

Deep Learning im

Ab-initio Electr



ray Photoelectron

Advisor : Heung-Sik. Kim
tory : Seong-Heum. Park

contents

01. Introduce of xps, deep learning

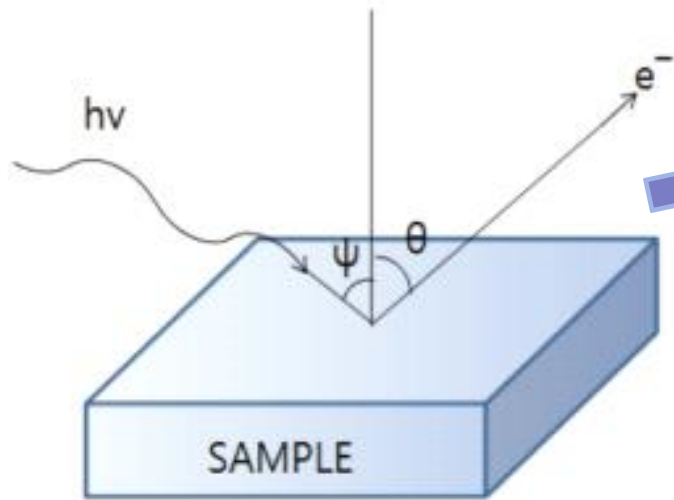
02. process of fitting program

03. result of fitting program

04. Conclusion

1-1.Introduction of xps

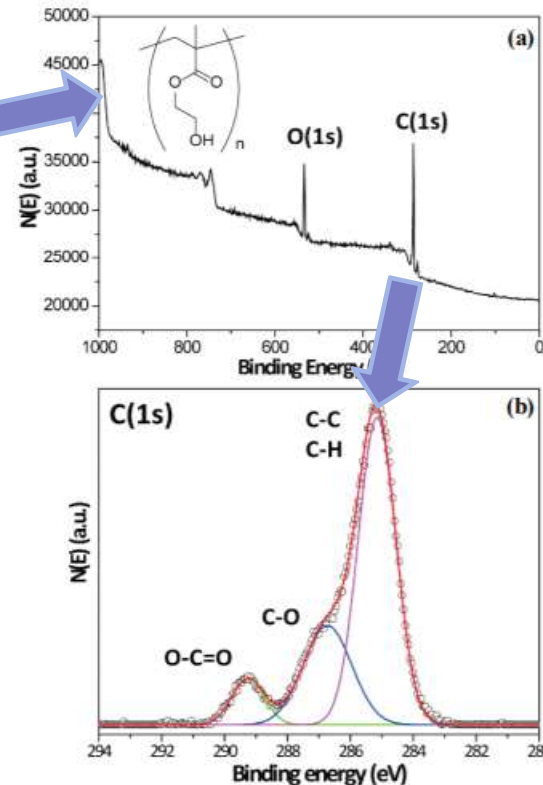
x-ray Photoelectron Spectroscopy(XPS)



$$E_K = h\nu - E_B - \phi$$

E_K = Kinetic Energy $h\nu$ = x-ray Energy

E_B = Binding Energy ϕ = work function



이전 선행연구 특징

*각 피크의 면적값(Area)

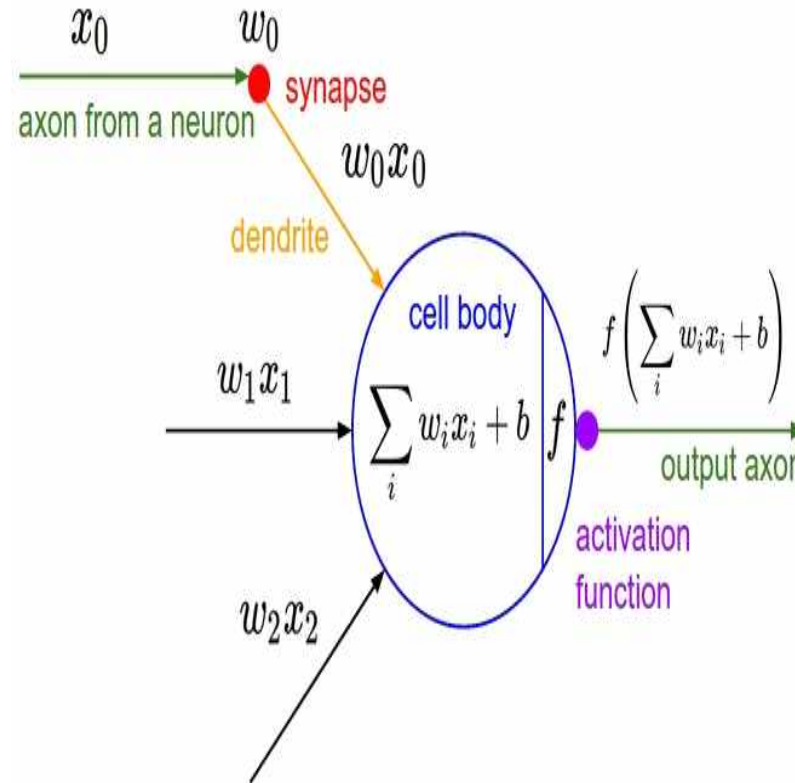
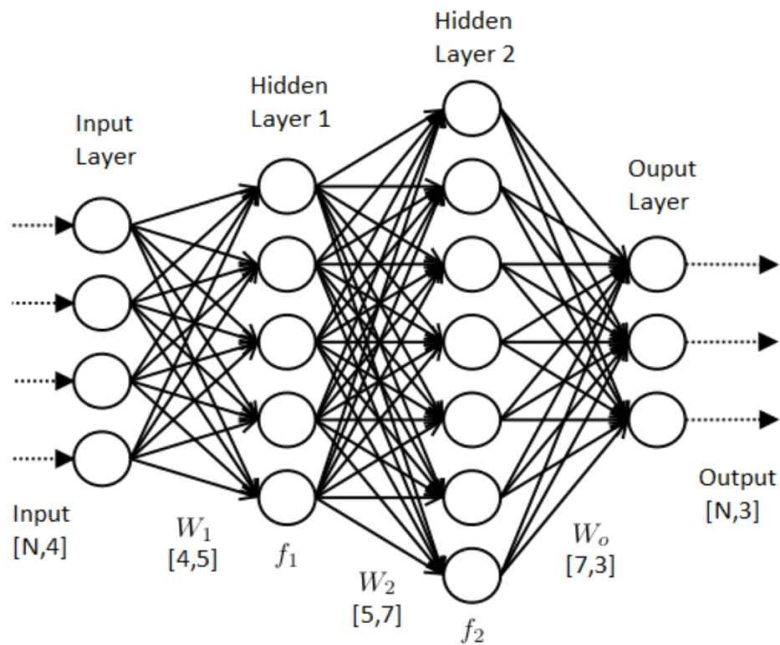
*피크의 개수,

*문턱값(Threshold)

