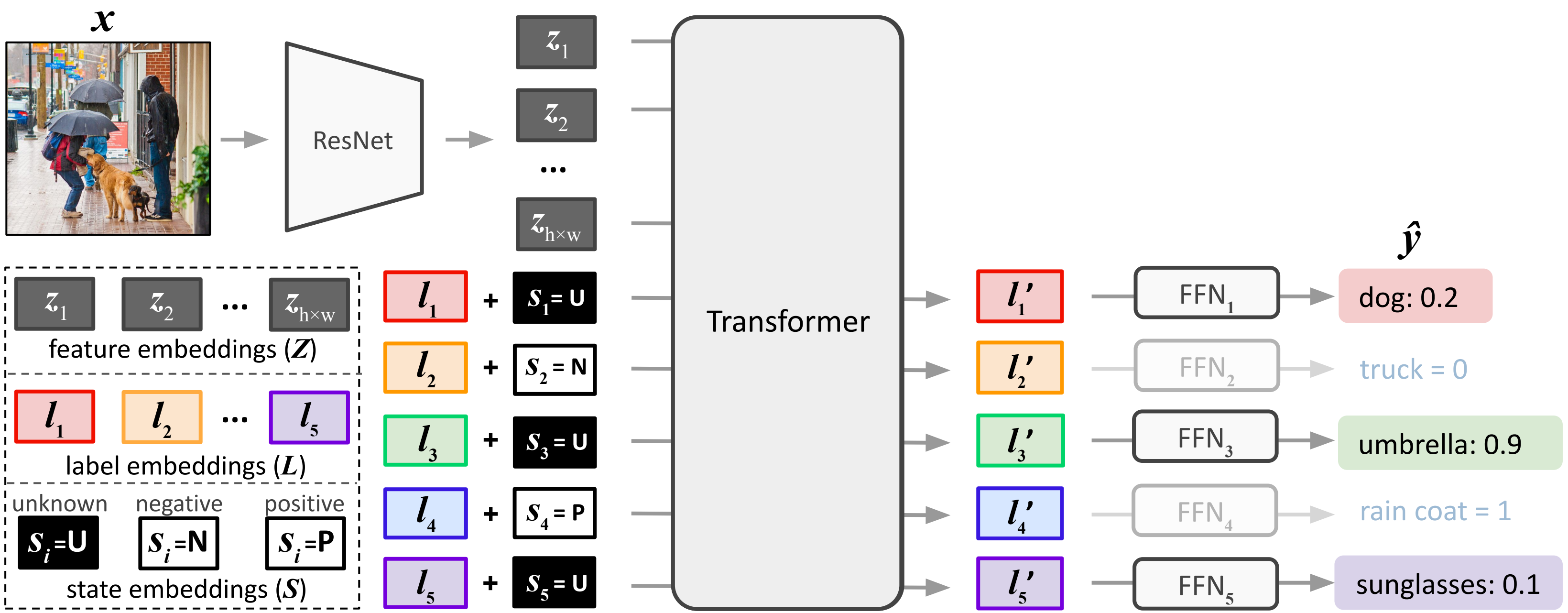


Wang et al. 2018

Research Question 3

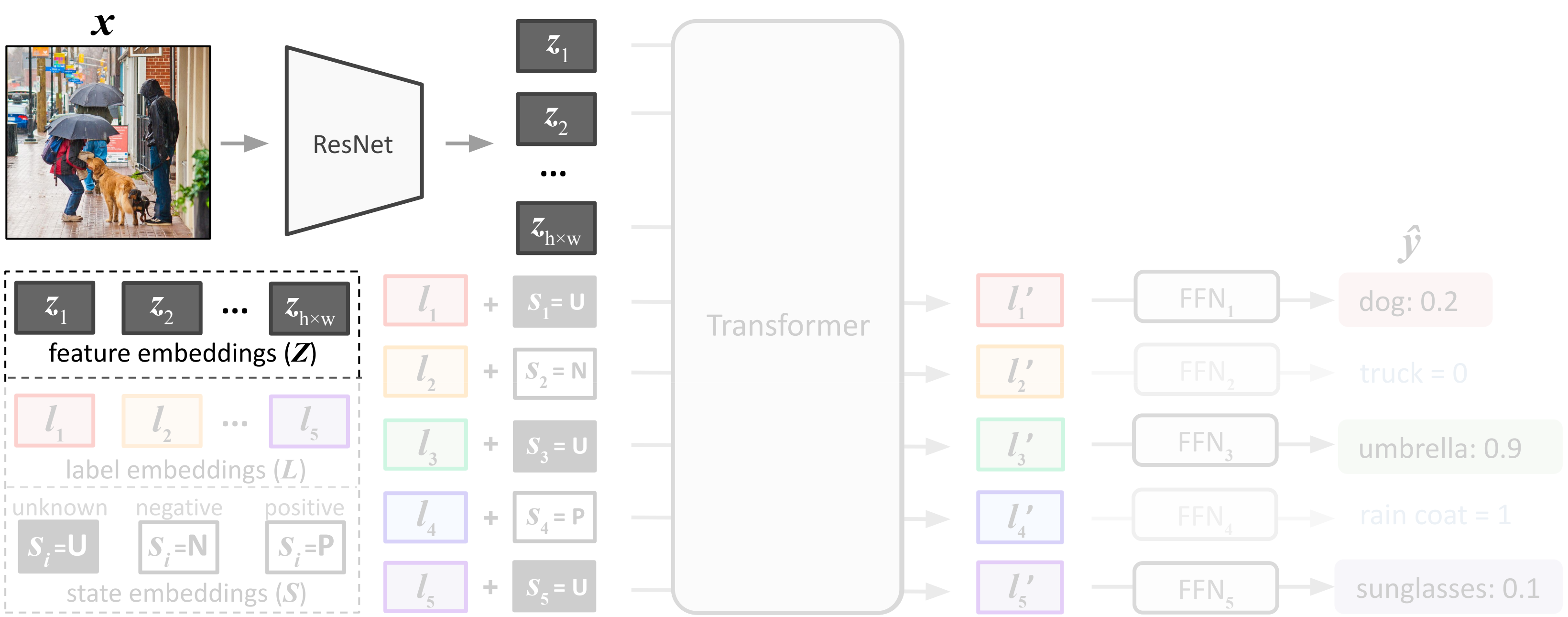
Can we model interactions between object labels, and also exploit the interactions from arbitrary amounts of known labels?

Classification Transformer (C-Tran)

