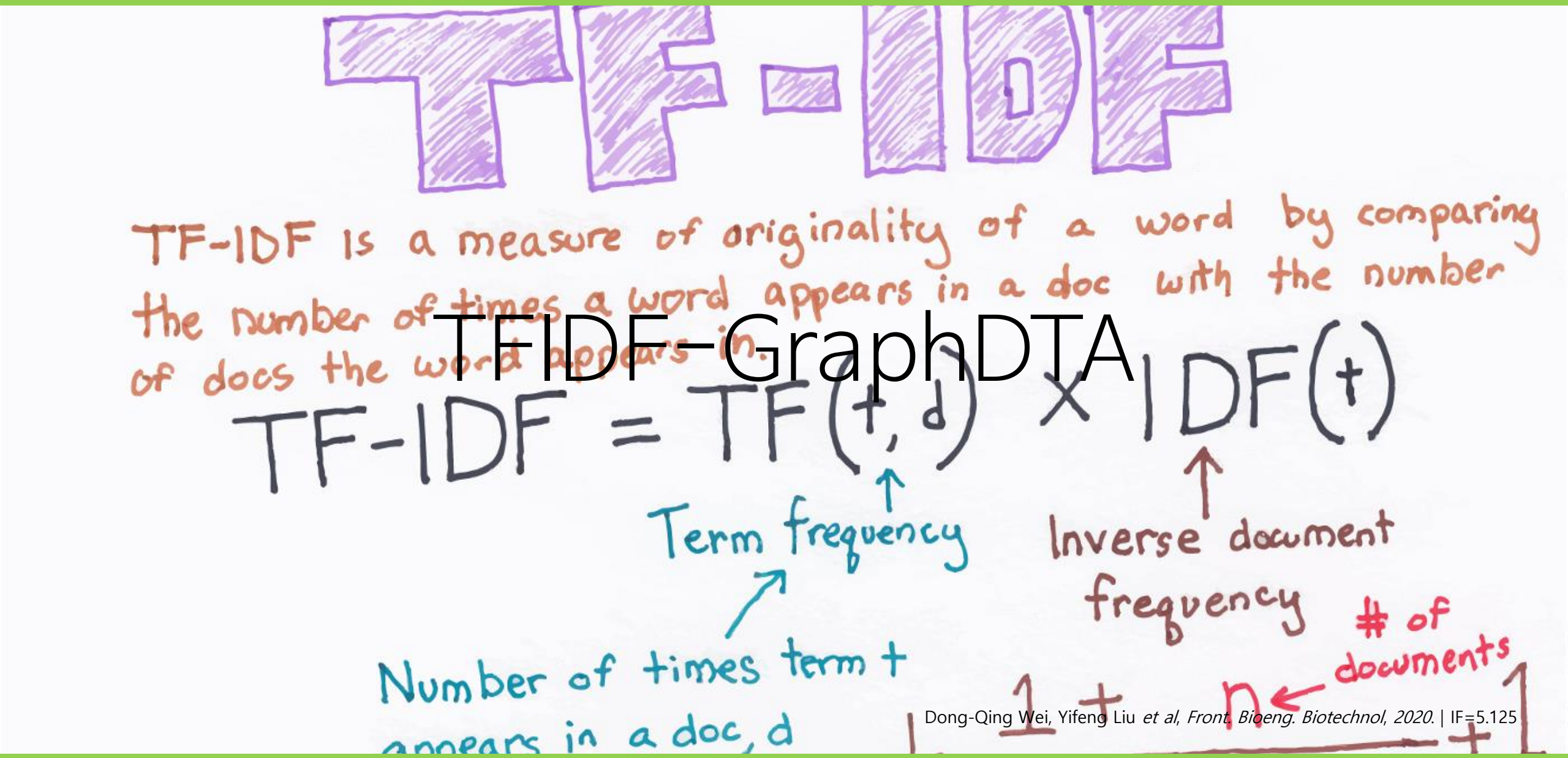

TFIDF-GraphDTA

Dong-Qing Wei, Yifeng Liu *et al*, *Front. Bioeng. Biotechnol*, *2020*. | IF=5.125

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METHODS
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Check for updates

Dipeptide Frequency of Word Frequency and Graph Convolutional Networks for DTA Prediction