*다음 피크선정의 최소높이값(prominences)등

다양한 parameter를 필요

1-2.Introduction of Artificial Neural Network

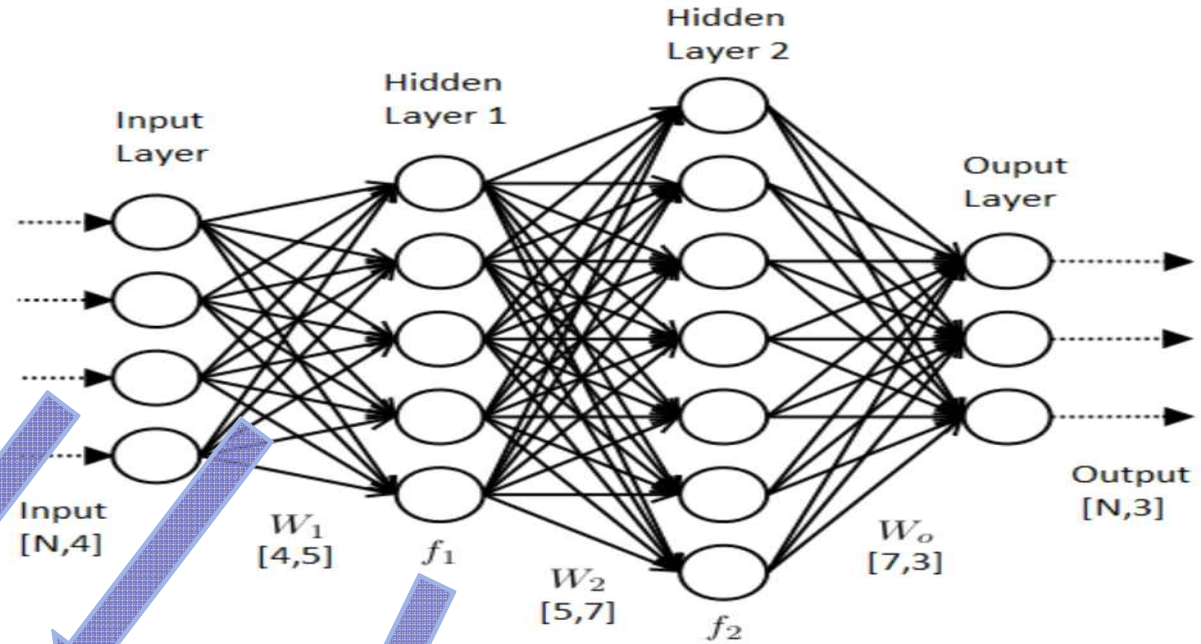
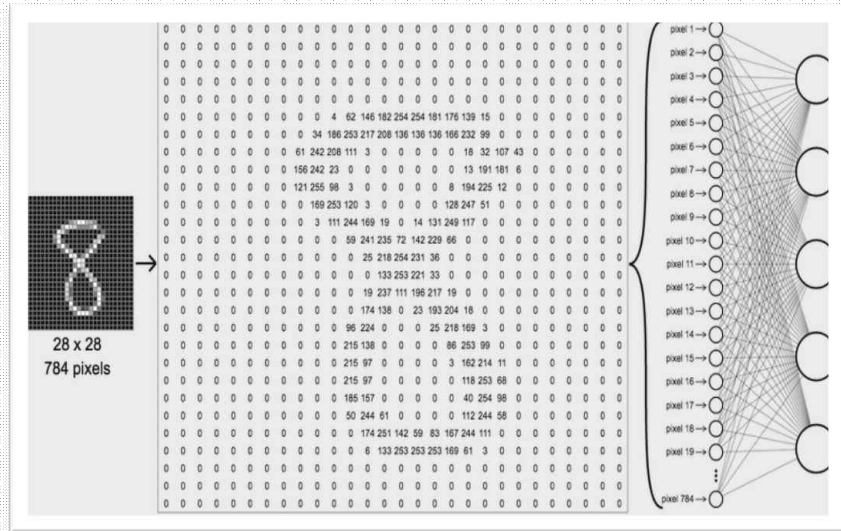


인공신경망을 통한 연구특징

*기본적인 peak의 amplitude, width, center, 등의 간단한 parameter만 학습에 필요

*학습후에는 parameter의 존재없이 data만으로 fitting 가능

1-2.Introduction of Artifical Neural Network



$$f \left[\begin{pmatrix} 8 & 7 & 4 & 9 \end{pmatrix}, \begin{pmatrix} 5 & 7 & 9 & 4 & 5 \\ 1 & 6 & 5 & 4 & 8 \\ 9 & 7 & 5 & 1 & 6 \\ 5 & 4 & 8 & 9 & 5 \end{pmatrix} \right] = (a, b, c, d, e)$$

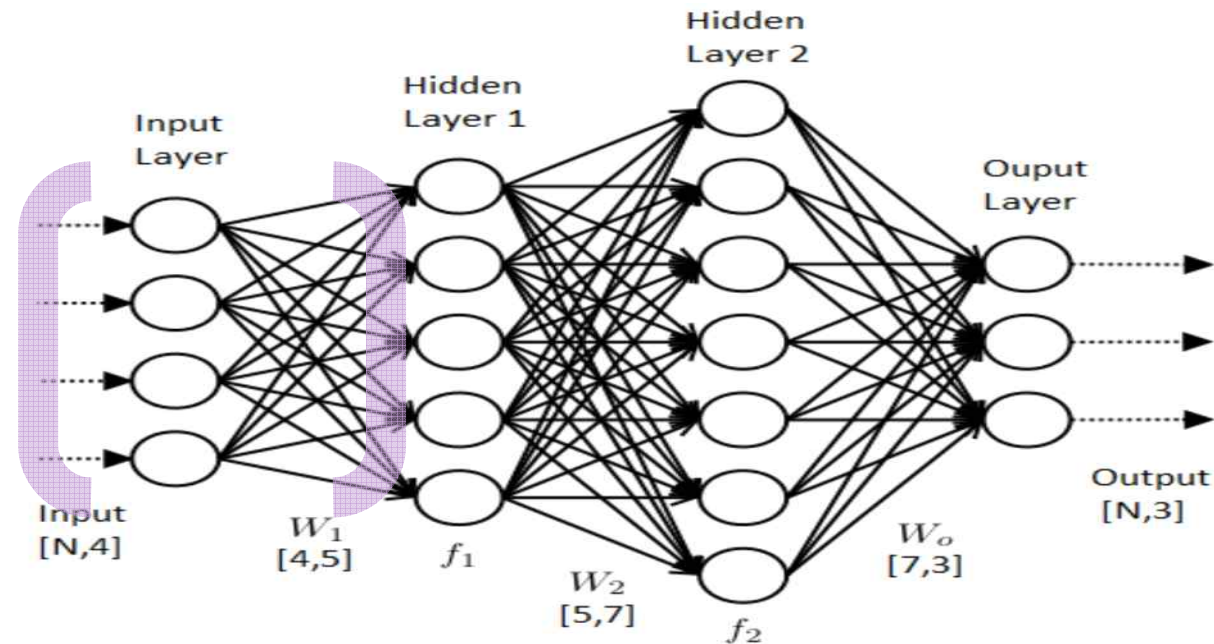
KEYWORD

1.WEIGHT

2.ACTIVATION FUNCTION

3.BACKPROPAGATION

1-2.Introduction of Artifical Neural Network



ACTIVATION FUCTION

$$f\left(\begin{bmatrix} 5 & 7 & 9 & 4 & 5 \\ 1 & 6 & 5 & 4 & 8 \\ 9 & 7 & 5 & 1 & 6 \\ 5 & 4 & 8 & 9 & 5 \end{bmatrix}\right) = (a, b, c, d, e)$$

