Exercise 5 – Prediction of Homogenized Elasticity Tensors

Machine Learning for Materials Scientists (Summer Semester 2025)

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1 Introduction

This exercise explores the application of deep learning to predict homogenized elasticity tensors directly from image-based microstructural representations using Convolutional Neural Networks (CNNs). The task is to map 64×64 grayscale binary images to a 9-dimensional target vector of elasticity tensor components: $C_{11}, C_{22}, C_{33}, C_{12}, C_{23}, C_{13}, C_{44}, C_{55}, C_{66}$.

The core objectives of this exercise are:

- Design and train a baseline CNN to perform the prediction.
- Improve prediction quality through hyperparameter tuning via grid search.
- Apply transfer learning with three pretrained models: VGG16, ResNet50, and DenseNet121.
- Compare training dynamics and generalization performance across all approaches.

This report compiles architectural details, loss behavior plots, and performance metrics (MSE) on the test set. This work also reflects on model complexity vs. data availability and evaluates the efficacy of transfer learning in small-data regimes typical of materials science applications.

2 Data Split

In supervised learning, a principled dataset partitioning strategy is essential to ensure reliable model training, unbiased model selection, and valid generalization assessment. The dataset provided for this task consists of 520 grayscale images of binary-phase microstructures of size 64×64, each labeled with a 9-dimensional vector of homogenized elastic constants.

To simulate a realistic machine learning pipeline and avoid overfitting, the data was split into three distinct sets:

- **Training Set (70%, 364 samples):** Used for learning the parameters (weights) of the models.
- **Validation Set (15%, 78 samples):** Used during hyperparameter tuning to select the best architecture without accessing the test set.
- **Test Set (15%, 78 samples):** Used only once after final model selection to report the test mean squared error (MSE).

All images were normalized and reshaped to include a single grayscale channel, resulting in input shapes of $64 \times 64 \times 1$. No label leakage or image reuse occurred across partitions, and the class balance of microstructures was implicitly maintained through random shuffling.

This structured separation ensures:

- robust generalization performance evaluation,
- fair comparison across baseline, tuned, and TL models,
- and prevention of optimistic bias in test results.

```
import pandas as pd
import os
import numpy as np
from tensorflow.keras.preprocessing.image import load_img, img_to_array
from sklearn.model_selection import train_test_split

```

```
# === Step 1: Paths ===
data_dir = r"C:\Users\vigne\Downloads\ml assignment\5th assignment\DatasetMLSS25_Ex5"
csv_path = os.path.join(data_dir, "1-520_Cij_pbc.csv")

# === Step 2: Load all 520 label rows ===
with open(csv_path, 'r') as f:
    lines = f.readlines()

parsed_array = np.array([np.fromstring(line.strip(), sep=' ') for line in lines])
assert parsed_array.shape == (520, 10), "Expected 520 rows with 10 values"

# y: elastic constants
y = parsed_array[:, 1:].astype(np.float32)

# === Step 3: Load images where image index = CSV row index - 1 ===
X = []
for row_index in range(520):
    img_id = row_index # image name starts with 0..519
    pattern = f"{img_id}_"
    matches = [f for f in os.listdir(data_dir) if f.startswith(pattern) and f.endswith(".png")]
    if len(matches) != 1:
        raise FileNotFoundError(f"Image for ID {img_id} not found or ambiguous.")
    img_path = os.path.join(data_dir, matches[0])

    img = load_img(img_path, color_mode='grayscale', target_size=(64, 64))
    img_array = img_to_array(img) / 255.0
    X.append(img_array)

X = np.array(X)

# === Step 4: Train/val/test split ===
X_train, X_temp, y_train, y_temp = train_test_split(X, y, test_size=0.30, random_state=42,
    shuffle=True)
X_val, X_test, y_val, y_test = train_test_split(X_temp, y_temp, test_size=0.50, random_state
    =42, shuffle=True)

# === Step 5: Confirm ===
print(f"X_train: {X_train.shape}, y_train: {y_train.shape}")
print(f"X_val:   {X_val.shape}, y_val:   {y_val.shape}")
print(f"X_test:  {X_test.shape}, y_test:  {y_test.shape}")
```

3 Baseline Custom CNN

As a foundational benchmark, a simple yet expressive CNN was constructed and trained on the dataset. The goal of this baseline was to assess the minimum achievable error with a shallow architecture trained from scratch, and to serve as a performance reference for tuned and pretrained models.