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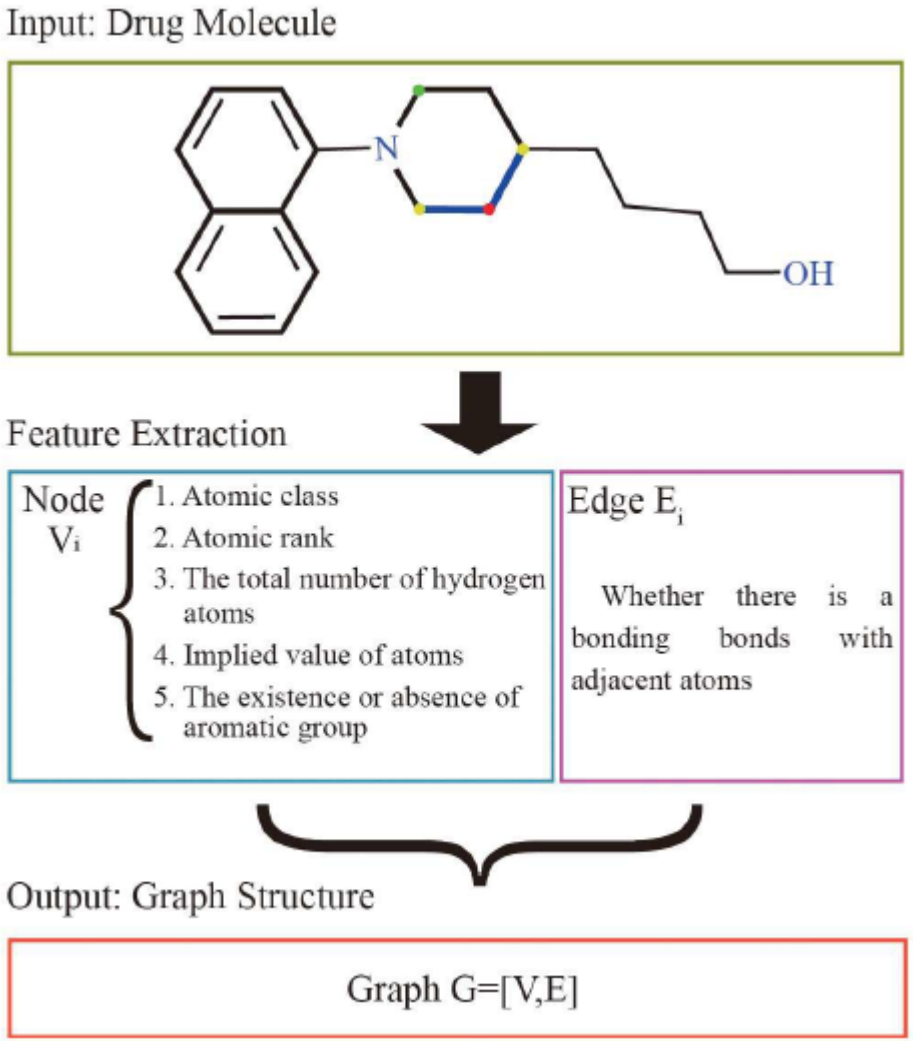
Outline

- Drug Molecular Feature Extraction
- Protein Sequence Feature Extraction
- Network Model Construction
- Results and Discussion