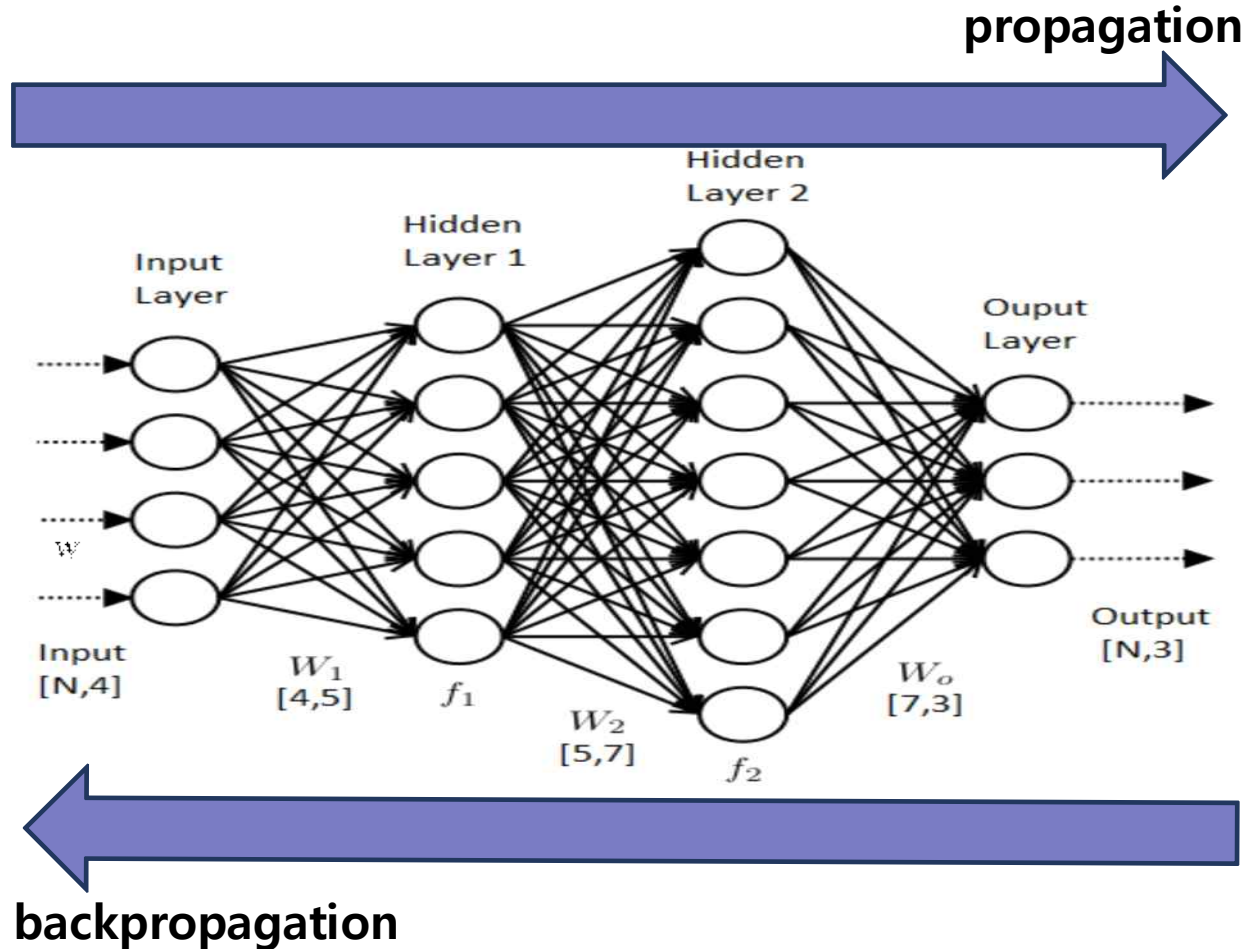
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1-2.Introduction of Artifical Neural Network



$$(1) \quad E_{o1} = \frac{1}{2} (target_{o1} - out_{o1})^2$$

$$(2) \quad W_5(t+1) = W_5(t) - \frac{\partial E_{total}}{\partial W_5}$$

$$(3) \quad \frac{\partial E_{total}}{\partial W_5} = \underbrace{\frac{\partial E_{total}}{\partial out_{o1}}}_{(1)} * \underbrace{\frac{\partial out_{o1}}{\partial net_{o1}}}_{(2)} * \underbrace{\frac{\partial net_{o1}}{\partial W_5}}_{(3)}$$

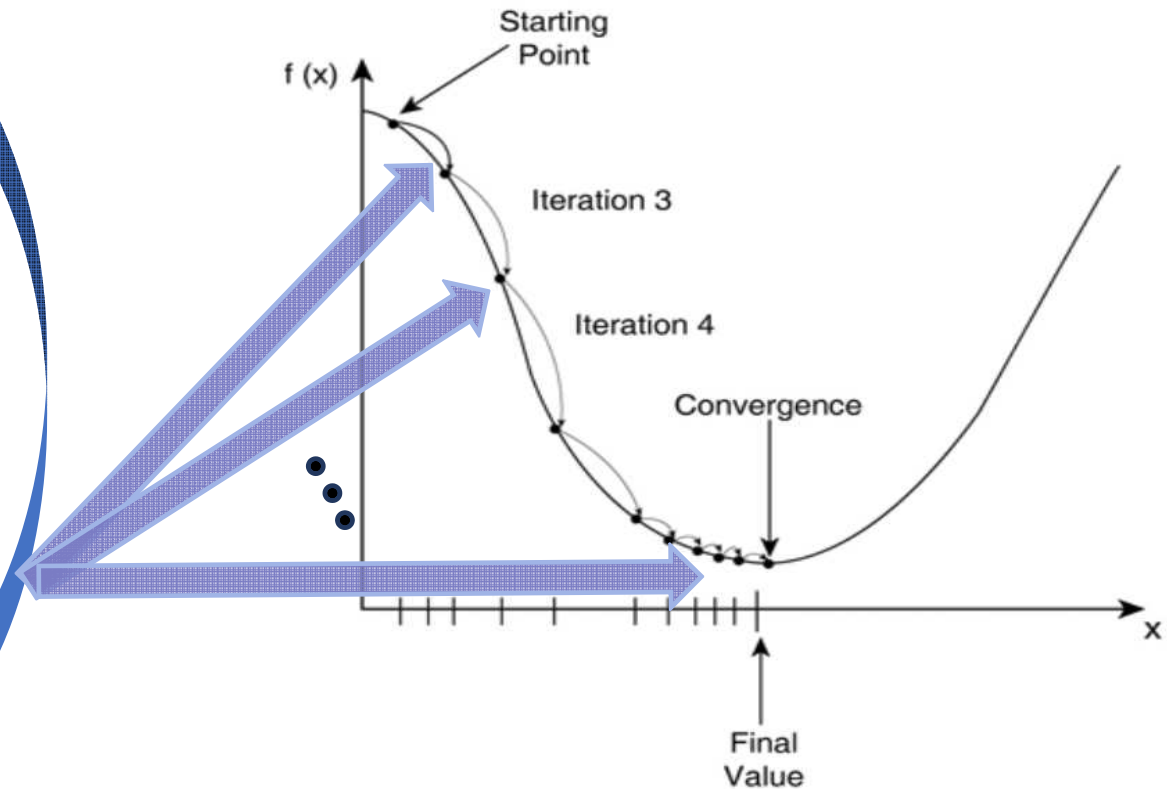
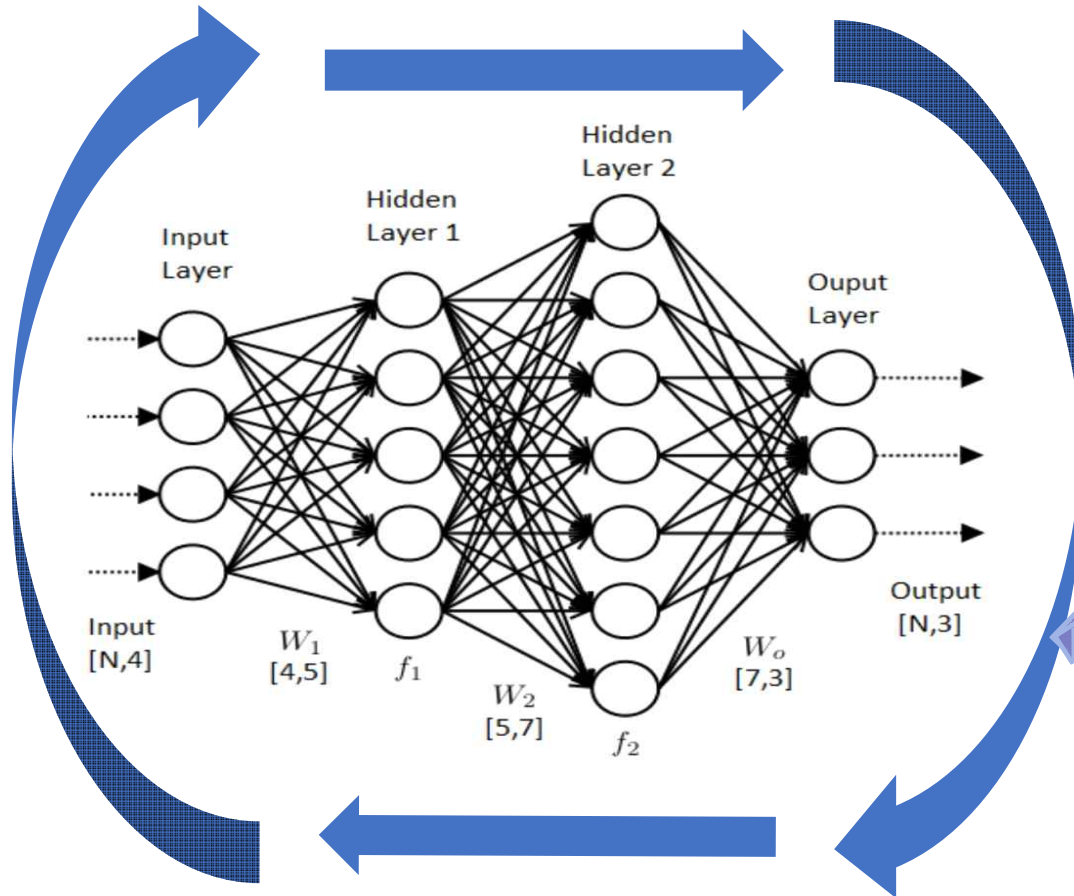
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02. process of fitting program

