Predicting properties of porous structure using three-dimensional convolutional neural networks with cuboid filter

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***Abstract*—The goal of this research is to predict Young's Modulus of porous structure and comparing the accuracy and efficiency between cube-shape and cuboid-shape Convolutional Neural Network filter.**

I. Introduction

Last 10 years, 3-D printer has taken one of the major roles in the industry. The main trade-off in 3-D printing is the 'time' and the 'strength & stiffness'. If the printed stuff is filled with 100% density, It might take too much time to print and consume too much materials even though it can assure the strength.

So most of the commercial 3-D printing software gives the options of filling with simple, regular patterned grids, whose characteristic can be analyzed linearly. A structure with irregular patterns take more computational costs to analyze the characteristic and it's not commonly supported in the normal 3-D printing software.

Still, irregular patterns like porous structure are useful in many cases, especially in medical industry and space industry since it can give many practical aspects like low thermal conductivity, light weight, similarity with human tissue(e.g. bone).

The conventional method to analyze the characteristic of the complex structure is a numerical method, Finite Element Analysis. It subdivides a large system into smaller parts(finite elements) and nodes, enables to change the complex, non-linear system into the assembly of simple linear equations. This method assures accuracy if the structure is divided into smaller units, which cause heavy computational cost.

So we found the demand of the faster and reliable way to analyze the characteristic of the non-linear structure, compared to the conventional method.

Nowadays, applying deep learning method is becoming a trend in many research field, especially when it comes to classification and numerical prediction. And the invention of the Convolutional Neural Network(CNN) led vision-based research in another level.

Sometimes we roughly predict the strength of the structure just by looking. Getting insight from this concept, many researches has been held using 3-D CNN to predict the characteristic of the structure. [1-4]

Conventional CNN use cube shaped filters which have same length in every axis. We thought the connection between the elements in the direction of the external force(e.g. x) affects more than the connection in perpendicular direction(e.g. y or z).

In this research, we predict the Young's modulus of the representative volume element(RVE) of porous structure by using 3-D CNN with cuboid shaped filter which has longer side in the direction of the external force. Thereby we achieve less computational cost and higher accuracy simultaneously.

II. Related Works

Yang, Zijiang, et al. have suggested applying 3-D CNN to predict properties of RVEs exceeds simple physics-based approaches by 54% in 2018 [1]. And compared 3-D CNN method against traditional machine learning method with fully connected layers, suggesting the potential to apply the transfer learning in 2019. [2] Cecen, Ahmet, et al. have suggested to utilize both CNN and higher order spatial statistics to predict the properties of the material in 2018. [3] We could get insights on training neural network with small dataset by using shallow network.

III. Dataset Generation

Using a commercial material analysis software 'Digimat', we generated RVEs with porous structure. Since Digimat only runs on GUI environment, we made a script using python package 'pyautogui' to automate to produce datasets by controlling the mouse and keyboard.

The matrix material is Acrylonitrile Butadiene Styrene copolymer(ABS). The density of it is in range of 1010 1210 (kg/m3), the Young's Modulus is in range of 1.19×10^9 - $2.9 \times 10^9 (Pa)$, and the Poisson's ratio is 0.35 [4]. We use approximations of these as shown in the table **??**.

ABS Material Properties	
Density	1100 (kg/m^3)
Young's Modulus	2 $\times 10^9 (Pa)$
Poisson's ratio	0.35

Each RVE has 30-50 void ellipsoid inclusions whose aspect ratio is between 1 - 4 with total 5% - 20% of volume fraction.

The reason of the small volume fraction is the error of Digimat while consisting the geometry with bigger volume fraction.

Fig. 1: Inclusion shape change by aspect ratio

The number of inclusions, total volume fraction, aspect ratio of each RVE are distributed based on random uniform distribution. The size of the mesh is 30 x 30 x 30 and consisted with voxels. It is converted into numpy array whose elements are filled with 1 if there is a material, and 0 if there is not.

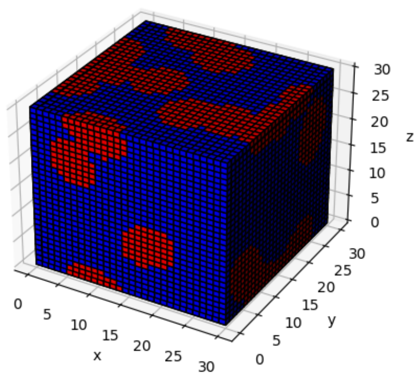


Fig. 2: Visualized numpy array of mesh data

The target data(label) is the Young's modulus of the RVE in x direction, $E11$. Total dataset size is 6000. 4720 of them are used as training data, 1280 as validation data, 100 as test data. It took 1.5 minutes of computing time to generate a data (150 hours totals)

IV. Method

A. 3-D Convolution

$$(f * g)(t) = \int_0^t f(\tau)g(t-\tau)d\tau$$

The convolution is defined as the integral of the product of the two functions after one is reversed and shifted. The expression above is a discrete form. It is well known in deep learning that the use of a convolutional layer rather than a fully connected layer allows the model to be more flexible and retain more geometric data. We apply 3-D convolutional layer with filters that moves in three perpendicular directions to keep the valuable data of connections between voxels.