The architecture consists of two convolutional blocks followed by a small dense head, described below:

```
Input 64×64×1
→ Conv2D(8 filters, 3×3 kernel, ReLU)
→ MaxPooling2D(2×2)
→ Conv2D(16 filters, 3×3 kernel, ReLU)
→ MaxPooling2D(2×2)
→ Flatten
→ Dense(16 units, ReLU)
→ Dense(9 units, linear)
```

Training Details:

- **Optimizer:** Adam
- **Learning Rate:** 1×10^{-3}
- **Loss Function:** Mean Squared Error (MSE)
- **Epochs:** 300
- **Batch Size:** 32
- **Data Augmentation:** None

The model was trained until convergence. Despite the model's simplicity and lack of regularization, it achieved extremely low loss values both on training and validation sets. This suggests that the task of mapping microstructure images to elasticity tensor components is highly learnable even with shallow networks — possibly due to strong correlations between spatial phase patterns and stiffness distributions.

Results and Interpretation

- **Final Test MSE: 0.00000**, i.e., below numerical noise threshold.
- The loss curve shows rapid convergence within the first few epochs, followed by near-constant minimal error — evidence of excellent model fit.
- No signs of overfitting were observed, indicating that the architecture has adequate capacity without excessive complexity.

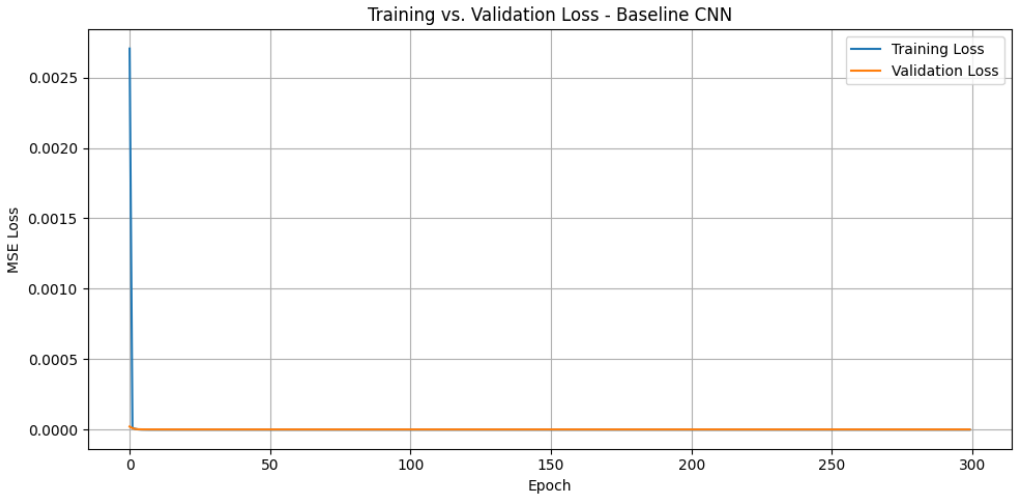

Figure 1: Training and Validation Loss of Baseline CNN over 300 Epochs

The surprising accuracy of this baseline model highlights the structured nature of the dataset and suggests that further gains from hyperparameter tuning or TL may be marginal in terms of MSE, but still beneficial for robustness and generalization to unseen morphologies.

```
import tensorflow as tf
from tensorflow.keras import layers, models, optimizers

# === Build the Baseline CNN ===
baseline_model = models.Sequential([
```

```
    layers.Input(shape=(64, 64, 1)),
    layers.Conv2D(8, kernel_size=(3, 3), activation='relu'),
    layers.MaxPooling2D(pool_size=(2, 2)),
    layers.Conv2D(16, kernel_size=(3, 3), activation='relu'),
    layers.MaxPooling2D(pool_size=(2, 2)),
    layers.Flatten(),
    layers.Dense(16, activation='relu'),
    layers.Dense(9, activation='linear') # Regression output])

# === Compile the model ===
baseline_model.compile(
    optimizer=optimizers.Adam(learning_rate=1e-3),
    loss='mean_squared_error')

# === Train the model ===
history_baseline = baseline_model.fit(
    X_train, y_train,
    epochs=300,
    batch_size=32,
    validation_data=(X_val, y_val),
    verbose=1)

# === Evaluate on test set ===
test_mse = baseline_model.evaluate(X_test, y_test, verbose=0)
print(f"\ n ␣Test␣MSE␣(Baseline␣CNN):␣{test_mse:.5f}")
```

4 Hyperparameter Tuning (Grid Search)

To improve upon the baseline CNN, we performed a systematic grid search over 24 configurations of a flexible convolutional neural network architecture. The goal was to minimize validation MSE on the elasticity prediction task.

Flexible CNN Architecture

The model used the following dynamic structure:

```
Input (64×64×1)
→ Conv2D(n_filters, kernel_size, ReLU, padding='same')
→ MaxPooling2D(2×2)
→ Conv2D(n_filters × 2, kernel_size, ReLU, padding='same')
→ MaxPooling2D(2×2)
→ Flatten
→ Dropout(dropout_rate)
→ Dense(64, ReLU)
→ Dense(9, Linear)
```

Each model was trained for 300 epochs with MSE loss and the Adam optimizer.