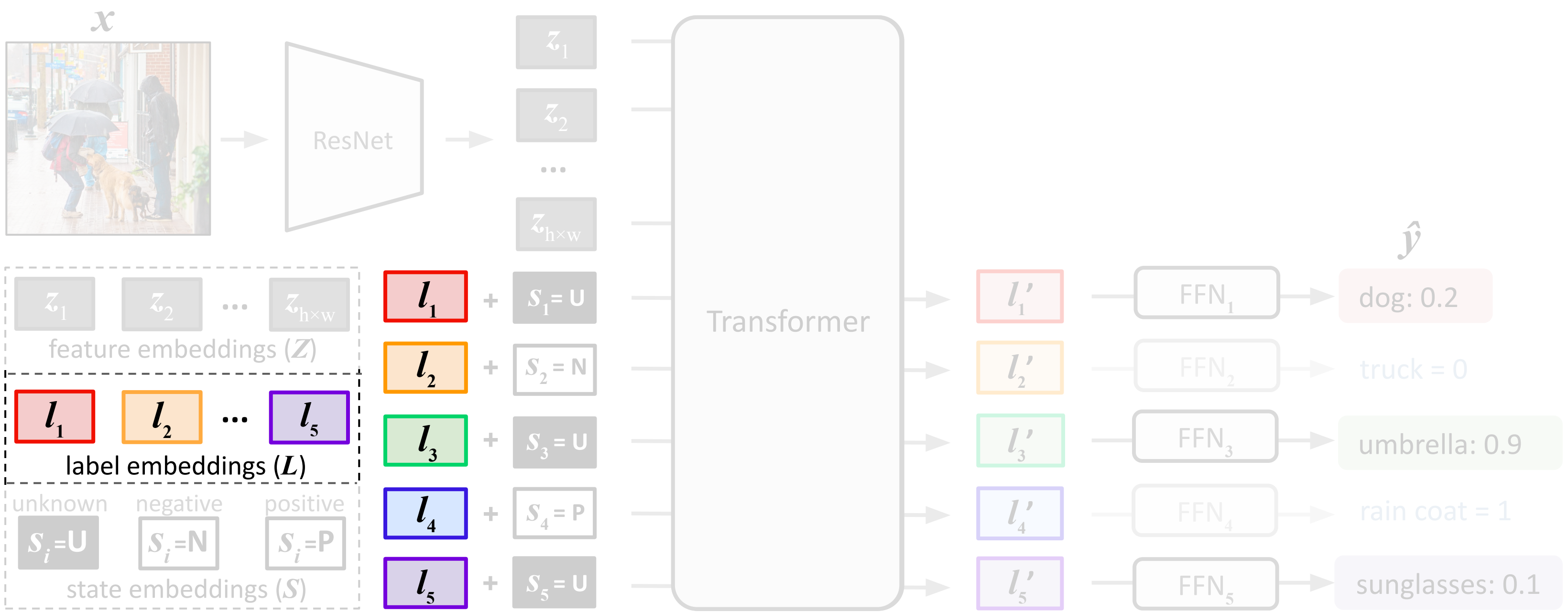


Lanchantin, Wang, Ordoñez, Qi - CVPR 2021

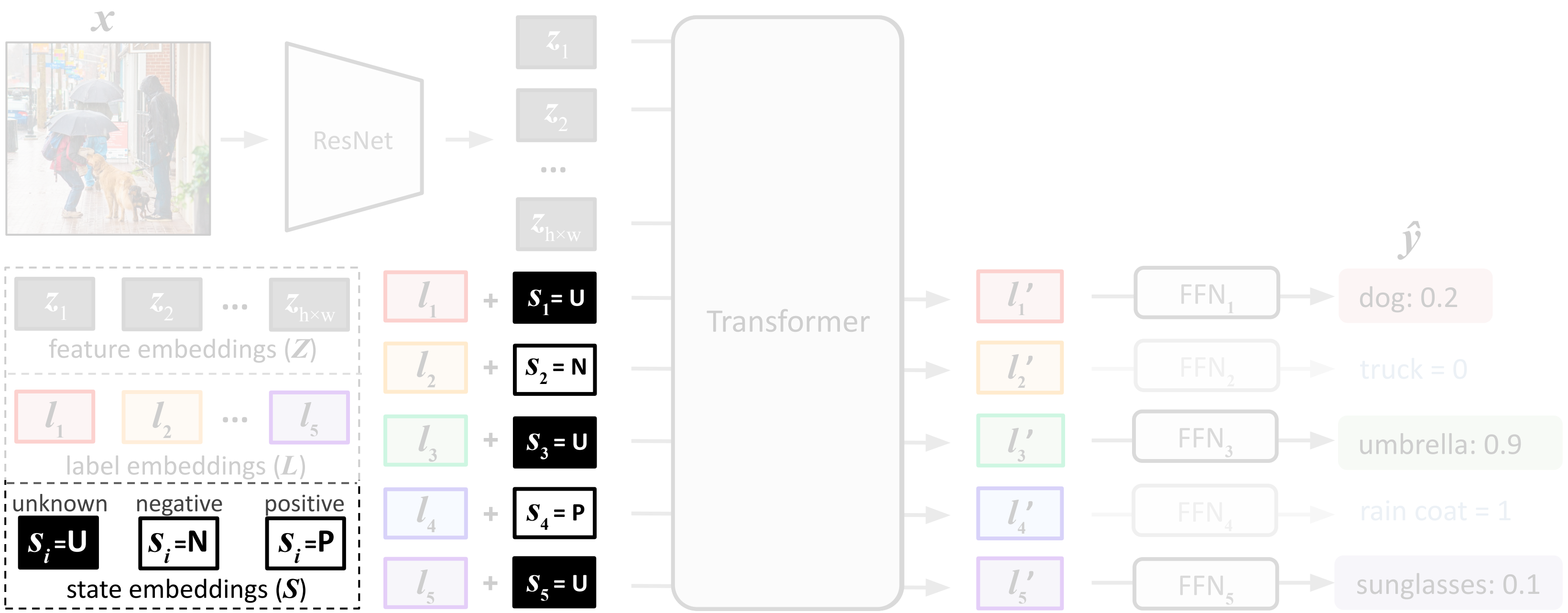
Classification Transformer (C-Tran)



Classification Transformer (C-Tran)



Classification Transformer (C-Tran)



Lanchantin, Wang, Ordoñez, Qi - CVPR 2021

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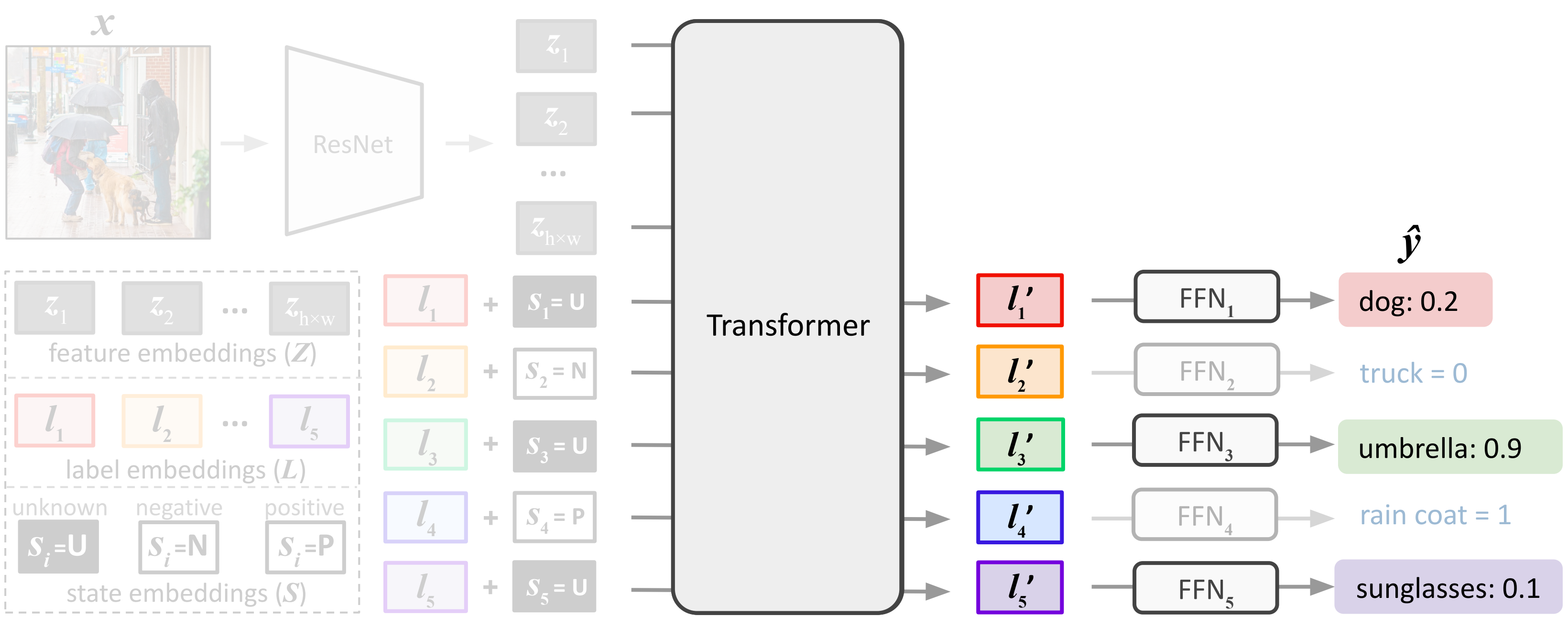

Lanchantin, Wang, Ordoñez, Qi - CVPR 2021

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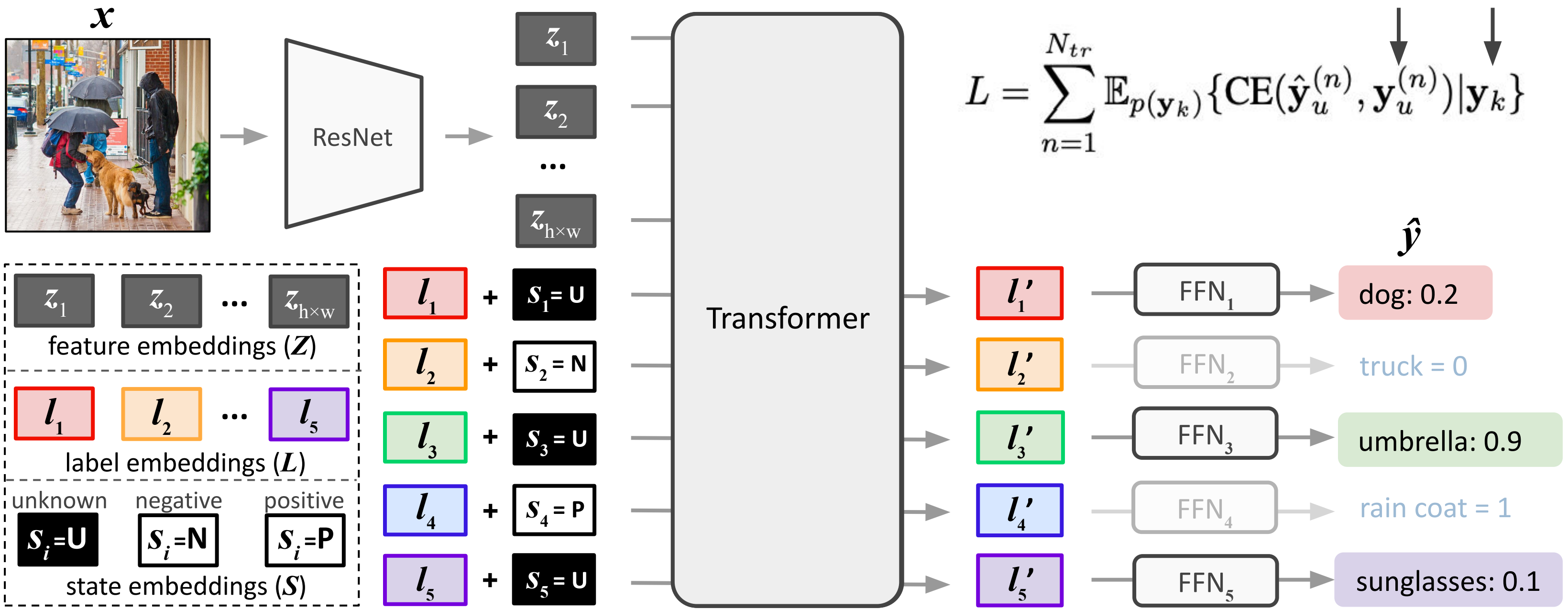
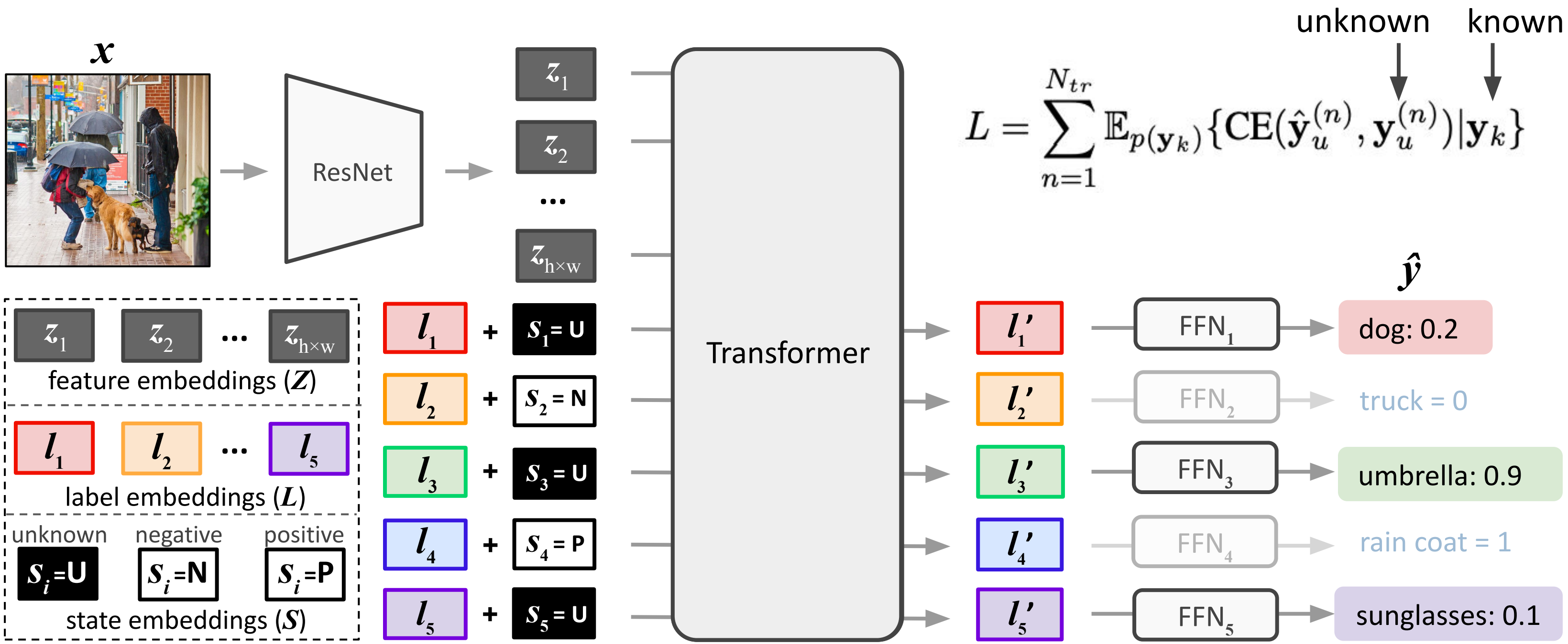


$$L = \sum_{n=1}^{N_{tr}} \mathbb{E}_{p(\mathbf{y}_k)}\{\text{CE}(\hat{\mathbf{y}}_u^{(n)}, \mathbf{y}_u^{(n)})|\mathbf{y}_k\}$$

randomly sample a random amount of known labels

Classification Transformer (C-Tran)



$$L = \sum_{n=1}^{N_{tr}} \mathbb{E}_{p(\mathbf{y}_k)} \{ \mathrm{CE}(\hat{\mathbf{y}}_u^{(n)}, \mathbf{y}_u^{(n)}) | \mathbf{y}_k \}$$