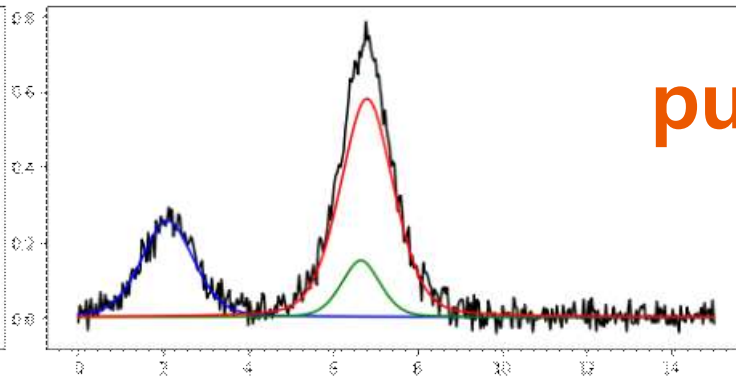
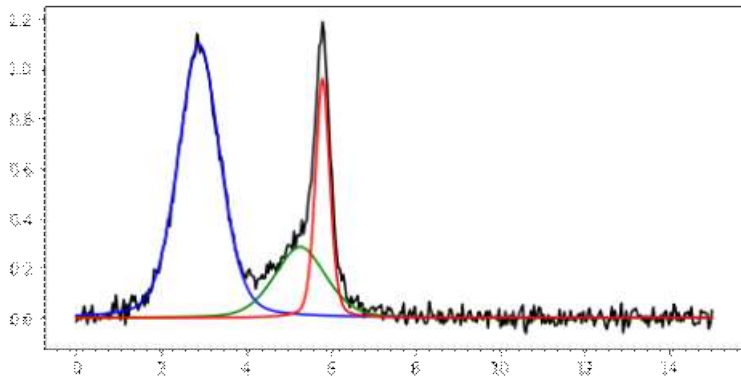
03. result of fitting program

04. Conclusion

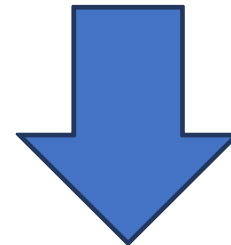
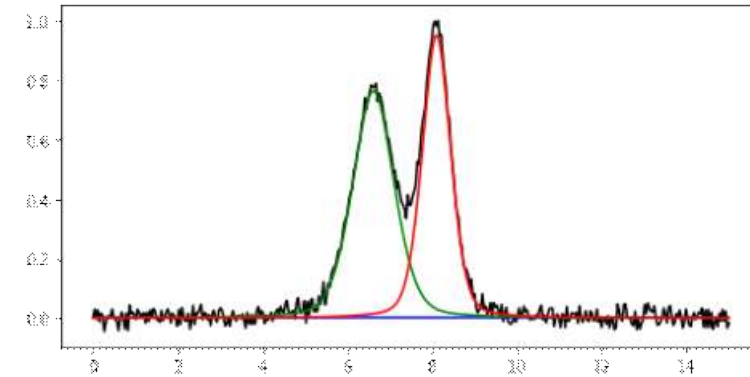
2-1. process of fitting program

voigt function:

$$f(w; w_0, I_0, w) = 0.7 e^{-\frac{w_G^2 (w - w_0)^2}{w^2}} + 0.3 \frac{1}{1 + \frac{w_L^2 (w - w_0)^2}{w^2}}$$