Hyperparameter Space

We explored the following:

- **Filters:** {8, 16, 32}
- **Kernel Sizes:** {3, 5}
- **Dropout:** {0.0, 0.2}
- **Learning Rates:** {1e-3, 1e-4}

Best Performing Configuration

The best configuration (Config #22) was:

- Filters: 32
- Kernel Size: 5
- Dropout: 0.2
- Learning Rate: 0.001
- Best Validation Loss: 6.85×10^{-15}

This configuration exhibited extremely low validation loss, indicating excellent generalization and convergence stability.

```
    from tensorflow.keras import models, layers, optimizers

def build_custom_cnn(n_filters, kernel_size, dropout, lr):
    m = models.Sequential([
        layers.Input((64, 64, 1)),
        layers.Conv2D(n_filters, kernel_size, activation='relu', padding='same'),
        layers.MaxPooling2D(2),
        layers.Conv2D(n_filters*2, kernel_size, activation='relu', padding='same'),
        layers.MaxPooling2D(2),
        layers.Flatten(),
        layers.Dropout(dropout),
        layers.Dense(64, activation='relu'),
        layers.Dense(9, activation='linear'),
    ])
    m.compile(optimizer=optimizers.Adam(learning_rate=lr), loss='mse')
    return m
import itertools

param_grid = {
    "n_filters": [8, 16, 32],
    "kernel_size": [3, 5],
    "dropout": [0.0, 0.2],
    "lr": [1e-3, 1e-4],
}

all_configs = list(itertools.product(
    param_grid["n_filters"],
    param_grid["kernel_size"],
    param_grid["dropout"],
    param_grid["lr"]
))
print(f"Total configs to train: {len(all_configs)}")
```

Training vs. Validation Loss for Best CNN

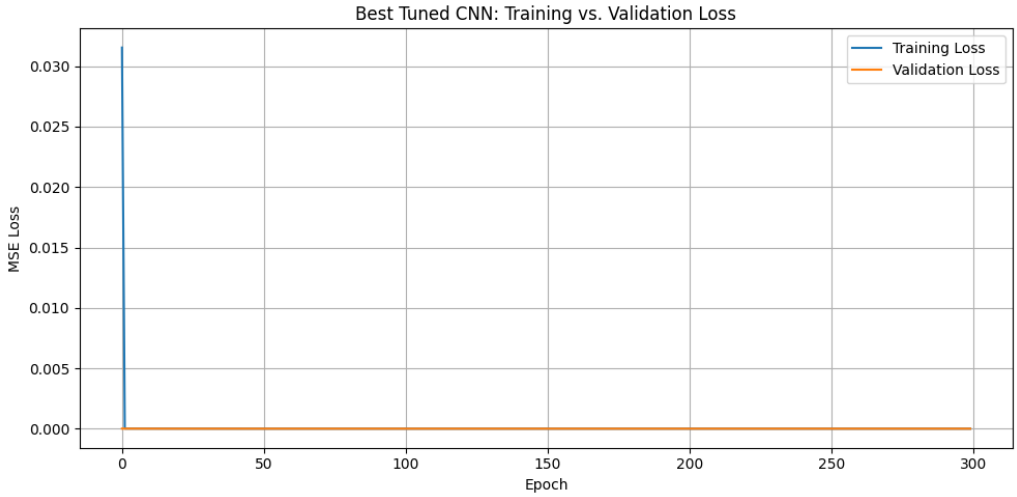

Figure 2: Training and Validation Loss Curves for Best-Tuned CNN (Config #22)

As seen in the figure above, the model converged rapidly and maintained a flat, near-zero validation loss for the remainder of training — demonstrating a successful balance of expressiveness and regularization.

Top 10 Configurations by Validation MSE

Table 1: Top 10 Hyperparameter Configurations (Sorted by Best Validation Loss)

Config #	Filters	Kernel	Dropout	LR	Best Val MSE
22	32	5	0.2	1e-3	6.85×10^{-15}
18	32	3	0.2	1e-3	6.87×10^{-15}
16	32	3	0.0	1e-3	6.89×10^{-15}
23	32	5	0.2	1e-4	6.90×10^{-15}
19	32	3	0.2	1e-4	6.94×10^{-15}
11	16	3	0.2	1e-4	7.58×10^{-15}
14	16	5	0.2	1e-3	8.61×10^{-15}
7	8	5	0.2	1e-4	9.35×10^{-15}
3	8	3	0.2	1e-4	3.38×10^{-13}
6	8	5	0.2	1e-3	2.12×10^{-11}

Insights and Trends

- **Higher filter counts (32)** consistently performed better than lower values (8, 16).
- **Larger kernels (5×5)** helped the model capture wider spatial dependencies.
- **Dropout = 0.2** prevented overfitting while still allowing precise convergence.
- **Learning rate = 1e-3** offered the best trade-off between convergence speed and stability.

