

A Multi-fidelity Prediction with Convolutional Neural Networks Using High-Dimensional Data¹

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Outline

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Introduction



- Multi-fidelity (MF) = High-fidelity (HF) + Low-fidelity (LF)
- Low number of high-fidelity data, high number of low-fidelity data
- > Predictions as accurate as high-fidelity data
- Relatively cheaper than high-fidelity data
- Highly appealed in design optimization and uncertainty quantification due to efficiency.
- Multi-fidelity deep neural networks¹ (MFDNN) was proposed recently.
- In this study, we propose two novel neural network architectures tailored for high-dimensional inputs.
- The proposed architectures outclasses the MFDNN in the high-dimensional aerodynamic problem.



¹Meng, X., and Karniadakis, G. E., "A composite neural network that learns from multi-fidelity data: Application to function approximation and inverse PDE problems," Journal of Computational Physics, Vol. 401, 2020, p. 109020.3

Multi-fidelity Deep Neural Networks

- It makes both LF and HF predictions with a model.
- An MFDNN model consists of 3 subnetworks
 - > NN_L : Low-fidelity estimator
 - **NN_{H1} :** Linear correlation network
 - **NN_{H2} :** Nonlinear correlation network
- NN_L takes low-fidelity inputs and makes low-fidelity predictions.
- Correlation networks take the stacked high-fidelity input and low-fidelity predictions.
- NN_{H1} approximates the linear correlation between HF and LF data.
- NN_{H2} approximates the nonlinear correlation between HF and LF data.



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Figure: A generic MFDNN architecture.

Autoregressive scheme¹:

 $y_H(x,y_L) = \omega \mathcal{F}_l(x,y_L) + (1-\omega) \mathcal{F}_{nl}(x,y_L)$

- $\succ \text{ NN}_{\text{H1}} = \mathcal{F}_l(x, y_L), \text{ NN}_{\text{H2}} = \mathcal{F}_{nl}(x, y_L)$
- NN_{H1} only consists of linear layers because it is supposed to learn the linear correlation.
- NN_{H2} consists of the combination of linear and nonlinear layers.
- MFDNNs work very well with lowdimensional inputs and predictions.



¹Meng, X., and Karniadakis, G. E., "A composite neural network that learns from multi-fidelity data: Application to function approximation and inverse PDE problems," Journal of Computational Physics, Vol. 401, 2020, p. 109020.5 Multi-fidelity Deep Neural Networks – Drawback 1

The input of correlation networks use the concatenated high-fidelity input $\mathbf{x}_{\mathbf{H}} \in \mathbb{R}^{N_{H}}$ and low-fidelity predictions $\mathbf{\hat{y}}_{\mathbf{L}} \in \mathbb{R}^{M_{L}}$.

 $\mathbf{x}_{\mathbf{C}} \in \mathbb{R}^{N_H + M_L}$

If the input size N_H is larger enough than the prediction size M_L ($M_L << N_H$), the prediction is ignored during training.

This is an issue in case of highdimensional inputs such as flow fields.

$$y_H(x, y_L) = \omega \mathcal{F}_l(x, y_L) + (1 - \omega) \mathcal{F}_{nl}(x, y_L)$$



Figure: A generic MFDNN architecture.



As a remedy of the first drawback,

- We adapted the MFDNN by adding a fullyconnected encoder.
 - > NN_{xH} : A fully-connected encoder
- NN_{XH} contains only linear layers and maps high-dimensional inputs onto lowerdimensional subspaces.
- > Thus, input sizes get closer to the low-fidelity predictions $\mathbf{\hat{y}}_{L} \in \mathbb{R}^{M_{L}}$.

$$NN_{XH}: \mathbb{R}^{N_H} \to \mathbb{R}^{\tilde{N}_H}$$

$$\mathbf{x}_{\mathbf{H}} \in \mathbb{R}^{N_{H}} \longrightarrow \tilde{\mathbf{x}}_{\mathbf{H}} \in \mathbb{R}^{\tilde{N}_{H}}$$

$$\tilde{N}_{H} \approx M_{L} << N_{H}$$

This architecture improves the multi-fidelity prediction.



- In addition, MFDNN can only process vector or scalar inputs.
- Flow fields compose highly correlated regions and are represented with matrix/tensor notation.
- Thus, each flow field must be vectorized to be processed by an MFDNN.
- Vectorization dislocates highly correlated vertices on a flow field.
- Thus, it causes a loss of correlation information on the data.