Drug Molecular Feature Extraction

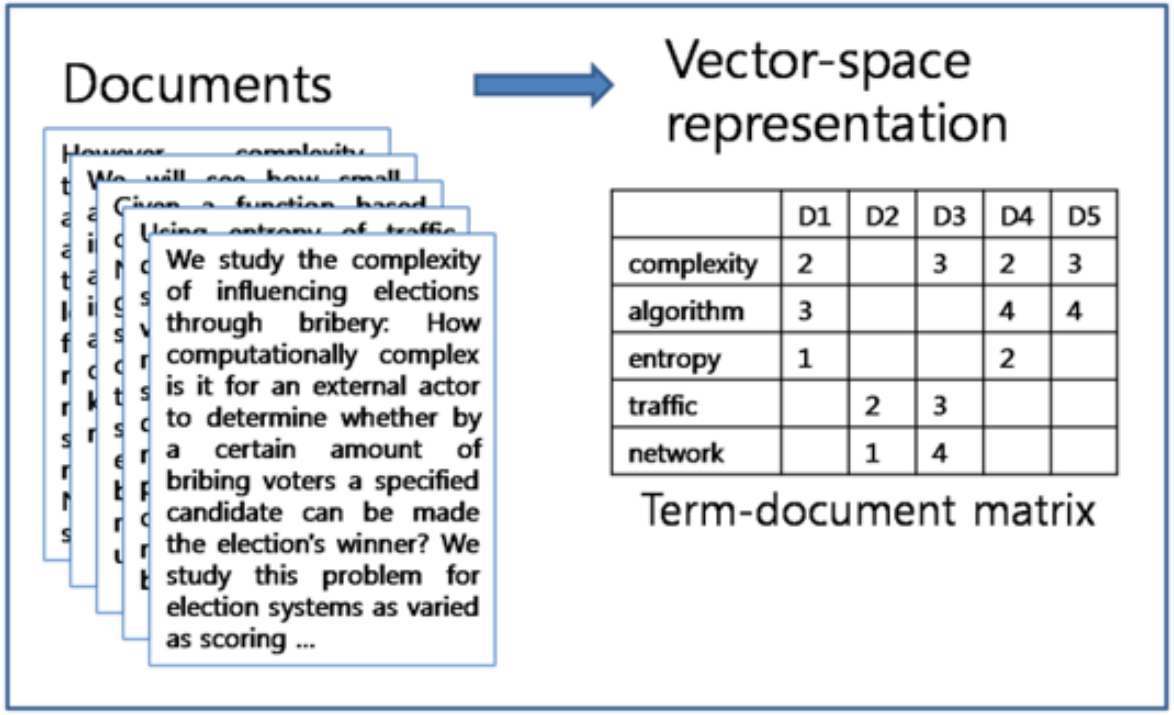


$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \quad (8, 8)$$

$$\begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ \vdots & \vdots & \vdots \\ x_{81} & x_{82} & x_{83} \end{bmatrix} \quad (8, 3)$$

Protein Sequence Feature Extraction

- term frequency - inverse document frequency (TF-IDF) algorithm is employed.
- This algorithm plays an important role in natural language process (NLP)
- polypeptide frequency is similar to the calculation process of TF in bioinformatics.



	D1	D2	D3	D4	D5
complexity	2		3	2	3
algorithm	3			4	4
entropy	1			2	
traffic		2	3		
network		1	4		

term	df_t	idf_t
car	18,165	1.65
auto	6723	2.08
insurance	19,241	1.62
best	25,235	1.5