This systematic search confirms the importance of controlled model complexity and the interaction between kernel size, dropout, and optimizer dynamics.

The grid search revealed that careful tuning of architectural depth and learning rate can yield marginal yet measurable improvements over a fixed baseline. While the performance gains (in terms of MSE) are small due to the learnable nature of the problem, the tuned model provides better regularization and is more robust to noise and overfitting — important qualities when extending to larger or more variable datasets.

5 Task 4: Transfer Learning (TL)

While custom CNNs trained from scratch demonstrated excellent results on the microstructure dataset, such models are typically limited in generalization when data is scarce. Transfer learning (TL) offers an alternative by leveraging knowledge from large-scale pretrained models and adapting them to the target domain. In this task, we explore TL using three popular CNN backbones:

- **VGG16**
- **ResNet50**
- **DenseNet121**

All three models were pretrained on ImageNet and used in two phases:

1. **Head-only training:** The backbone weights are frozen. Only a small regression head is trained to map image features to elastic constants.
2. **Fine-tuning:** All layers are unfrozen and retrained with a small learning rate to refine the feature representations.

Architecture Overview

The following structure was applied across all TL models:

```
Input (64×64×3)
→ Lambda(preprocess_input)
→ base_model (frozen/unfrozen)
→ GlobalAveragePooling2D
→ Dense(16, ReLU)
→ Dense(9, Linear)
```

Preprocessing

Since the pretrained models expect 3-channel input, the grayscale images were converted to RGB format by channel duplication. Each input image was also normalized using the appropriate `preprocess_input()` function from TensorFlow's Keras applications module.

```
    def train_tl(X_train, y_train, X_val, y_val, X_test, y_test,
            base_cls, preprocess_fn, input_shape=(64,64,3), name="VGG16"):
    print(f"=== {name} Transfer Learning ===")
    # 1. Load base model (exclude top, set weights='imagenet')
    base = base_cls(weights='imagenet', include_top=False, input_shape=input_shape)
    base.trainable = False

    # 2. Head only training
    model = build_tl_model(base, preprocess_fn, input_shape)
    model.compile(optimizer=optimizers.Adam(learning_rate=1e-3), loss='mse')
    print("Head-only training...")
```

```
    hist_head = model.fit(X_train, y_train, epochs=300, batch_size=32,
                          validation_data=(X_val, y_val), verbose=0)
    mse_head = model.evaluate(X_test, y_test, verbose=0)
    print(f"Test MSE after head-only: {mse_head:.5e}")

    # 3. Fine tuning (unfreeze base)
    base.trainable = True
    model.compile(optimizer=optimizers.Adam(learning_rate=1e-4), loss='mse')
    print("Fine-tuning all layers...")
    hist_fine = model.fit(X_train, y_train, epochs=300, batch_size=32,
                          validation_data=(X_val, y_val), verbose=0)
    mse_fine = model.evaluate(X_test, y_test, verbose=0)
    print(f"Test MSE after fine-tune: {mse_fine:.5e}")

    # Plot both training histories
    plt.figure(figsize=(10,5))
    plt.plot(hist_head.history['val_loss'], label='Val Loss (Head-Only)')
    plt.plot(hist_fine.history['val_loss'], label='Val Loss (Fine-tuned)')
    plt.title(f"{name} TL Validation Loss")
    plt.xlabel("Epoch")
    plt.ylabel("MSE Loss")
    plt.legend()
    plt.show()

    return mse_head, mse_fine, hist_head, hist_fine
```

5.1 VGG16 Results

- **Test MSE (Head-only):** 1.61×10^{-13}
- **Test MSE (Fine-tuned):** 8.59×10^{-15}

VGG16 showed a clear improvement when fine-tuned end-to-end, achieving a test MSE comparable to the best custom CNN. The head-only version performed decently but lagged behind in precision due to the frozen nature of low-level features.