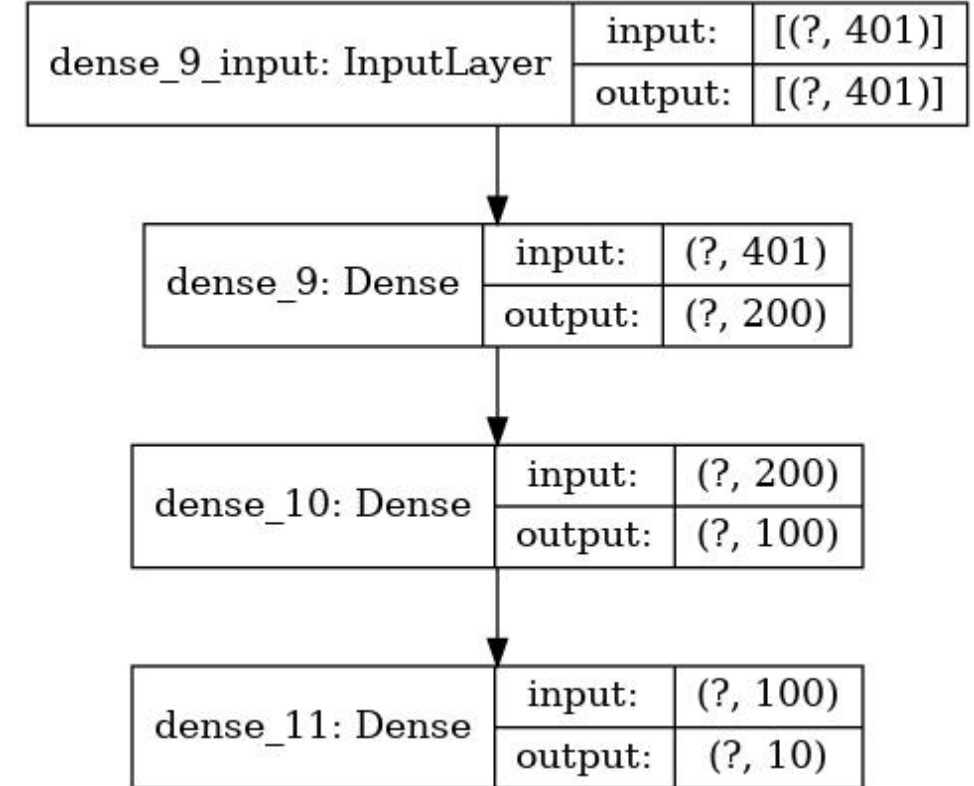
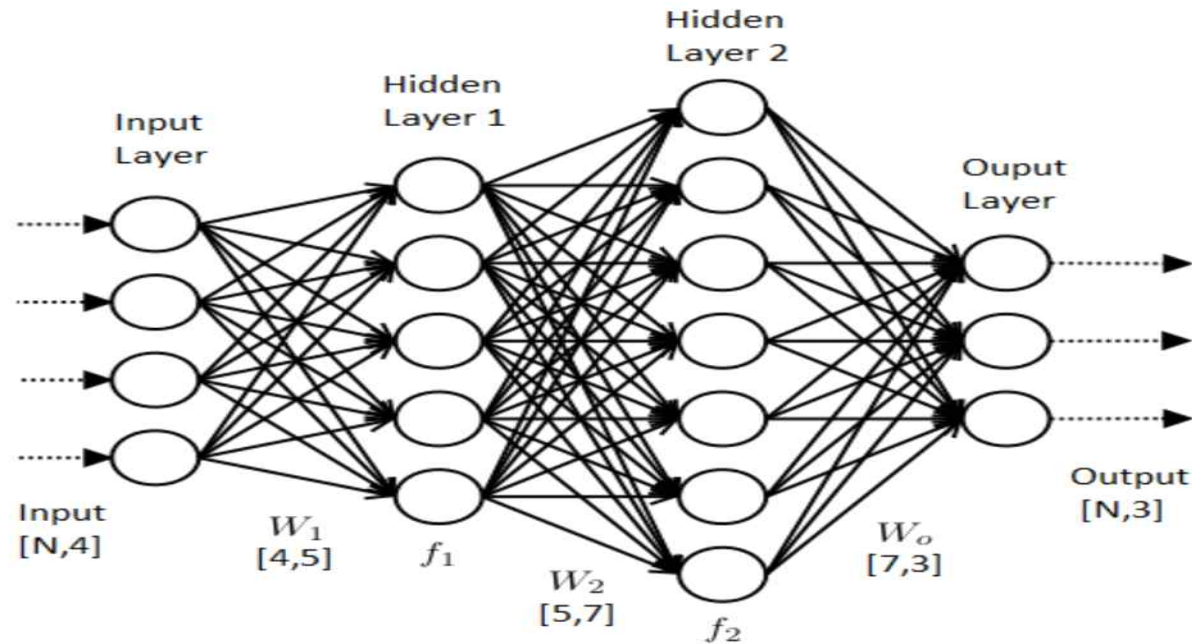


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200만개의 data 준비

2-1. process of fitting program



2-1. process of fitting program

200만개의 data



model1

dense_9_input: InputLayer	input:	[(?, 401)]
	output:	[(?, 401)]



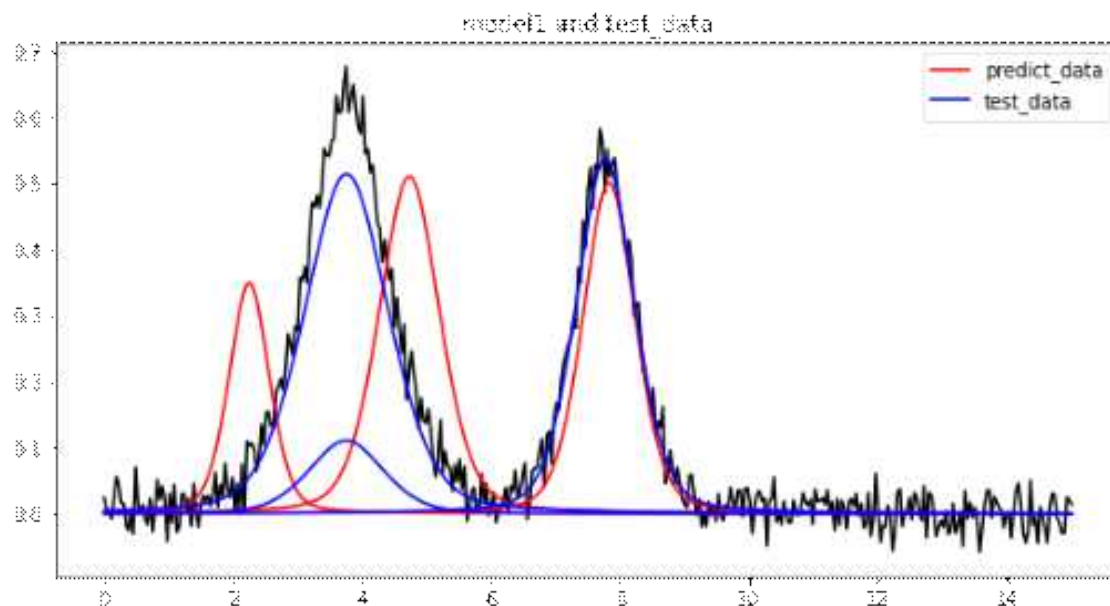
dense_9: Dense	input:	(?, 401)
	output:	(?, 200)



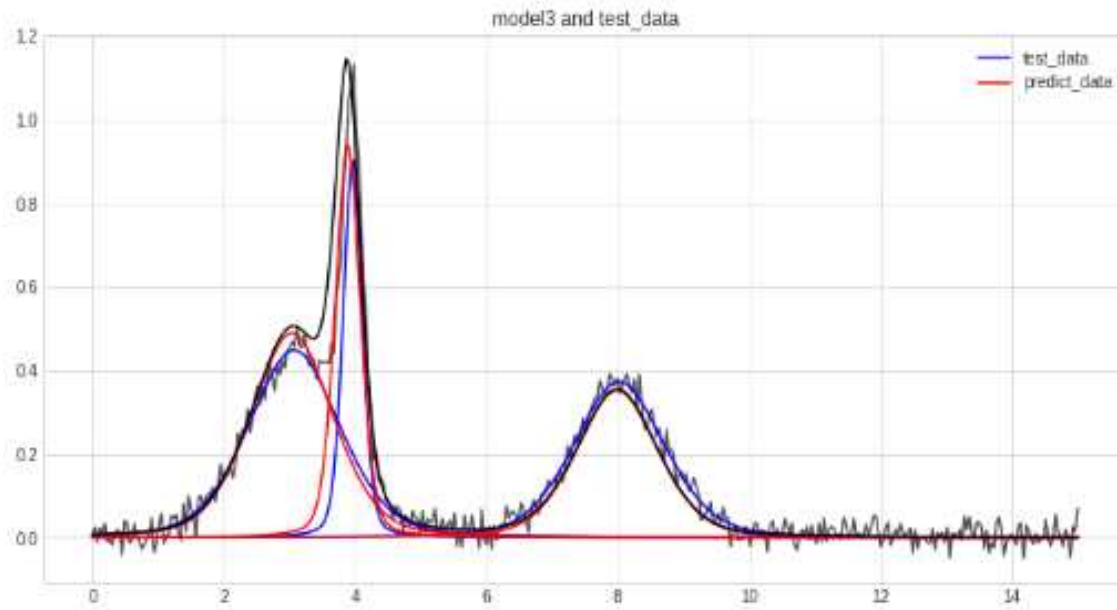
dense_10: Dense	input:	(?, 200)
	output:	(?, 100)



dense_11: Dense	input:	(?, 100)
	output:	(?, 10)