<u>randomly</u> sample a <u>random</u> amount of known labels

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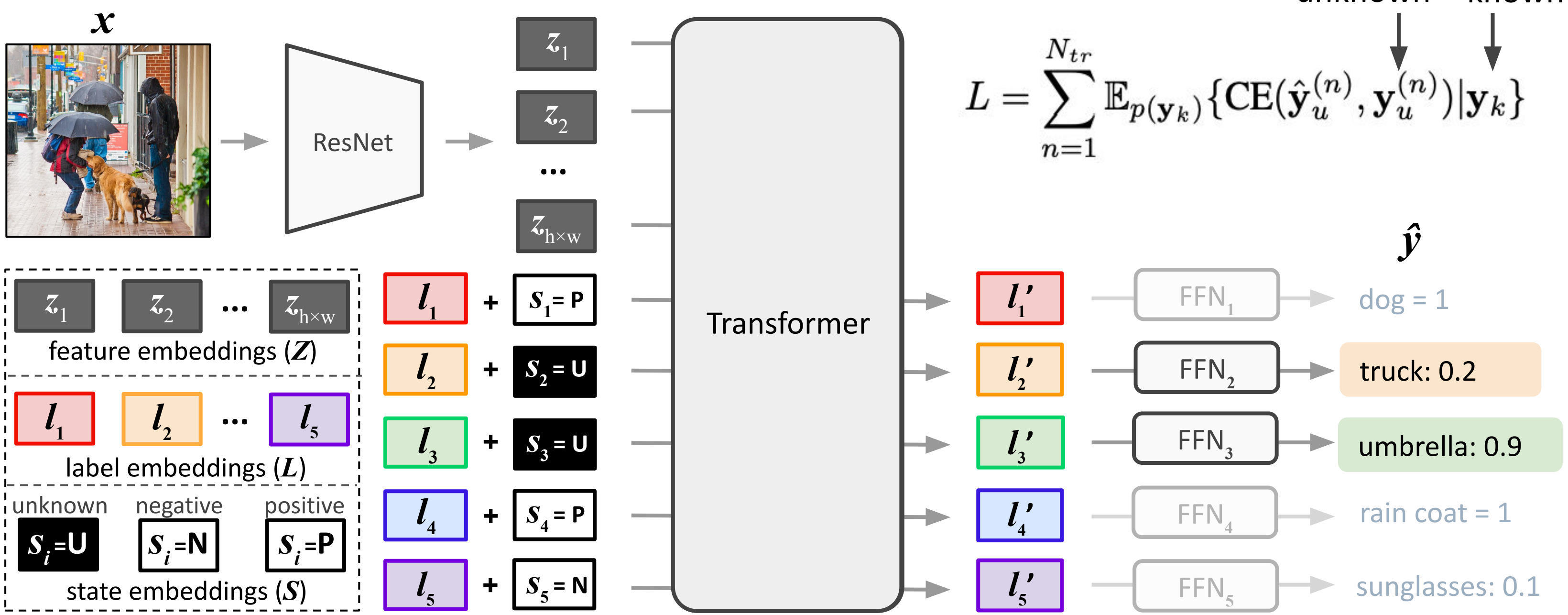

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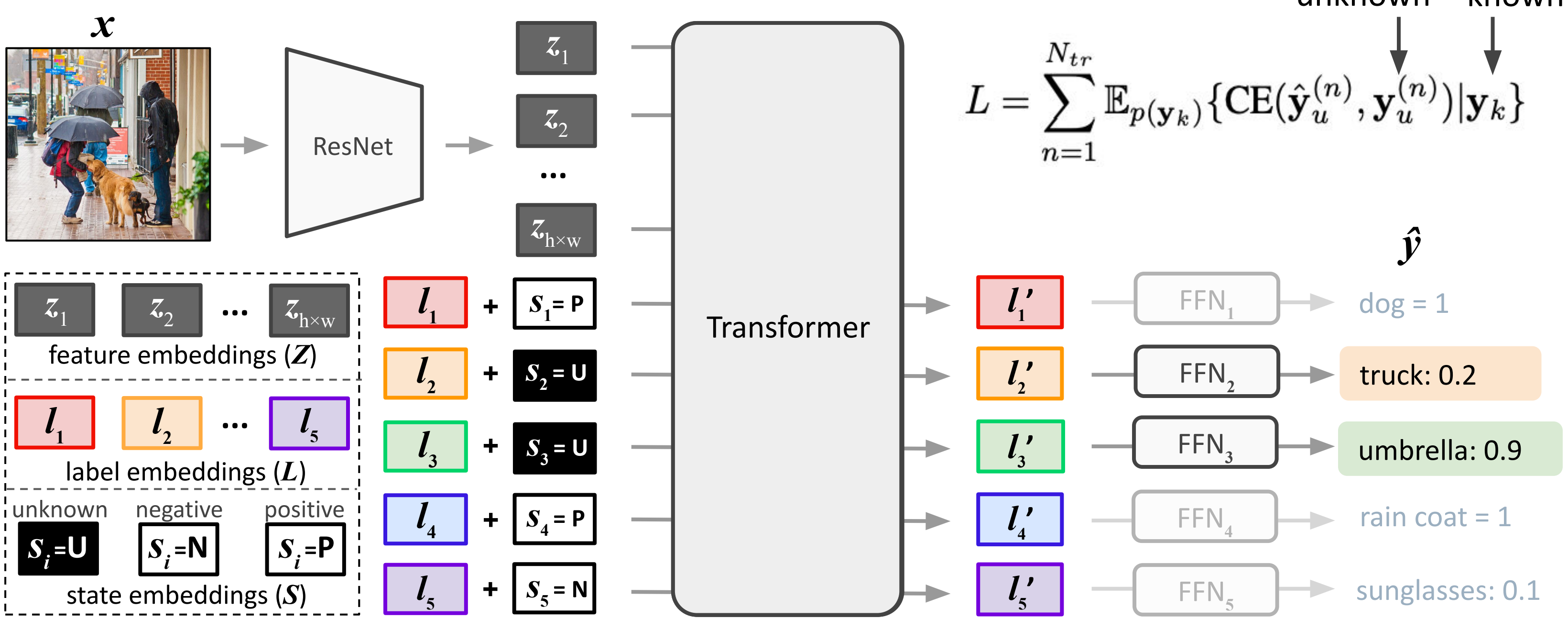

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randomly sample a random amount of known labels