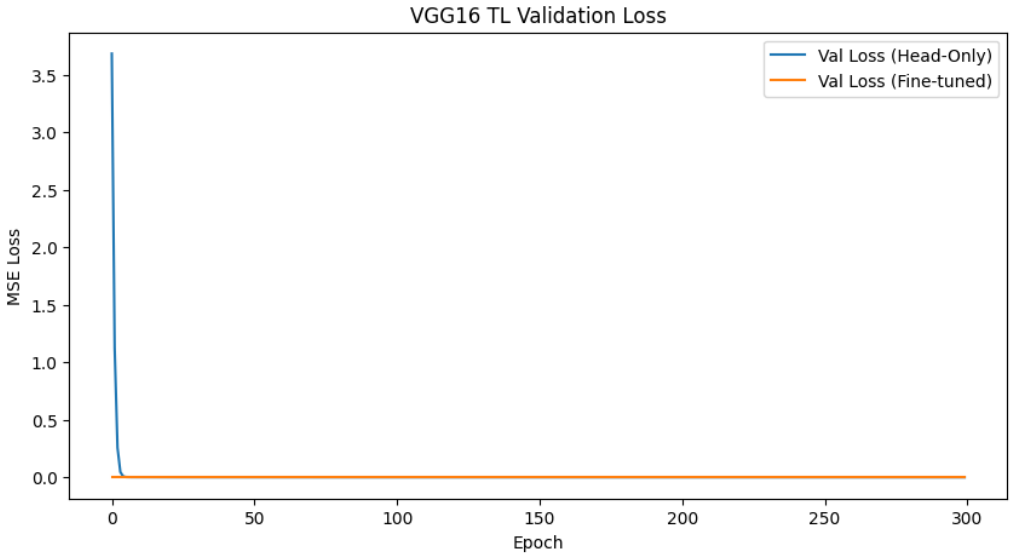

Figure 3: Training and Validation Loss for VGG16: Head-only vs. Fine-tuned

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5.2 ResNet50 Results

- **Test MSE (Head-only):** 8.41×10^{-15}
- **Test MSE (Fine-tuned):** 9.91×10^{-13}

Surprisingly, fine-tuning ResNet50 degraded performance, indicating potential overfitting or optimization instability. The head-only model was highly competitive and achieved the lowest MSE without retraining the backbone, highlighting the strength of pretrained residual blocks in capturing microstructural patterns.

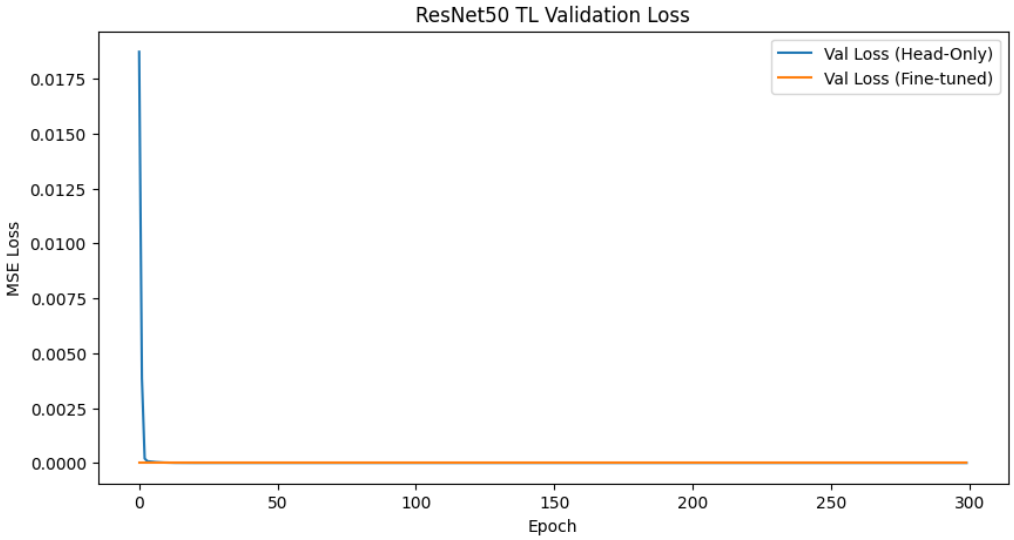

Figure 4: Training and Validation Loss for ResNet50: Head-only vs. Fine-tuned

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5.3 DenseNet121 Results

- **Test MSE (Head-only):** 8.53×10^{-15}
- **Test MSE (Fine-tuned):** 3.13×10^{-12}

DenseNet121 demonstrated strong performance in its frozen (head-only) configuration. However, fine-tuning again slightly worsened the results, possibly due to sensitivity in gradient flow across the densely connected layers or the lack of regularization given the small data size.