2-1. process of fitting program



2000만개의 data

model3



contents

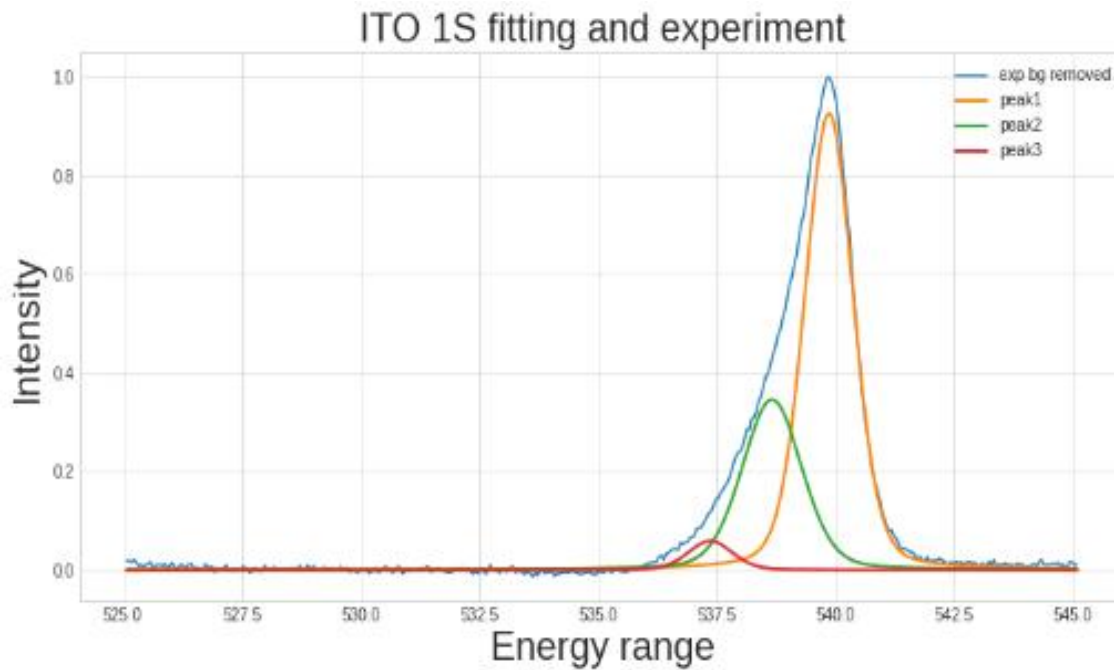
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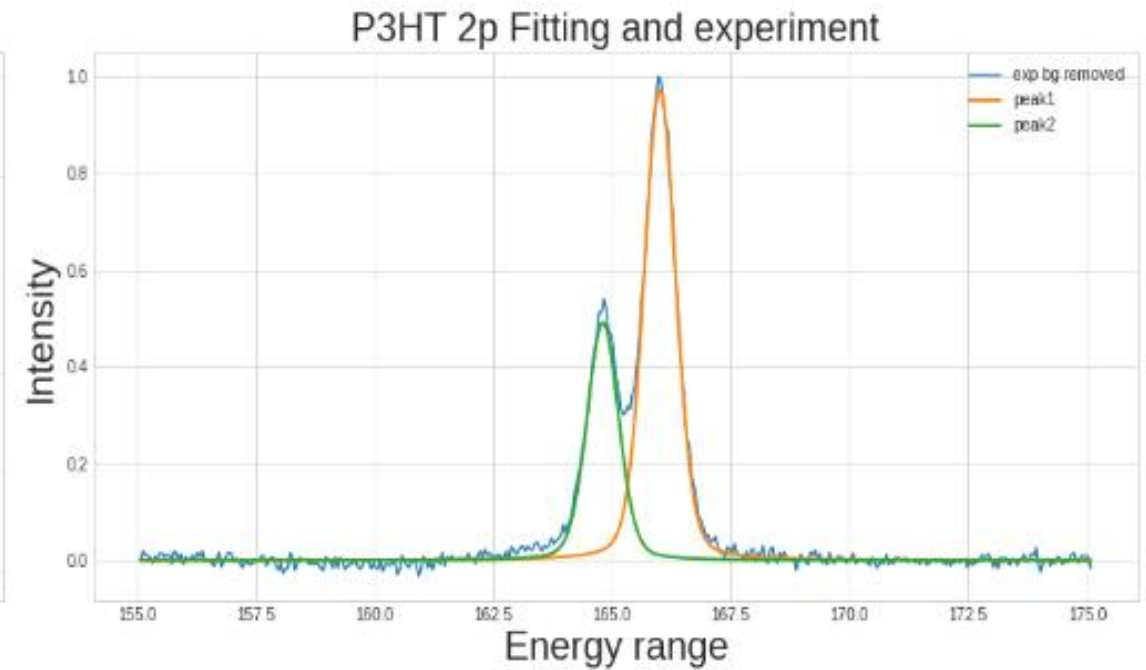
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04. result of fitting program