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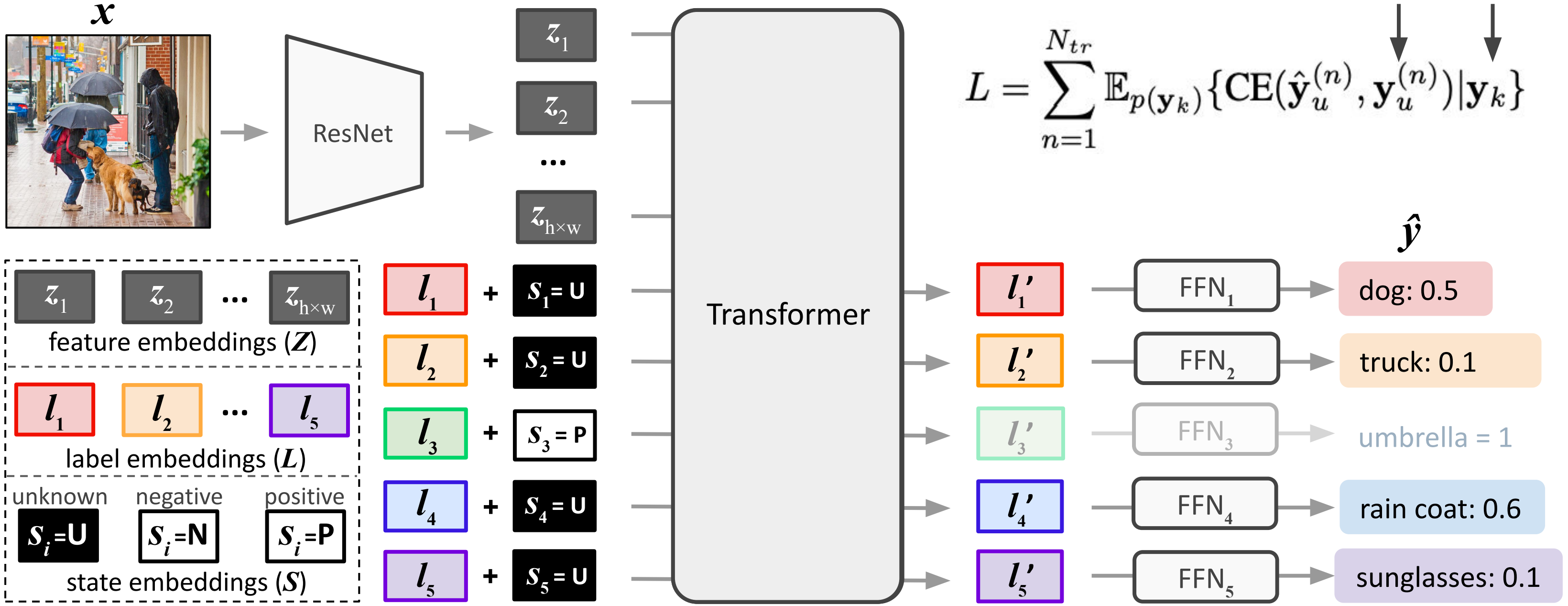
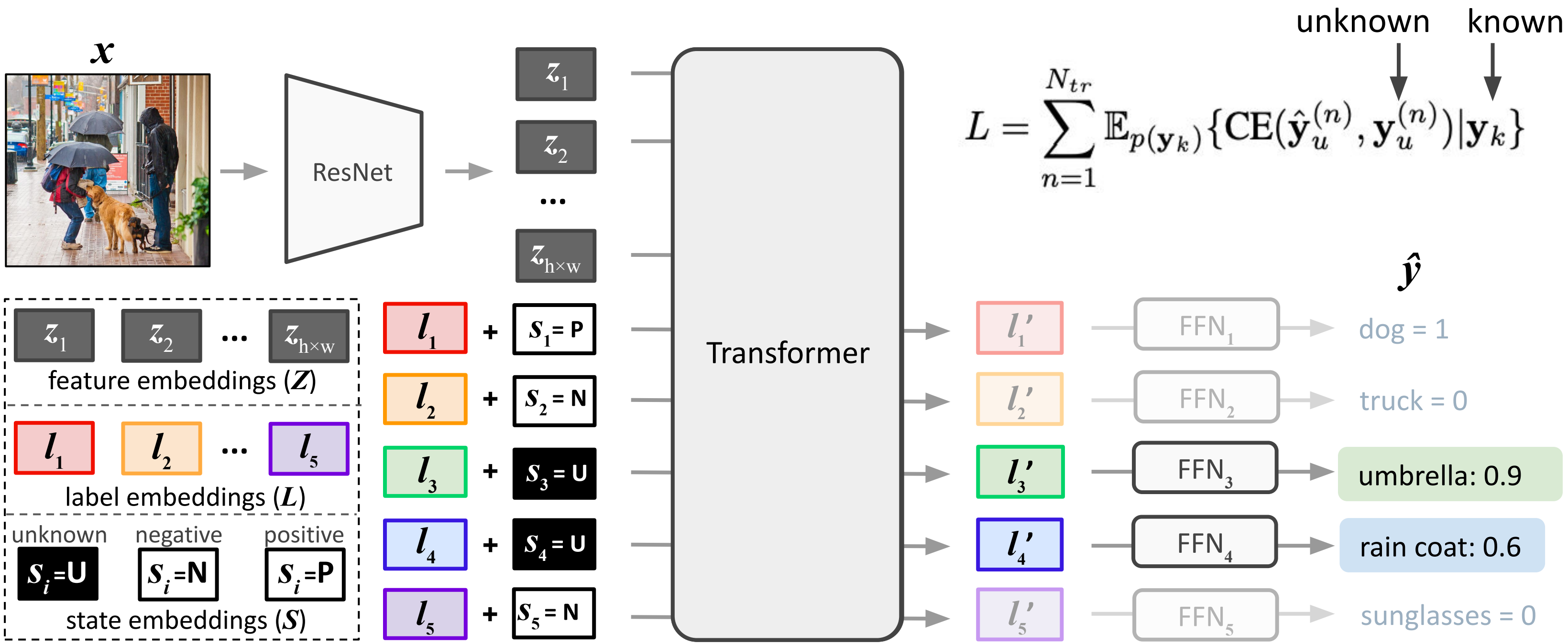


$$L = \sum_{n=1}^{N_{tr}} \mathbb{E}_{p(\mathbf{y}_k)}\{\mathrm{CE}(\hat{\mathbf{y}}_u^{(n)}, \mathbf{y}_u^{(n)})|\mathbf{y}_k\}$$

<u>randomly</u> sample a <u>random</u> amount of known labels

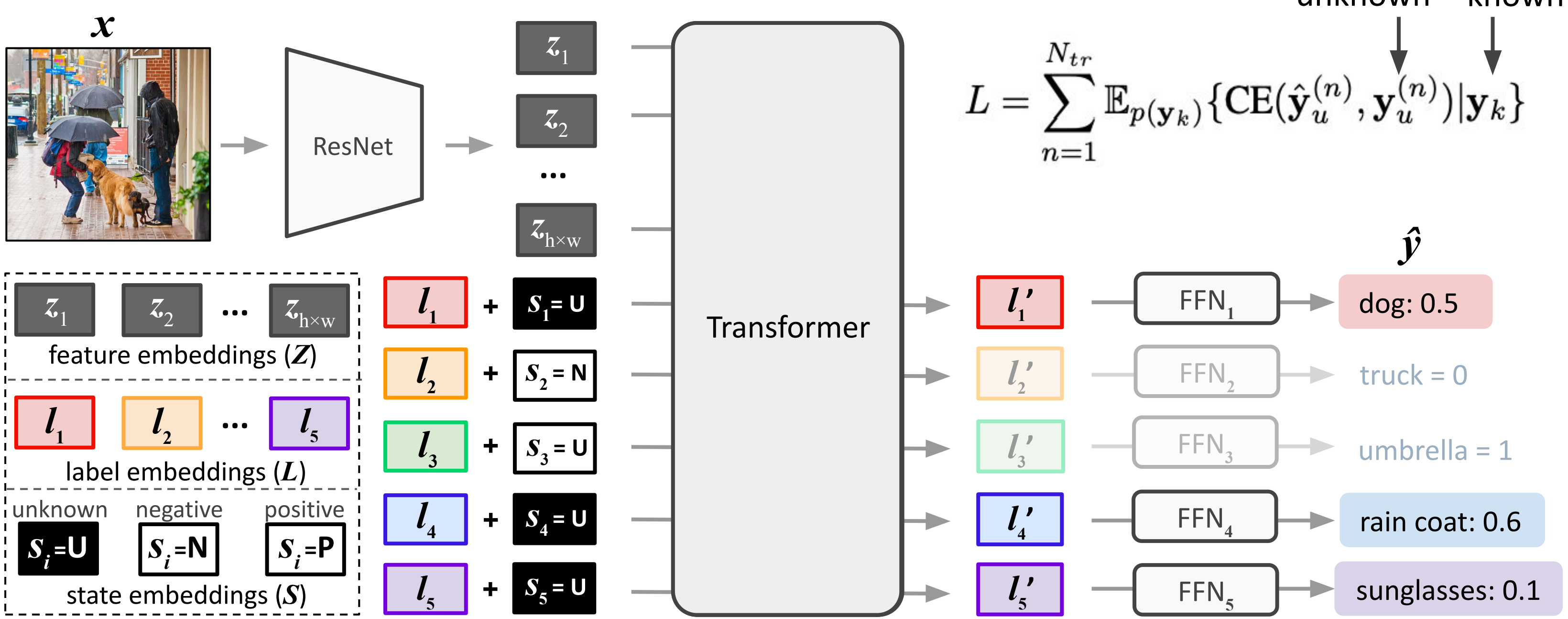
Classification Transformer (C-Tran)



$$L = \sum_{n=1}^{N_{tr}} \mathbb{E}_{p(\mathbf{y}_k)} \{ \mathrm{CE}(\hat{\mathbf{y}}_u^{(n)}, \mathbf{y}_u^{(n)}) | \mathbf{y}_k \}$$

randomly sample a random amount of known labels

Classification Transformer (C-Tran)



$$L = \sum_{n=1}^{N_{tr}} \mathbb{E}_{p(\mathbf{y}_k)} \{ \mathrm{CE}(\hat{\mathbf{y}}_u^{(n)}, \mathbf{y}_u^{(n)}) | \mathbf{y}_k \}$$

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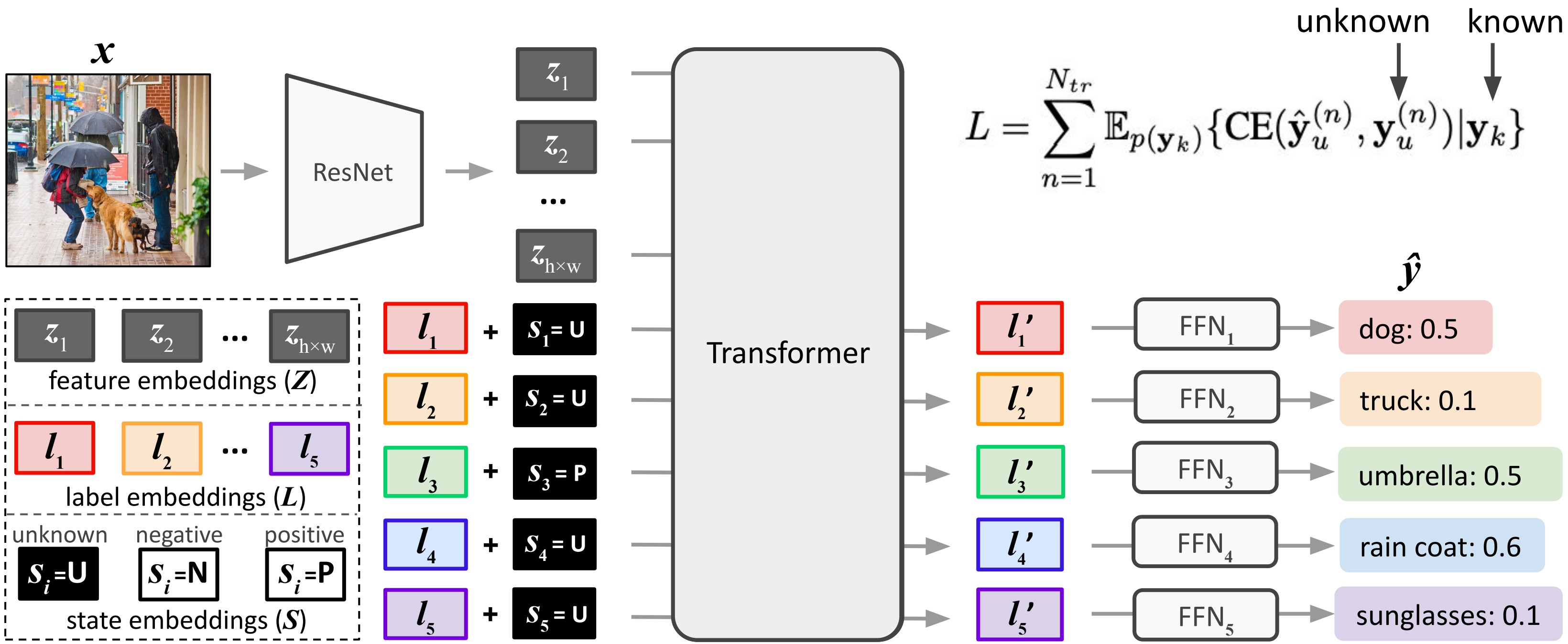
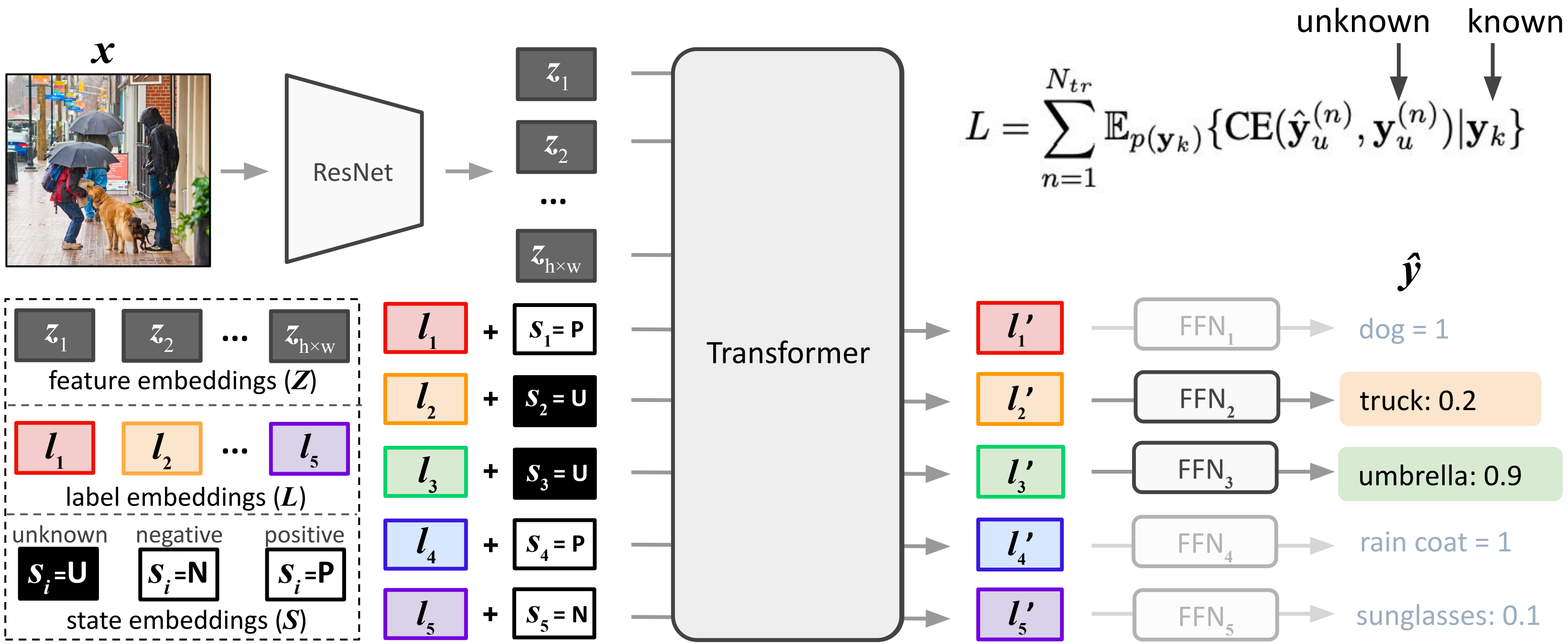
Classification Transformer (C-Tran)