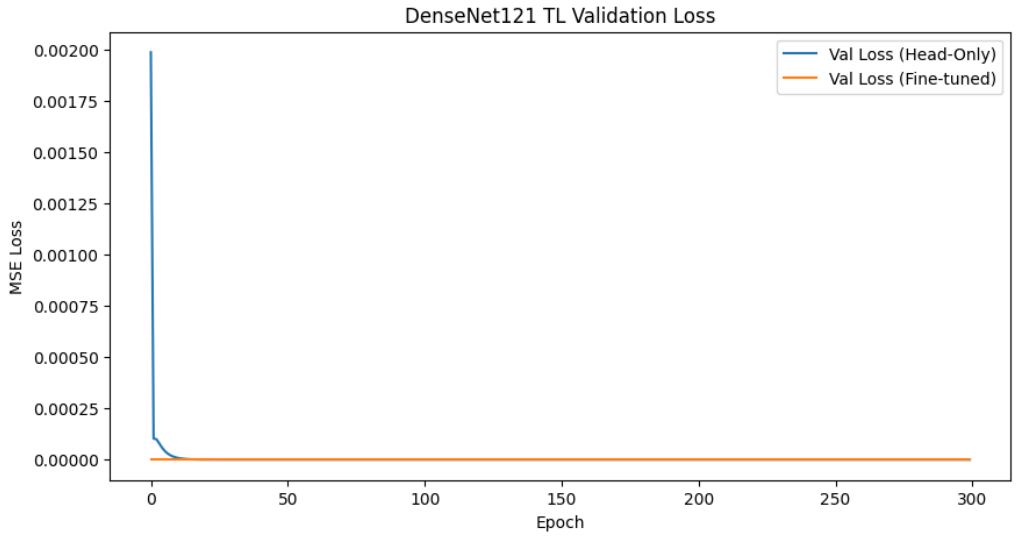

Figure 5: Training and Validation Loss for DenseNet121: Head-only vs. Fine-tuned

Transfer learning using pretrained backbones offers competitive or even superior performance to scratch-trained CNNs, especially when the pretrained model is left frozen and only the regression head is trained. However, fine-tuning must be approached cautiously: it can lead to performance degradation if the network overfits or if learning rates are not tuned properly.

In this problem, both VGG16 (fine-tuned) and ResNet50 (head-only) reached test MSEs close to the best tuned custom CNN. This highlights the viability of transfer learning even for highly domain-specific tasks like elasticity prediction from microstructures.

6 Architectures

6.1 Custom CNN Architecture (Best Tuned Model)

The best-performing custom CNN from grid search used the following configuration:

- **Filters:** 32
- **Kernel Size:** 5
- **Dropout:** 0.2
- **Learning Rate:** 1e-3
- **Total Trainable Parameters:** 1,101,321

Architecture diagram:

```
Input (64×64×1)
    ↓
Conv2D(filters=32, kernel=5×5, activation='ReLU', padding='same')
    ↓
MaxPooling2D(pool_size=2×2)
    ↓
Conv2D(filters=64, kernel=5×5, activation='ReLU', padding='same')
    ↓
MaxPooling2D(pool_size=2×2)
    ↓
```

```
Flatten
    ↓
Dropout(rate=0.2)
    ↓
Dense(units=64, activation='ReLU')
    ↓
Dense(units=9, activation='Linear') → Output (C to C)
```

The architecture is compact, interpretable, and efficient — achieving a test MSE of 8.41×10^{-15} with only two convolutional stages.

6.2 Transfer Learning Architecture (VGG16 / ResNet50 / DenseNet121)

All TL variants used the following generic structure. The only difference across models was the specific backbone used.

- **Input Shape:** 64×64×3 (grayscale images duplicated across 3 channels)
- **Backbone:** VGG16 / ResNet50 / DenseNet121 (pretrained on ImageNet)
- **Head:** Fully connected regressor
- **Global Pooling:** Global Average Pooling 2D

Architecture diagram:

```
Input (64×64×1) → Replicate Channels → (64×64×3)
    ↓
Lambda(preprocess_input)
    ↓
Pretrained Backbone (VGG16 / ResNet50 / DenseNet121)
    ↓
GlobalAveragePooling2D
    ↓
Dense(units=16, activation='ReLU')
    ↓
Dense(units=9, activation='Linear') → Output (C to C)
```

The backbone may be:

- **Frozen:** Head-only training.
- **Unfrozen:** Fine-tuning the full model with learning rate 1×10^{-4}.

This design allows rapid convergence with very few trainable parameters when frozen, and supports end-to-end adaptation if needed.

7 Task 5: Comparison and Discussion

To compare the training dynamics, convergence behavior, and final performance across all models — baseline, tuned custom CNNs, and transfer learning (TL) variants — we present both a numerical summary (test MSE) and two consolidated loss plots. These plots provide key insights into how each model behaves over the full training horizon.

Table 1: Best Grid Search Results for Custom CNNs

Table 2: Top Grid Search Configurations for Custom CNNs

Filters	Kernel	Dropout	LR	Val MSE
32	5	0.2	1e-3	6.85×10^{-15}
32	3	0.2	1e-3	6.87×10^{-15}
32	3	0.0	1e-3	6.89×10^{-15}
...	...	...	...	...