Figure: A generic MFDNN architecture.



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As a remedy of the second drawback,

- We employed convolution layers to process inputs within a matrix/tensor form.
- Vectorization is prevented so does the loss of information.
- > It also includes a convolutional encoder, NN_{XH} .
 - NN_{XH} : Convolutional encoder
- NN_{XH} contains only convolution layers and maps high-dimensional inputs onto lower-dimensional subspaces similar to the modified-MFDNN.
- Unlike previously presented methods, lowfidelity estimator, NN_L, is a convolutional neural network.

$$y_H(x, y_L) = \omega \mathcal{F}_l(x, y_L) + (1 - \omega) \mathcal{F}_{nl}(x, y_L)$$



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> Pressure coefficient fields are used as the input.

Each flow domain is interpolated onto 64-by-64 Cartesian grid using linear interpolation.

Interpolation makes geometry obscure but preserves the gradients on the flow field well!

>Min-max normalization is used on the dataset.

<code>>Low-fidelity input data $\mathbf{x}_L \in \mathbb{R}^{300 imes 64 imes 64}$ </code>

<code>>High-fidelity input data $\mathbf{x}_{H} \in \mathbb{R}^{100 imes 64 imes 64}$ </code>

▶85%-15% training and test split ratio is used.
10



Figure: An interpolated flow domain.



MFDNNs with 3 set of learnable parameters are	$N_{ heta}$	NS_H	LF-RMSE	MF-RMSE
tested.		10	0.0177	0.0458
Parameter sizes: 2.4e6, 4.6e6, 10.9e6	2.4×10^{6}	50	0.0177	0.0483
		100	0.0177	0.0477
Linear layers and rectified linear units are employed.		150	0.0177	0.0296
Pressure coefficient fields are vectorized.		200	0.0177	0.0473
$\tilde{\mathbf{z}}$ \sim $\mathbb{D}300 \times 4096$ $\tilde{\mathbf{z}}$ \sim $\mathbb{D}100 \times 4096$		10	0.0142	0.0447
$\mathbf{x}_L \in \mathbb{R}$ $\mathbf{x}_H \in \mathbb{R}$	4.6×10^{6}	50	0.0142	0.0481
Increasing high-fidelity sample size, NS_H , is used.		100	0.0142	0.0475
All MFDNNs yields comparable and unsatisfactory results in terms of MF-RMSE.		150	0.0142	0.0330
		200	0.0142	0.0480
		10	0.0177	0.0449
Higher number of high-fidelity data does not affect the	10.9×10^{6}	50	0.0177	0.0484
prediction accuracy!		100	0.0177	0.0484
It can be concluded that the MFDNN is not able to		150	0.0177	0.0322
learn the correlation between the HF and LF data.		200	0.0177	0.0486
	MFDNNs with 3 set of learnable parameters are tested. > Parameter sizes: 2.4e6, 4.6e6, 10.9e6 Linear layers and rectified linear units are employed. Pressure coefficient fields are vectorized. $\tilde{\mathbf{x}}_L \in \mathbb{R}^{300 \times 4096}$ $\tilde{\mathbf{x}}_H \in \mathbb{R}^{100 \times 4096}$ Increasing high-fidelity sample size, NS_H , is used. All MFDNNs yields comparable and unsatisfactory results in terms of MF-RMSE. Higher number of high-fidelity data does not affect the prediction accuracy! It can be concluded that the MFDNN is not able to learn the correlation between the HF and LF data.	MFDNNs with 3 set of learnable parameters are tested. N_{θ} > Parameter sizes: 2.4e6, 4.6e6, 10.9e6 2.4×10^6 Linear layers and rectified linear units are employed. 2.4×10^6 Pressure coefficient fields are vectorized. $\mathbf{\tilde{x}}_L \in \mathbb{R}^{300 \times 4096}$ $\mathbf{\tilde{x}}_H \in \mathbb{R}^{100 \times 4096}$ Increasing high-fidelity sample size, NS_H , is used. 4.6×10^6 All MFDNNs yields comparable and unsatisfactory results in terms of MF-RMSE. 10.9×10^6 Higher number of high-fidelity data does not affect the prediction accuracy! 10.9×10^6 It can be concluded that the MFDNN is not able to learn the correlation between the HF and LF data. 10.9×10^6	MFDNNs with 3 set of learnable parameters are tested. N_{θ} NS_H > Parameter sizes: 2.4e6, 4.6e6, 10.9e610Linear layers and rectified linear units are employed.2.4 × 10^650Pressure coefficient fields are vectorized. $\mathbf{\tilde{x}}_L \in \mathbb{R}^{300 \times 4096}$ $\mathbf{\tilde{x}}_H \in \mathbb{R}^{100 \times 4096}$ 200Increasing high-fidelity sample size, NS_H , is used.10All MFDNNs yields comparable and unsatisfactory results in terms of MF-RMSE.10Higher number of high-fidelity data does not affect the prediction accuracy!10It can be concluded that the MFDNN is not able to learn the correlation between the HF and LF data.100200150200100200200	MFDNNs with 3 set of learnable parameters are tested. N_{θ} NS_H LF-RMSE> Parameter sizes: 2.4e6, 4.6e6, 10.9e6100.0177Linear layers and rectified linear units are employed.2.4 × 10 ⁶ 500.0177Pressure coefficient fields are vectorized. $\tilde{\mathbf{x}}_L \in \mathbb{R}^{300 \times 4096}$ $\tilde{\mathbf{x}}_H \in \mathbb{R}^{100 \times 4096}$ 2000.0177Increasing high-fidelity sample size, NS_H , is used.100.01424.6 × 10 ⁶ 500.0142All MFDNNs yields comparable and unsatisfactory results in terms of MF-RMSE.100.01422000.0142Higher number of high-fidelity data does not affect the prediction accuracy!100.0177100.0177It can be concluded that the MFDNN is not able to learn the correlation between the HF and LF data.1500.01771500.0177 200 0.01771000.01771000.01771000.0177 00 0.0177 0.0177 0.0177 0.0177 0.0177 0.0177 00 0.0177 0.0177 0.0177 0.0177 0.0177 00 0.0177 0.0177 0.0177 0.0177 00 0.0177 0.0177 0.0177 00 0.0177 0.0177 0.0177 00 0.0177 0.0177 0.0177 00 0.0177 0.0177 0.0177 00 0.0177 0.0177 0.0177 00 0.0177 0.0177 0.0177