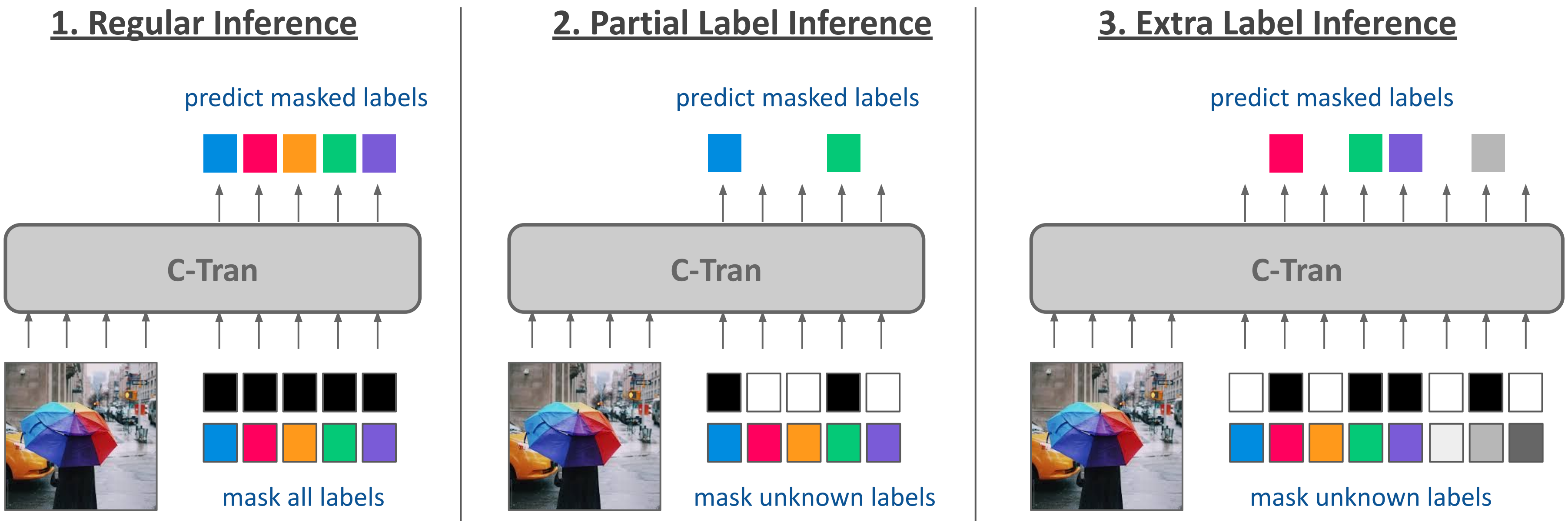
randomly sample a random amount of known labels

Classification Transformer (C-Tran)