3-1. result of fitting program

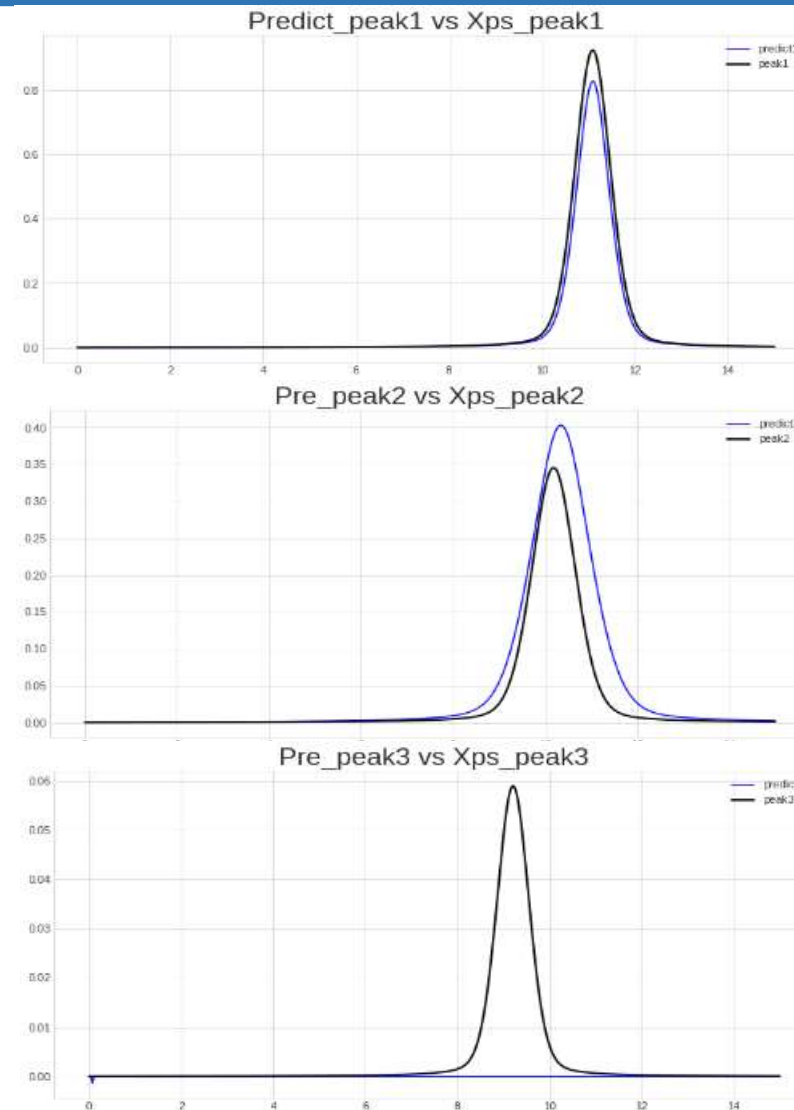
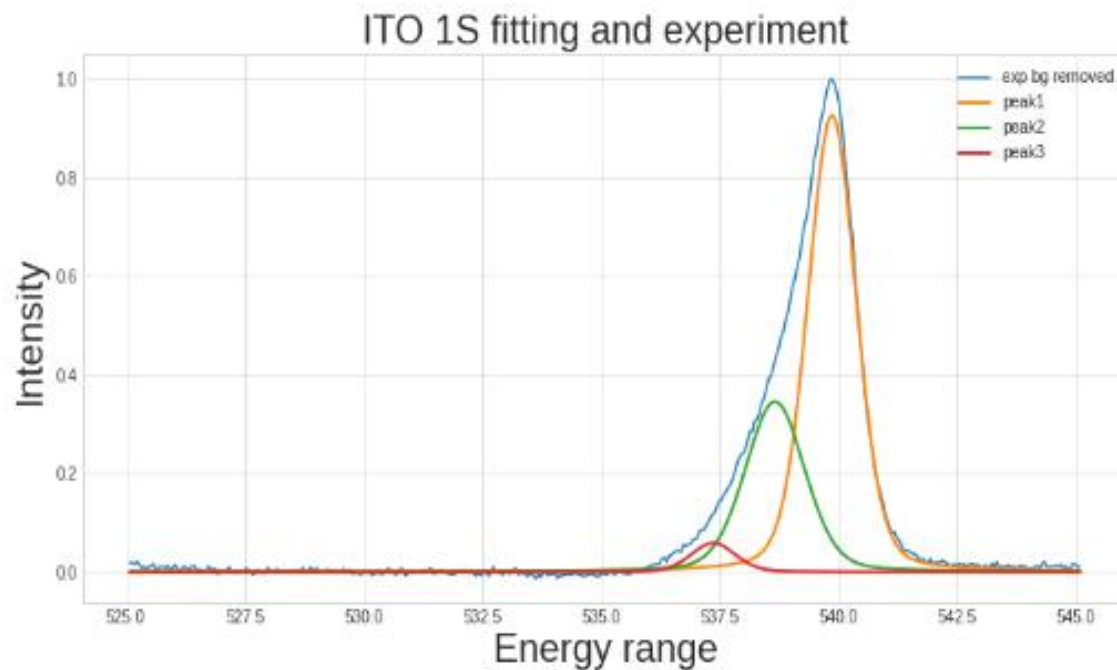


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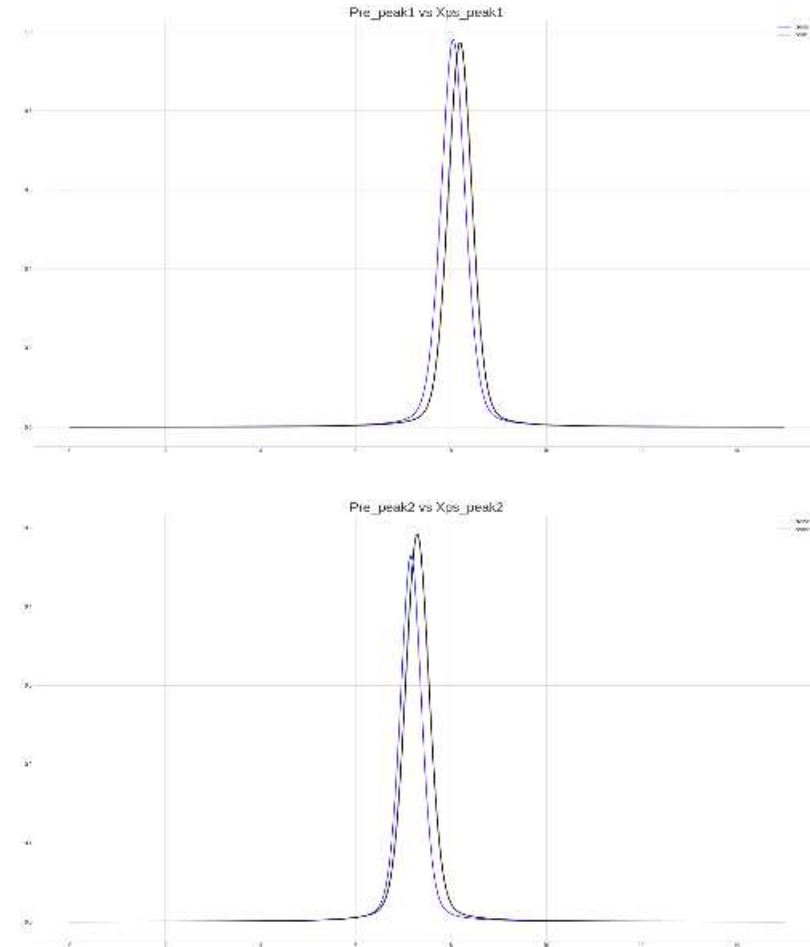
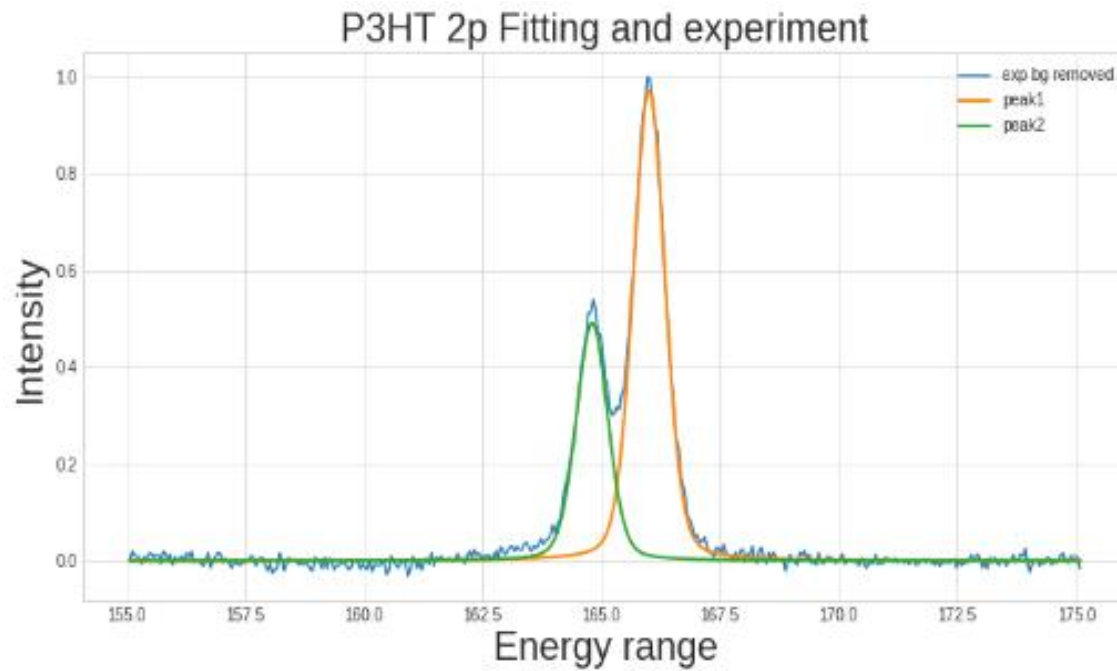