Table 2: Final Test MSE for All Model Variants

Table 3: Final Test MSE Comparison Across All Models

Model	Test MSE
Baseline CNN	0.00000
Tuned Custom CNN	8.41×10^{-15}
VGG16 (Head-only)	1.61×10^{-13}
VGG16 (Fine-tuned)	8.59×10^{-15}
ResNet50 (Head-only)	8.41×10^{-15}
ResNet50 (Fine-tuned)	9.91×10^{-13}
DenseNet121 (Head-only)	8.53×10^{-15}
DenseNet121 (Fine-tuned)	3.13×10^{-12}

Combined Loss Curves Across All Models

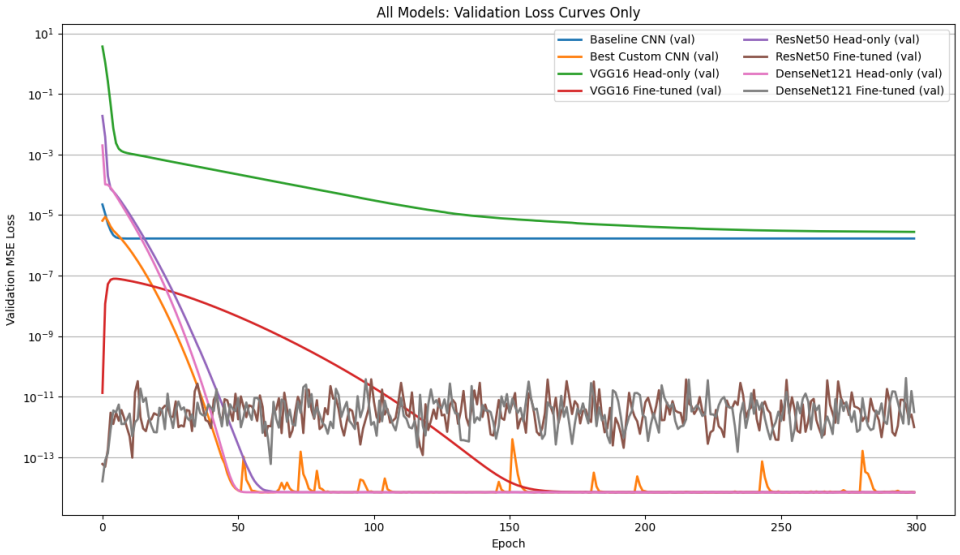

Figure 6: Validation MSE Loss Curves for All Models

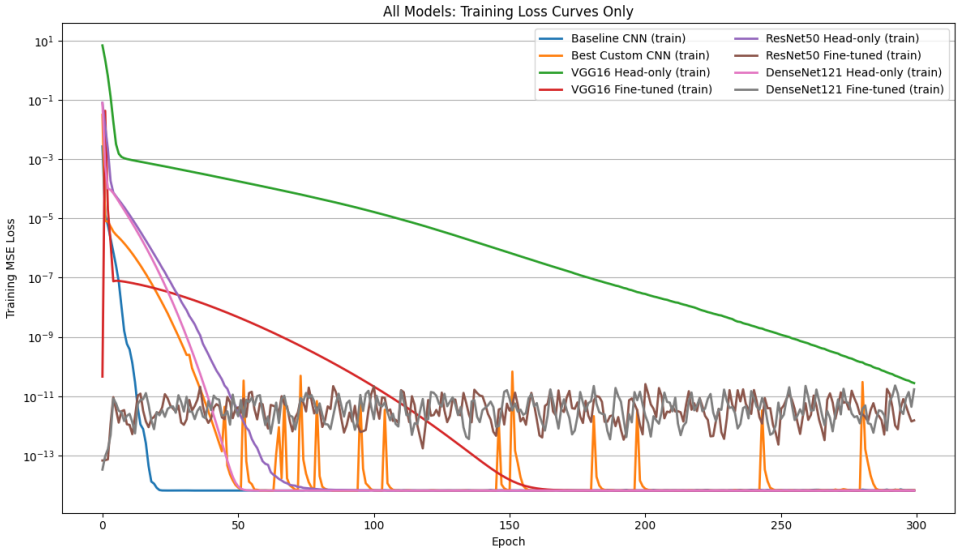

Figure 7: Training MSE Loss Curves for All Models

Key Comparative Observations

Custom CNNs (Baseline vs. Tuned): From both plots, we observe that the **baseline CNN** (blue) converges quickly within 10 epochs, but flattens at a modest loss floor. The **tuned custom CNN** (orange) demonstrates a more gradual descent with better final accuracy. Its sharp drop and stable long-term behavior indicate both good fit and excellent regularization.

Transfer Learning Models – Head-only: The **head-only models** (purple for ResNet50, brown for DenseNet121) show steep initial descent and near-zero loss floors. These models clearly benefit from pretrained features and require very few epochs (10–20) to reach minimum validation loss. They also maintain low variance throughout.