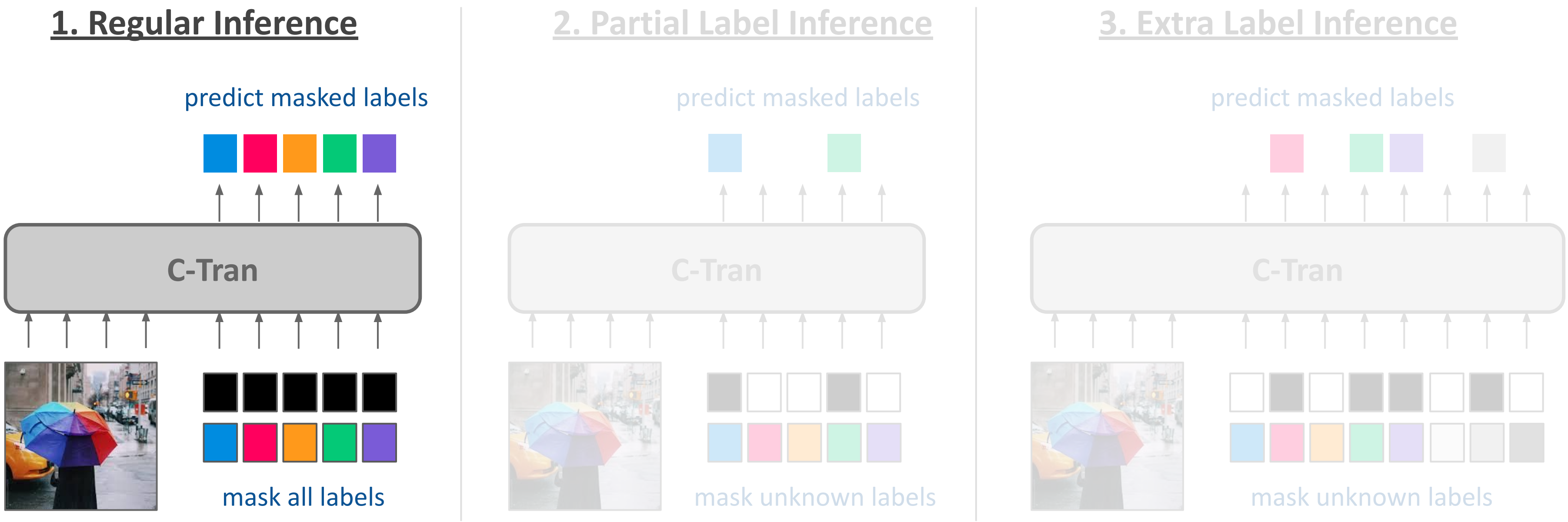


randomly sample a random amount of known labels

Three different inference settings



Three different inference settings



Regular inference setting

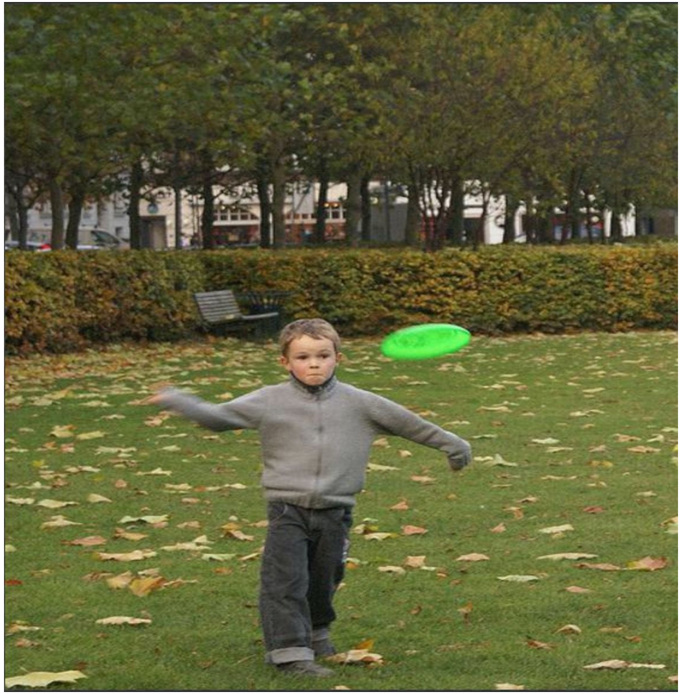
COCO
Common Objects in Context

0.8 improvement in mAP and F1 score

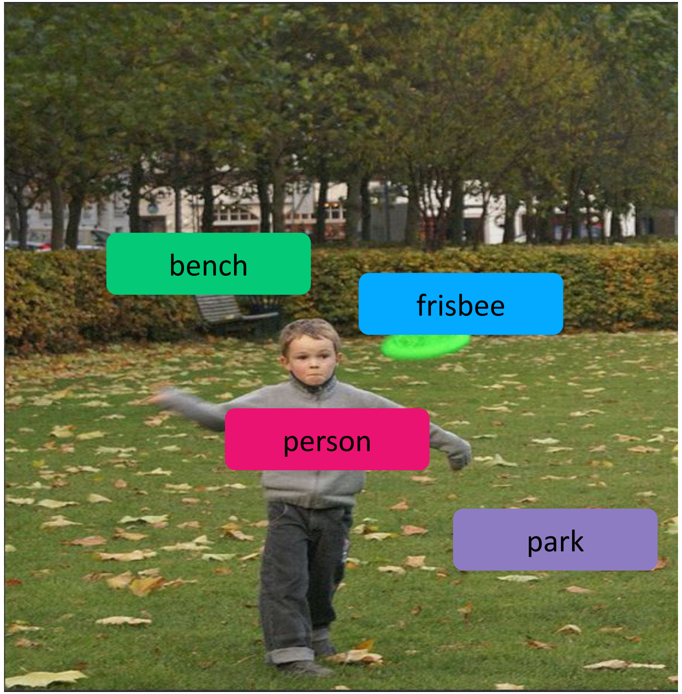
VISUALGENOME

1.0 improvement in mAP and F1 score

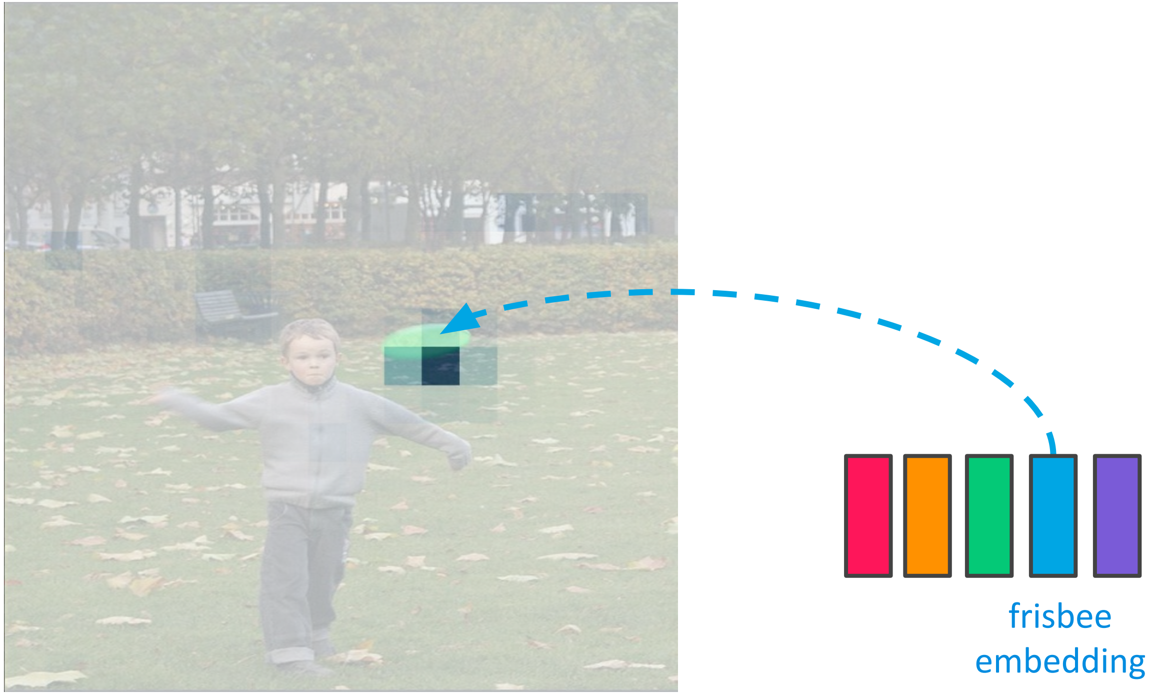
Attention Visualization



Attention Visualization

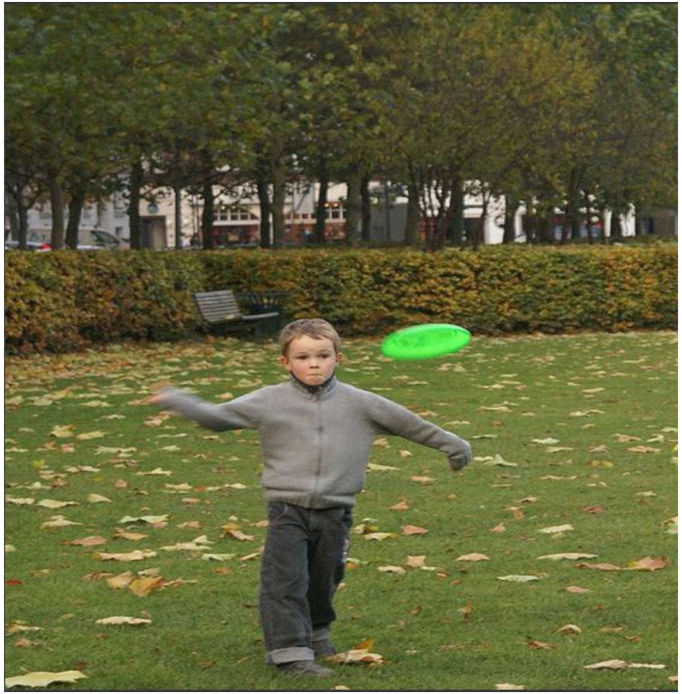


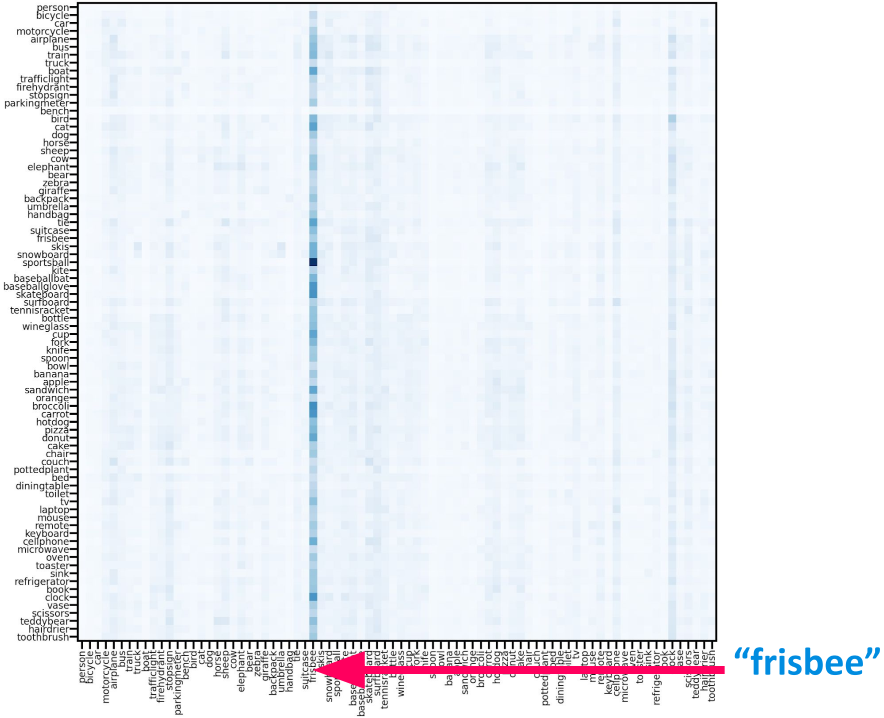
Dependencies between labels and image patches



frisbee-to-image attention

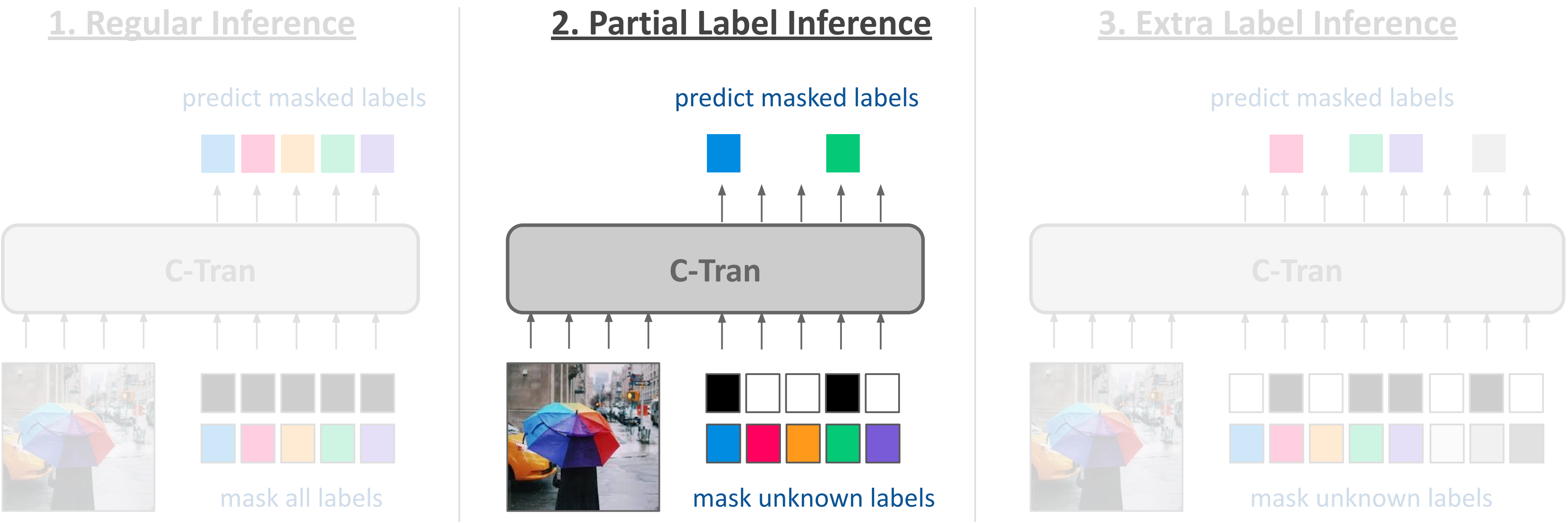
Dependencies between labels and other labels





label-to-label attention

Three different inference settings



Partial label inference setting

4 different percentages of known labels

	COCO-80				VG-500				NEWS-500				COCO-1000			
Partial Labels Known	0%	25%	50%	75%	0%	25%	50%	75%	0%	25%	50%	75%	0%	25%	50%	75%