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3-2. result of fitting program



3-2. result of fitting program



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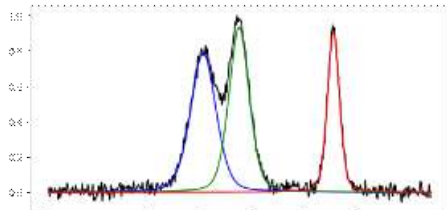
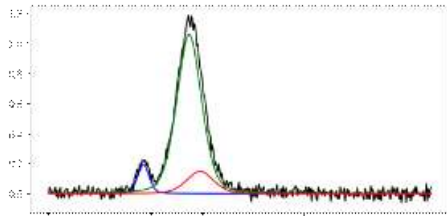
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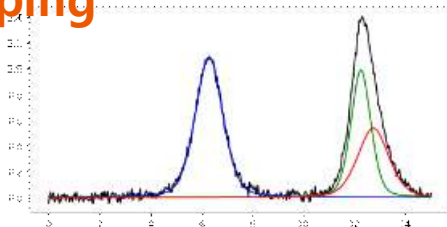
4. conclusion

$$f(w;w_0,I_0,w) = 0.7e^{-\frac{w_G^2(w-w_0)^2}{w^2}} + 0.3\frac{1}{1+\frac{w_L^2(w-w_0)^2}{w^2}}$$

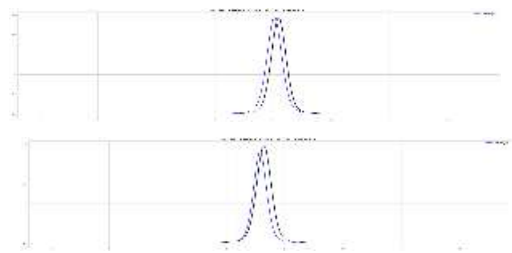
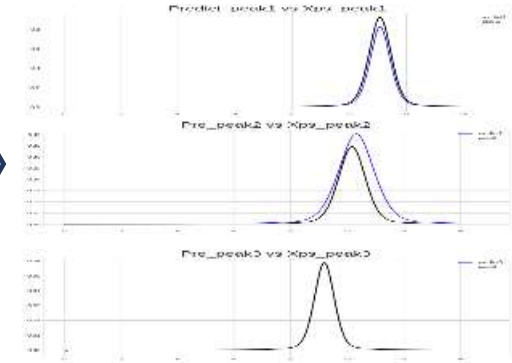
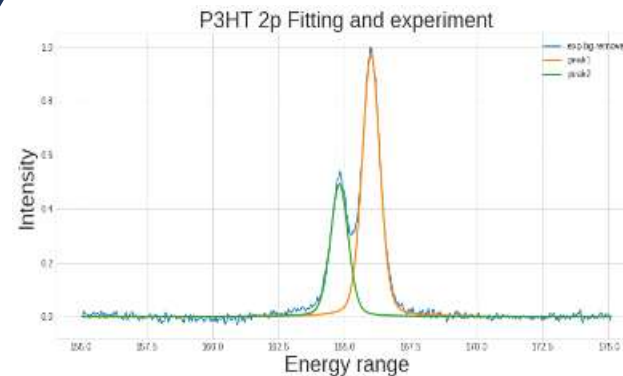
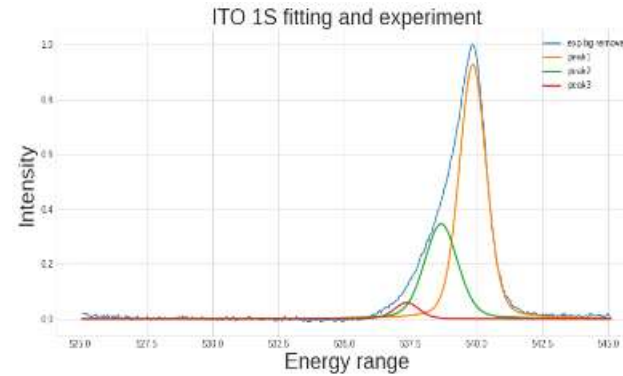
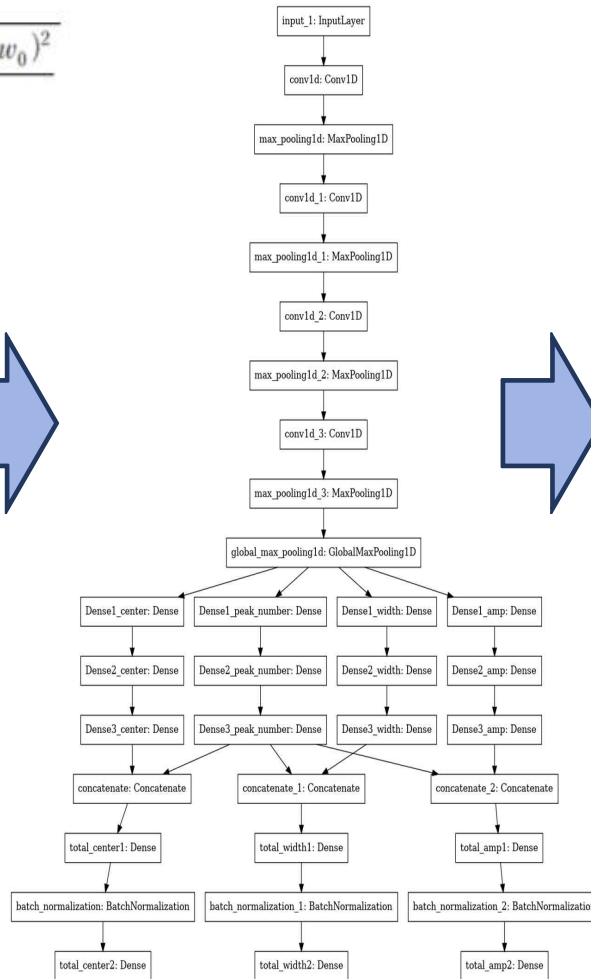


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model3



4. conclusion

앞으로의 방향과 개선점

- *데이터의 품질 개선

- *적절한 model을 design

- *Hyper parameter 설정

을 통해 더 높은 정확성을 올릴수 있도록 한다.

Q & A

Any Questions?



Thank you for your attention