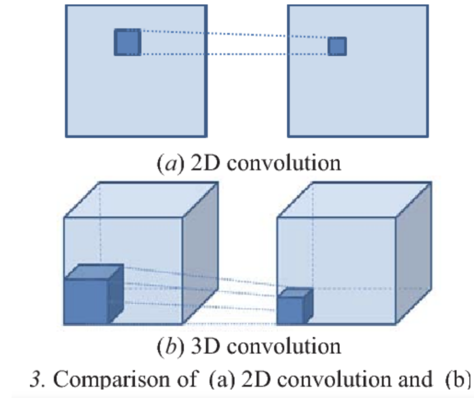


Fig. 3: Image: Lung nodule detection based on 3-D convolutional neural networks, Fan et al [5]

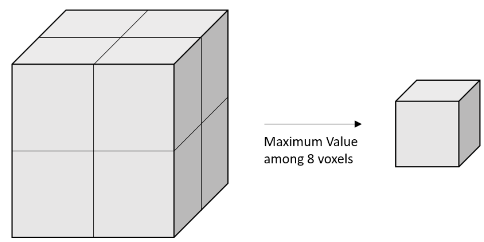


Fig. 4: 3D Max Pooling

B. 3-D Max Pooling

The max pooling helps to avoid overfitting by reducing parameters and leaving only important data(dominant value). We use 3-D max pooling method which convey the maximum value among 8 voxels.

C. Loss Function

We use Mean Absolute Percentage Error (MAPE) as our loss function. The major reason using the method is to regularize the loss. If not, the loss would explode because of the mesh size(27,000 voxels). The definition is as below.

$$loss = 100 \times \frac{|true - prediction|}{true}$$

D. Stochastic Gradient Descent

Because of the huge time spent on analyzing the structure with FEM, the size of the dataset is not big compared to most of the other deep-learning project. So we decided to use Stochastic Gradient Method(SGD), which updates parameters with every data. The problem of local minima can be solved by using SGD because every data has different vector space of loss. We applied Adam [6] as an updating method.

E. Rectified Linear Unit

Rectified Linear Unit(ReLU) is widely used activation function and defined as below.

$$f(x) = max(0, x)$$

It prevents the gradient descent problem which can appear in the deep neural network, and it is computationally efficient for simple calculation. Since our models don't have deep structure and use SGD which take time longer than Mini-batch Gradient Descent, we decided to use ReLU as the activation function to take advantage of calculation.

F. Models

Model: "model_basic"

Layer (type)	Output Shape	Param #
Conv3D	(None, 28, 28, 28, 32)	896
MaxPooling3D	(None, 14, 14, 14, 32)	0
Conv3D	(None, 12, 12, 12, 32)	27680
MaxPooling3D	(None, 6, 6, 6, 32)	0
Flatten	(None, 6912)	0
Dense	(None, 256)	1769728
Dense	(None, 1)	257

Total params: 1,798,561
Trainable params: 1,798,561
Non-trainable params: 0

Model: "model_advanced"

Layer (type)	Output Shape	Param #
Conv3D	(None, 19, 28, 28, 32)	3488
MaxPooling3D	(None, 9, 14, 14, 32)	0
Conv3D	(None, 4, 12, 12, 32)	55328
MaxPooling3D	(None, 2, 6, 6, 32)	0
Flatten	(None, 2304)	0
Dense	(None, 256)	590080
Dense	(None, 1)	257

Total params: 649,153
Trainable params: 649,153
Non-trainable params: 0

Fig. 5: Neural Network structures of basic(with cube filter) model and advanced(with cuboid filter) model

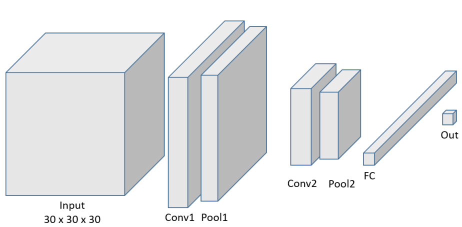


Fig. 6: Model visualization

We compared two different CNN models. Both are consisted with 2 Convolution & Max pooling layers and 2 Fully Connected layers as shown in Fig. 3. The only difference is the size of the filter. The basic model uses the cube-shape filter(3x3x3). The advanced model uses the cuboid-shape filter which is longer in the direction of the external force(in this case, x). The cuboid-shape filter has the length of 12 in the first convolution layer and 6 in the second.