Partial label inference setting

4 different percentages of known labels

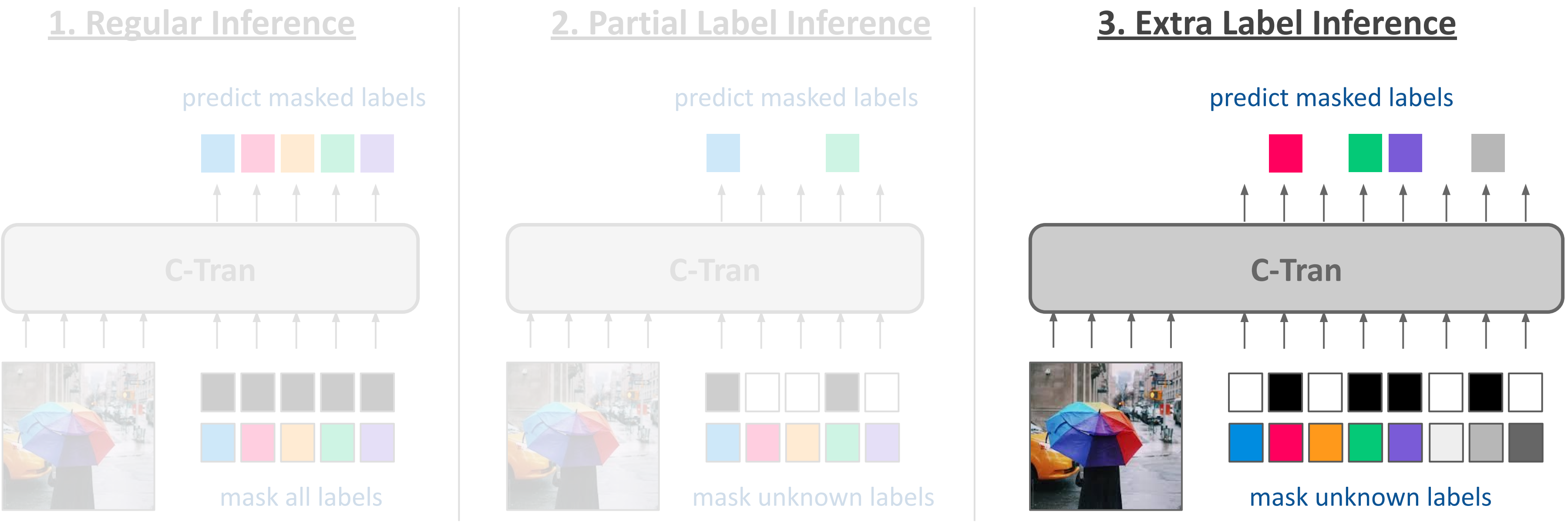
	COCO-80				VG-500				NEWS-500				COCO-1000			
Partial Labels Known	0%	25%	50%	75%	0%	25%	50%	75%	0%	25%	50%	75%	0%	25%	50%	75%
Feedbackprop [49]	80.1	80.6	80.8	80.9	29.6	30.1	30.8	31.6	14.7	21.1	23.7	25.9	29.2	30.1	31.5	33.0
C-Tran	**85.1**	**85.2**	**85.6**	**86.0**	**38.4**	**39.3**	**40.4**	**41.5**	**18.1**	**29.7**	**35.5**	**39.4**	**34.3**	**35.9**	**37.4**	**39.1**

C-Tran: improved accuracy with **any amount** of known labels

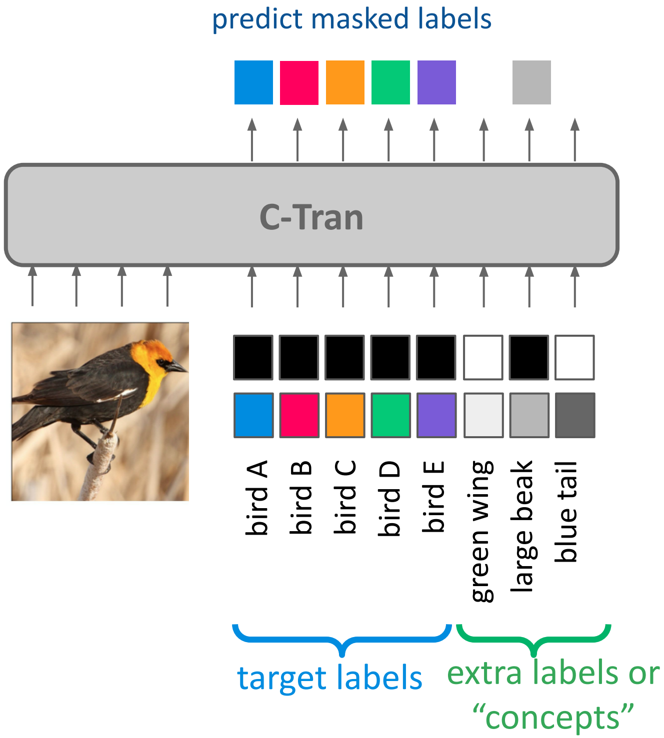
Partial label inference setting

Images	True Labels	ResNet-101	C-Tran	C-Tran + partial labels	
 ID:000000362831	fork knife, spoon, bowl, chair, diningtable	**fork,** sandwich, **diningtable,** **spoon,** cup	**fork,** **knife,** **diningtable,** person, cake	spoon=1, trafficlight=0, bench=0, dog=0, ...	**fork,** **knife,** **diningtable,** person, **bowl**

Three different inference settings



Extra label inference setting



Extra label inference setting on CUB bird classification dataset

4 different percentages of known extra labels

Extra Label Groups Known (ϵ)	0%	36%	54%	71%
Standard [23]	82.7	82.7	82.7	82.7
Multi-task [23]	**83.8**	83.8	83.8	83.8
ConceptBottleneck [23]	80.1	87.0	93.0	97.5
C-Tran	**83.8**	**90.0**	**97.0**	**98.0**

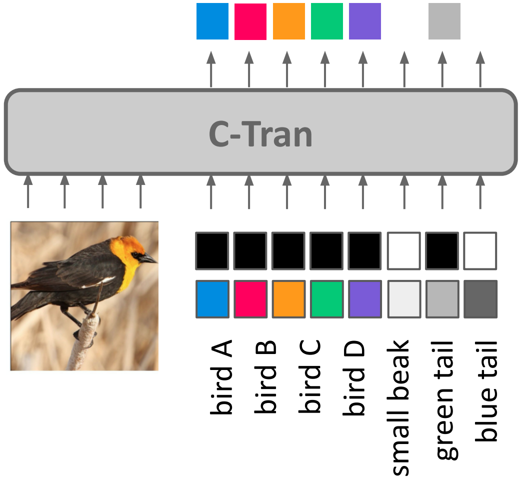
C-Tran: improved accuracy with **any amount** of extra attribute labels

Extra label inference setting

Image	True Label	C-Tran	C-Tran + Extra Labels	
	Anna Hummingbird	Rufous Hummingbird (96%)	has_bill_shape_needle = 1, has_wing_color_green=1, has_upperparts_color=green=1, has_back_color_blue=0, has_back_color_brown=0 ...	Anna Hummingbird (99%)

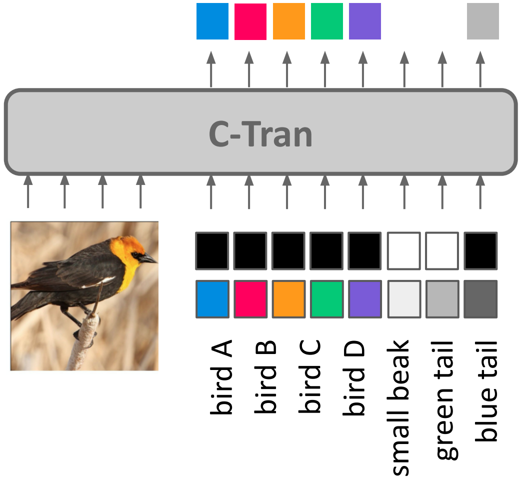
Model intervention

Given that I **know it has a blue tail,** what kind of bird is this?



Counterfactual testing

What kind of bird would this be **if it had a green tail**?

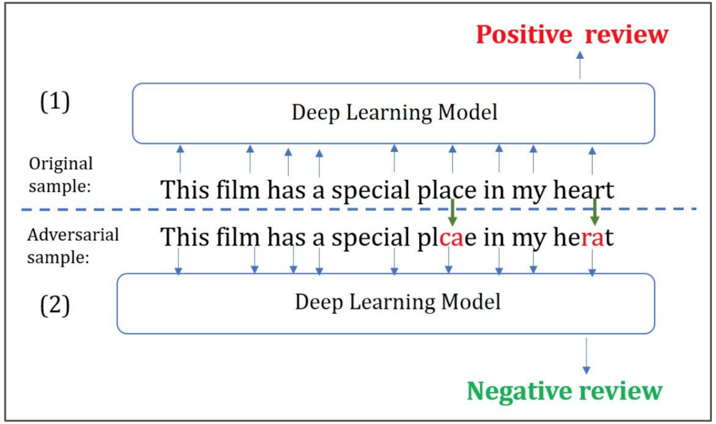


Drawback: over-relying on label interactions

Biased Model

Zhao et al. 2018

Prone to Adversarial Examples



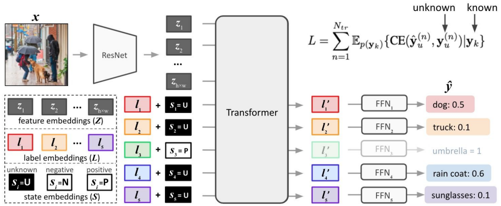
*Gao, **Lanchantin**, Soffa, Qi 2018*

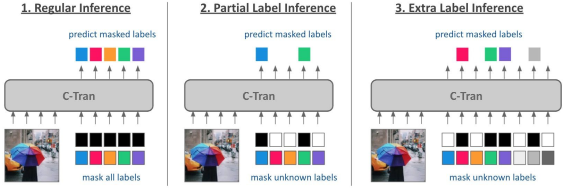
Contributions

1. Flexibility: multi-label image classification under **arbitrary subsets** of extra or partial labels

2. Accuracy: improved results on **six different datasets** across three inference settings

3. Interactivity: state embeddings enable users to easily interact with the model and **test counterfactuals**



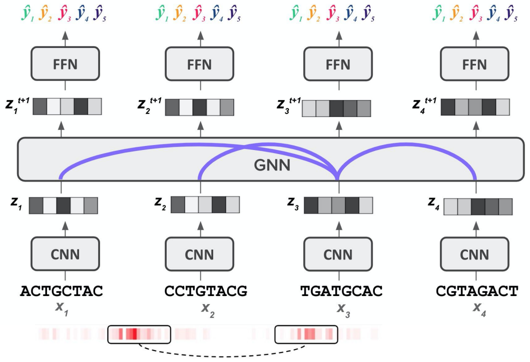


Concept Value	Class Prediction
has_yellow_underparts=1	Heermann_Gull
has_yellow_underparts=0	Glaucous_windged_Gull

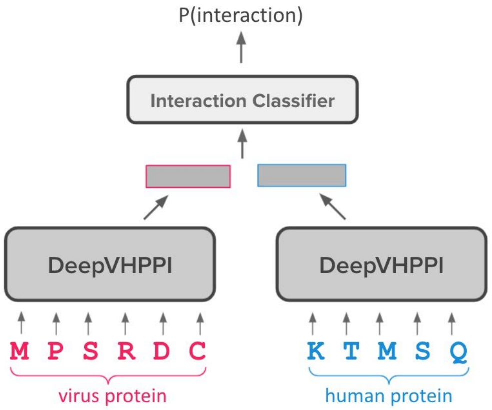
Transformers can be used to exploit interactions within image scenes for accurate multi-label image classification

Conclusions and Open Problems

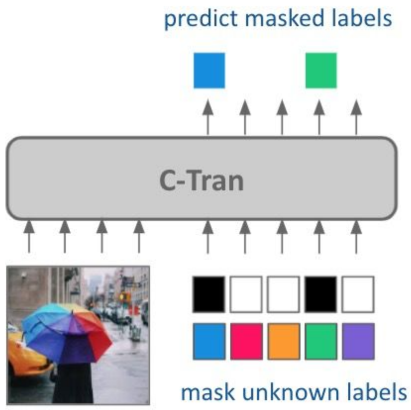
1. Using and discovering interactions between DNA subsequences



2. Predicting and analyzing interactions between proteins



3. Discovering and exploiting interactions between image labels



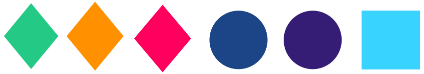
Incorporating structural interaction assumptions into the model can be extremely useful

Thesis Statement

This dissertation provides three deep learning frameworks with explicit structural assumptions to exploit, learn, predict, and understand important interactions in complex systems.