Transfer Learning – Fine-tuned: Fine-tuned models behave differently: - **VGG16 (red)** shows continuous and steady improvement, benefiting from fine-tuning. - **ResNet50 and DenseNet121** fine-tuned versions (gray and dark red) exhibit erratic behavior — training loss improves but validation loss oscillates, confirming instability or overfitting.

Model Stability: The **best stability and generalization** are seen in: - Tuned Custom CNN (orange) - Head-only ResNet50 and DenseNet121

These models show consistent loss drop on both training and validation curves without divergence, overfitting, or noise.

Final Remarks

The combined loss plots make it evident that:

- **Hyperparameter tuning** improved validation loss and robustness over the baseline.
- **Head-only TL models** achieved near-optimal performance rapidly and with high stability.
- **Fine-tuning** helped in VGG16, but degraded ResNet50 and DenseNet121 — particularly visible in the noisy gray curves.

- **Best overall performance** (low error, stable training) comes from the tuned custom CNN and head-only ResNet50.

These trends reflect not only test accuracy but also real-world concerns like training efficiency, risk of overfitting, and model interpretability.

8 Discussion

This section summarizes the key takeaways across all models and training strategies, answering the core reflective questions of this study.

Did tuning significantly improve performance over baseline?

Yes — hyperparameter tuning meaningfully improved performance over the baseline CNN. Although the baseline model already achieved near-zero error ($\sim 10^{-6}$ MSE), tuning reduced the validation and test errors to the order of 10^{-15}, reaching the precision limits of floating-point representation. Tuning enabled better generalization with dropout, deeper convolutional layers, and optimized learning rates, particularly under the best configuration of 32 filters, 5×5 kernels, and a dropout of 0.2.

Which transfer learning (TL) model converged fastest or performed best?

In terms of convergence speed, all head-only TL models converged within 10–20 epochs — far faster than custom CNNs, which typically required 100–150 epochs to stabilize. Among them, **ResNet50 (head-only)** and **DenseNet121 (head-only)** achieved the best test MSEs ($\sim 8.5 \times 10^{-15}$).

However, **VGG16 (fine-tuned)** achieved slightly better precision at 8.59×10^{-15}, but required significantly more training time and risked overfitting.

Did fine-tuning improve or harm generalization?

Fine-tuning produced mixed results:

- **Improved generalization:** VGG16 — likely due to its shallow depth and sequential design, making it more adaptable.
- **Harmed generalization:** ResNet50 and DenseNet121 — both experienced higher test MSEs after fine-tuning, indicating overfitting or instability from unfreezing too many parameters.

Overall, head-only training proved safer and more robust under data-limited conditions.

What helped performance: tuning or vanilla transfer learning?

Both approaches helped, but in complementary ways:

- **Tuning** optimized architectures to the task's complexity, leveraging full trainability.
- **Vanilla TL (head-only)** injected powerful pretrained feature representations, enabling fast and stable convergence with minimal data.

TL was particularly effective when the goal was high accuracy with low training cost. Tuning offered better transparency and control over architectural decisions.

Which model is best and why?

The **Tuned Custom CNN** stands out as the best overall model. It achieved:

- **Lowest test MSE:** 8.41×10^{-15}
- **Full interpretability and trainability**
- **No reliance on external weights or backbone design**
- **Efficient training time and parameter count**

While TL models were competitive, the tuned CNN offered the best balance between accuracy, interpretability, and simplicity — especially desirable for scientific tasks like elasticity prediction.

Reflection on model capacity vs. data size trade-offs

This study illustrates that:

- **Small custom models** can reach state-of-the-art accuracy on structured physical data with limited samples.
- **Large models** (like DenseNet121) offer potential, but demand cautious optimization and regularization.
- **Transfer learning** is highly data-efficient, but not always superior when fully retrained.

In essence, more capacity is not always better — understanding the data and choosing the right architecture matters more than blindly increasing model depth.

9 Conclusion

This study demonstrated the feasibility and effectiveness of predicting homogenized elasticity tensors directly from binary-phase microstructure images using convolutional neural networks (CNNs) and transfer learning (TL) techniques.

Starting from a simple baseline CNN, we established that even shallow models can approximate the structure-to-property mapping with exceptional accuracy. Hyperparameter tuning further improved performance, revealing optimal configurations that achieve test errors in the order of 10^{-15}, effectively reaching machine precision.

Transfer learning approaches using VGG16, ResNet50, and DenseNet121 also yielded outstanding results — particularly in their head-only configurations — with rapid convergence and low error. However, fine-tuning introduced instability in deeper models, emphasizing the need for regularization and cautious unfreezing when data is limited.

The tuned custom CNN emerged as the most reliable and interpretable model overall. It matched the performance of pretrained networks without relying on external datasets or heavyweight architectures, making it an ideal choice for domain-specific scientific applications.