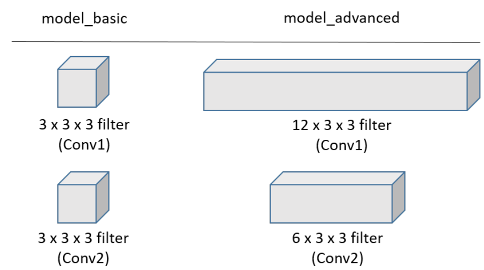
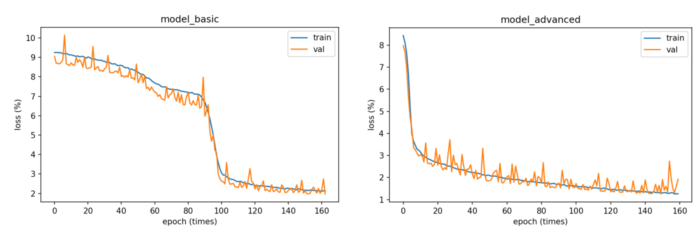


Fig. 7: cube cuboid shape filters

V. Results



(a) model with cube filter (b) model with cuboid filter

Fig. 8: Loss vs Epochs graph

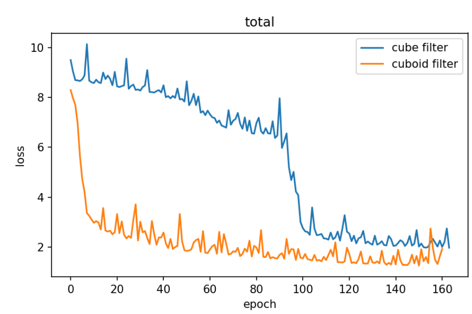


Fig. 9: Comparison of loss vs epochs between both models

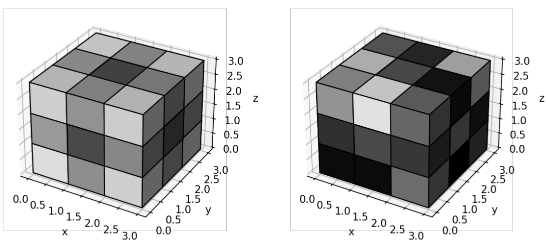
As shown in Fig.8-9, the model with cuboid shape CNN filter shows better learning characteristics and less loss(thus, the accuracy is higher), compared to the model with cube shape filter. Both model shows stable learning curve without gross overfitting and converge at epochs of 160 170.

average error rate	
cube filter	1.99 %
cuboid filter	1.84 %

The average error rate on 100 test dataset is as above. The measuring method is MAPE. The model with cuboid filters outperforms others by 8% in relatively.

Computing time	
FEM	32.51 s
CNN	0.047 s

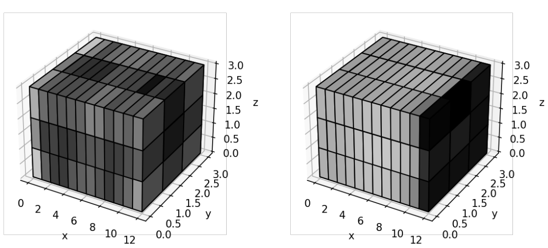
Both models also show much faster computing time than the conventional method, FEM.



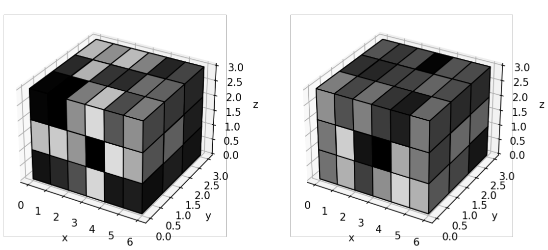
(a) Conv1 (b) Conv2

Fig. 10: Visualization of cube filters (basic model)

We can check filters of the basic model in Fig. 10. In the first layer, each filter looks similar. But in second layer, filters shows widespread distribution and various shapes compare to other filters in the same layer.



(a) Conv1 (b) Conv1



(c) Conv2 (d) Conv2

Fig. 11: Visualization of cuboid filters (advanced model)

Similar happens in the advanced model(Fig. 11). We can infer that filters in the deeper layer are trained to detect more specific characteristics.

VI. Conclusion

In this research, we verified our assumption that the cuboid CNN filter, which is longer in the direction of external force, can achieve better learning characteristic and higher prediction accuracy. The visualization of filters shows that filters are trained to detect characteristics of the structure. It seems that the filter works well because the connection between elements in the direction of external force delivers a greater impact. Applying 3-D CNN on analyzing characteristics of the structure has a great advantage in time compared to the conventional method. Though it shows lower accuracy than the conventional method until now, the neural network offers a great potential because it has proved that the performance of it increases in proportion with the size of the dataset. We expect more sophisticated neural networks that can analyze the complex material with lower computing power and higher accuracy in further research.

References

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