Opportunities in Genomics

expression/repression

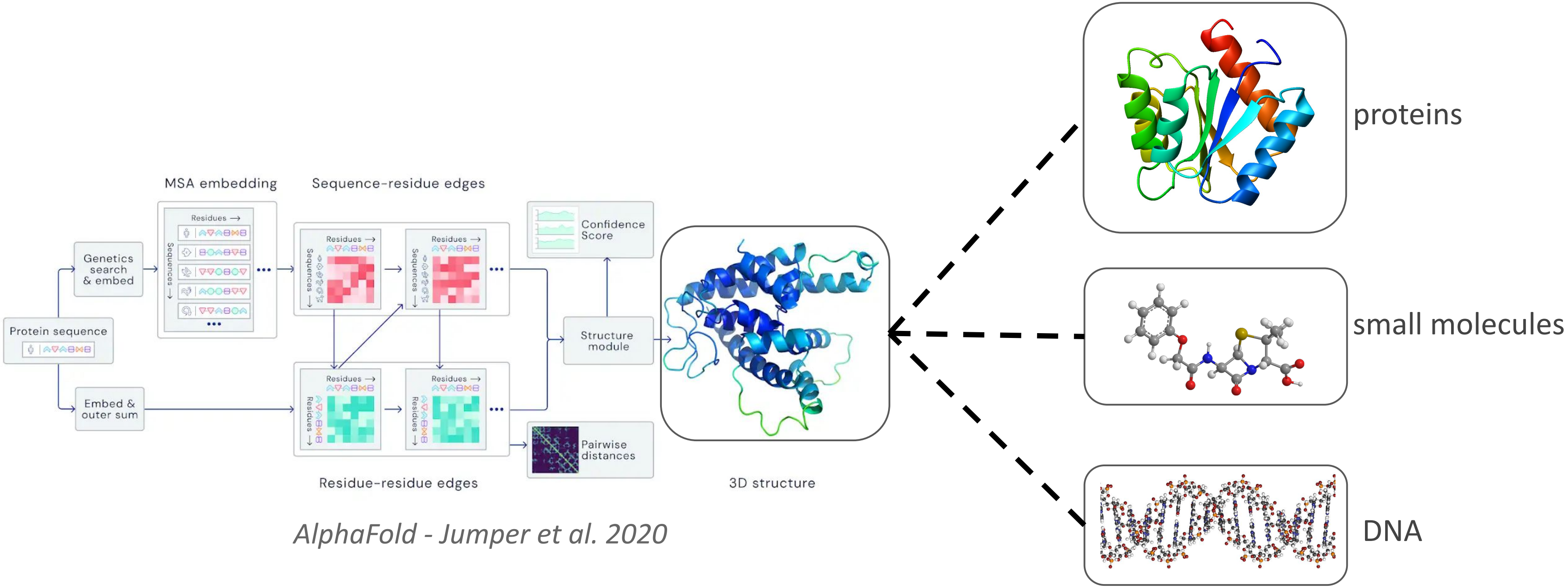


chromatin profile

CACTATACGACTGACTACTGAGC

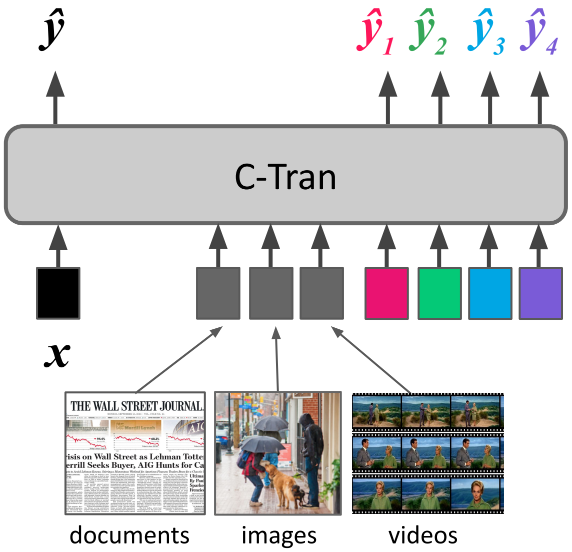
DNA

Opportunities in Proteomics



AlphaFold - Jumper et al. 2020

Opportunities in Images and Natural Language

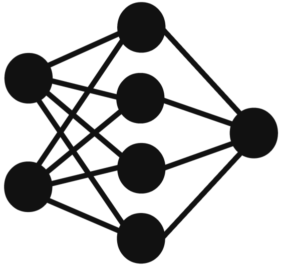


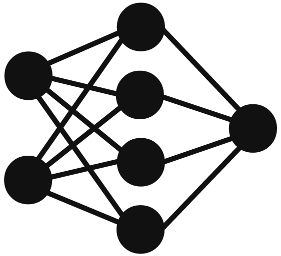
Context-dependent representations

Reflections

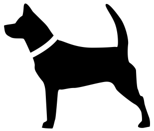
Genomics / Proteomics

Images / Natural Language





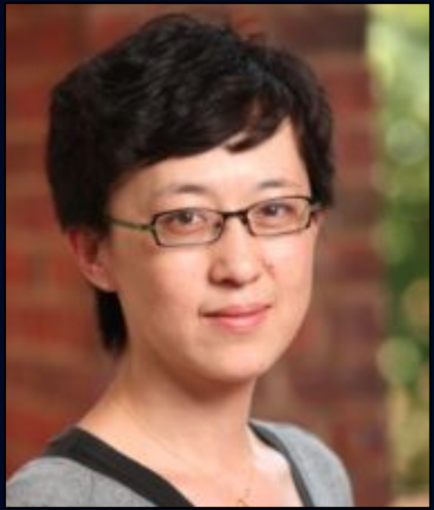
ACTGACATCG **MPGKQTVKE**



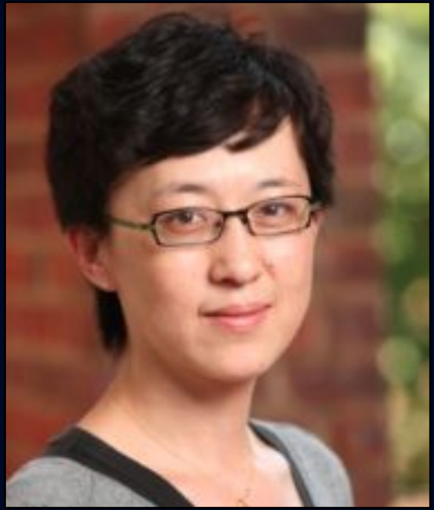
this movie
is great!

Acknowledgements

Yanjun Qi



Yanjun Qi



"My feeling is that a good scientist has a great deal of what we can call curiosity. They're just curious how things tick and they want to know the answers to questions.

- Claude Shannon

Committee


Vicente Ordoñez


Yanjun Qi

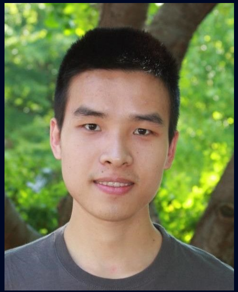

Yangfeng Ji


Clint Miller


Casey Greene

Lab-mates

Ritambhara Singh

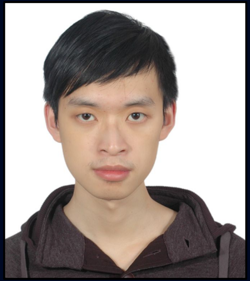


Weilin Xu

Arshdeep Sekhon

Zeming Lin

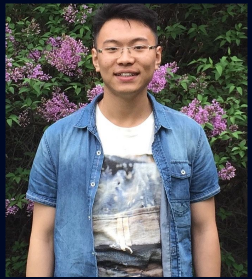
Beilun Wang



Ji Gao

Derrick Blakely

Jack Morris



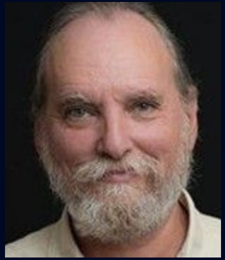
Zhe Wang

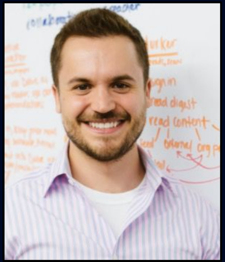
Dmitry Diochnos

Teachers, Mentors, Collaborators

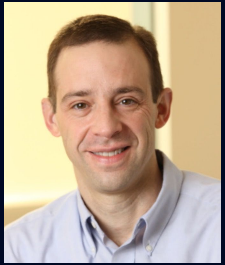

Gabe Robins

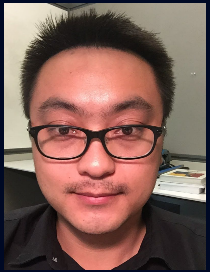

Mary-Lou Soffa


Worthy Martin


Tom Weingarten


Hongning Wang


Kevin Skadron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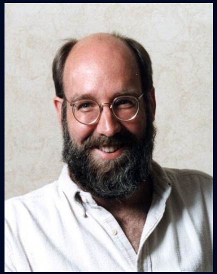
Mark Fowler


Scott Craver


Carl Betcher


Malathi Veeraraghavan

Friends

....

Brothers

Parents

Questions