$$idf_j = log\left[\frac{n}{df_j}\right]$$

Protein Sequence Feature Extraction

- term frequency - inverse document frequency (TF-IDF) algorithm is employed.
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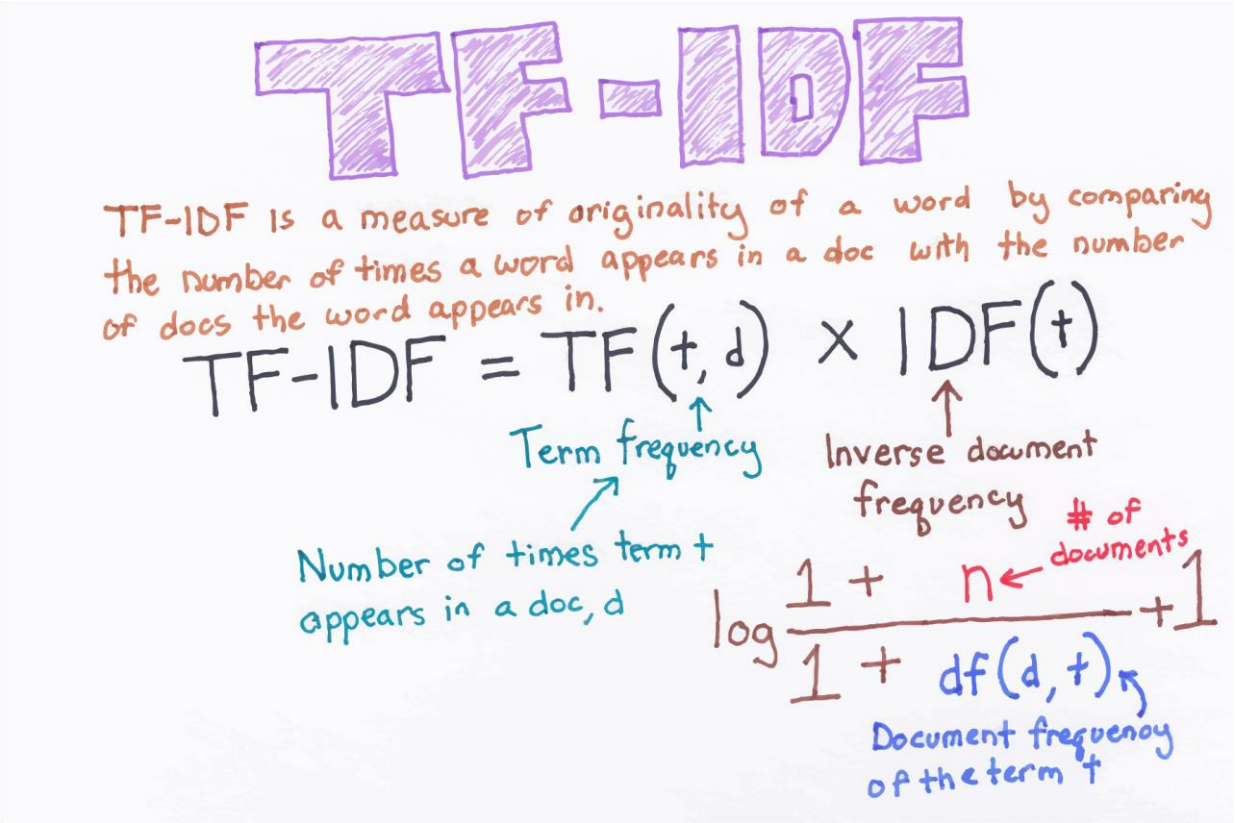
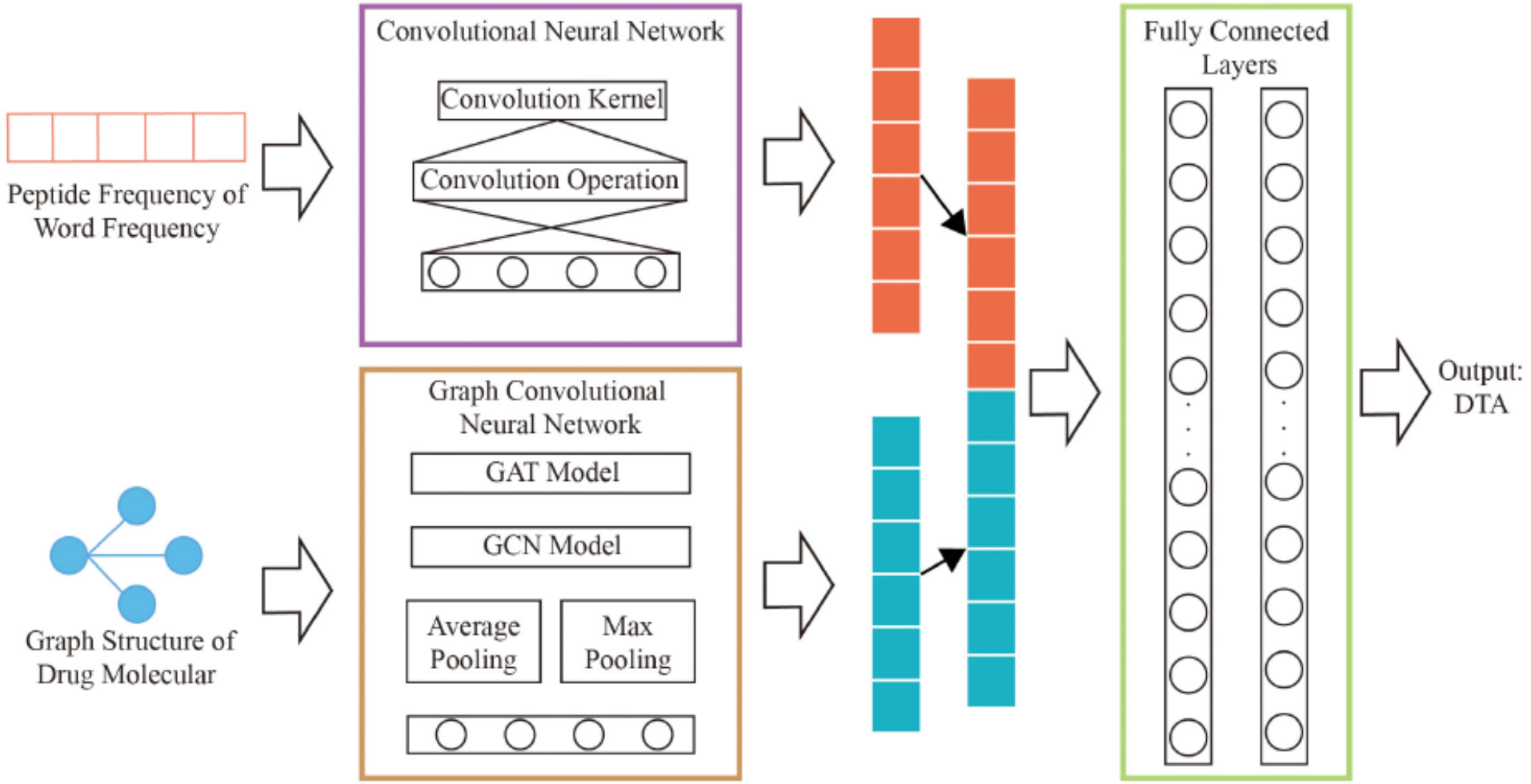


Network Model Construction



Result and Discussion

Features	KIBA		Davis	
	MSE	CI	MSE	CI
DeepDTA	0.194	0.863	0.261	0.878
WipeDTA	0.179	0.875	0.262	0.886
This model	**0.126**	**0.901**	**0.220**	**0.899**