- The modified-MFDNNs with 3 different latent vector sizes are investigated. \tilde{N}_{H} : 4,8,16
- Linear layers and rectified linear units are employed.
- Increasing high-fidelity sample size is used.
- > The lower the \tilde{N}_H is, the better multi-fidelity predictions we get!
- > Higher number of high-fidelity data does not affect the prediction accuracy!
- > Thus, compressing high-fidelity inputs causes the loss of information.
- > The modified-MFDNN outperforms the MFDNN up to 66%.

$N_{ ilde{H}}$	NS_H	LF-RMSE	MF-RMSE	MF-RMSE Improvement (%)
4	[10,200]	0.0155	0.0162	66.0
8	[10,200]	0.0208	0.0215	50.8
16	[10,200]	0.017	0.0240	45.1

Predictions with the MFCNN

- A single MFCNN model is constructed.
- Convolution layers and rectified linear units are employed.
- Higher number of high-fidelity data improves the prediction accuracy!
- The MFCNN is superior to the previously presented methods for the considered case.
- The MFCNN improves the multi-fidelity ¹/₁ predictions up to 78% in comparison of the ²/₂ MFDNN.
- It can also improves the multi-fidelity predictions up to 38% when compared to the modified-MFDNN.

	LF-RMSE	MF-RMSE	MF-RMSE Improvement (%)		
S_H			MFDNN vs. MFCNN	Modified-MFDNN vs. MFCNN	
10	0.0075	0.0225	50.9	-42.4	
50	0.0059	0.0113	76.5	30.0	
100	0.0060	0.0105	77.9	35.0	
150	0.0065	0.0100	66.2	38.3	
200	0.0075	0.0101	78.7	37.7	



Comparison

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- > MFCNN is the fastest learning method.
- MFCNN is the best in learning.
- > MFCNN is the best in making multi-fidelity predictions.



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Figure: The comparison of RMSE on the test data.

Conclusion

- MFDNN couldn't handle high-dimensional inputs with low-dimensional predictions.
- The modified-MFDNN enhances the MFDNN significantly in terms of multi-fidelity predictions.
- The MFCNN proves its efficacy on highdimensional inputs.

Thank you for listening!