Drive already mounted at /content/drive; to attempt to forcibly remount, call drive.mount("/content/drive", force\_remount=True).

📦 Installing dependencies...

━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 129.1/129.1 kB 4.0 MB/s eta 0:00:00

📁 Results will be saved to: /content/drive/MyDrive/AllergenAI-new/results

📊 Loading ESM-2 embedding data...

✅ Training set: 16120 samples (8060 positive)

✅ Test set: 4030 samples (2015 positive)

✅ Feature dimension: 1280

✅ Class balance - Train: 0.500, Test: 0.500

============================================================

📊 BASELINE: DUMMY CLASSIFIER

============================================================

Dummy Classifier (Stratified) - 5-Fold CV Results:

==================================================

Average Dummy Metrics

==================================================

Accuracy: 0.4991

Sensitivity: 0.4950

Specificity: 0.5031

Precision: 0.4991

F1-Score: 0.4970

MCC: -0.0019

AUC-ROC: 0.4991

==================================================

Dummy Classifier - Test Set Results:

==================================================

Test Set Dummy Metrics

==================================================

Accuracy: 0.4950

Sensitivity: 0.4948

Specificity: 0.4953

Precision: 0.4950

F1-Score: 0.4949

MCC: -0.0099

AUC-ROC: 0.4950

==================================================

============================================================

🔀 Y-SCRAMBLING NEGATIVE CONTROL

============================================================

============================================================

📊 EVALUATING: CNN

============================================================

Fold 1/5:

**101/101** ━━━━━━━━━━━━━━━━━━━━ **1s** 4ms/step

Accuracy: 0.7714, AUC: 0.8506, MCC: 0.5428

Fold 2/5:

**101/101** ━━━━━━━━━━━━━━━━━━━━ **1s** 3ms/step

Accuracy: 0.7764, AUC: 0.8671, MCC: 0.5559

Fold 3/5:

**101/101** ━━━━━━━━━━━━━━━━━━━━ **0s** 3ms/step

Accuracy: 0.7723, AUC: 0.8565, MCC: 0.5448

Fold 4/5:

**101/101** ━━━━━━━━━━━━━━━━━━━━ **0s** 3ms/step

Accuracy: 0.7255, AUC: 0.8260, MCC: 0.4558

Fold 5/5:

**101/101** ━━━━━━━━━━━━━━━━━━━━ **0s** 3ms/step

Accuracy: 0.7053, AUC: 0.8130, MCC: 0.4159

CNN - 5-Fold CV Summary:

==================================================

CNN Average Metrics

==================================================

Accuracy: 0.7502

Sensitivity: 0.7922

Specificity: 0.7082

Precision: 0.7330

F1-Score: 0.7607

MCC: 0.5030

AUC-ROC: 0.8426

==================================================

🔀 Y-Scrambling Test for CNN:

**101/101** ━━━━━━━━━━━━━━━━━━━━ **0s** 3ms/step

**101/101** ━━━━━━━━━━━━━━━━━━━━ **0s** 3ms/step

**101/101** ━━━━━━━━━━━━━━━━━━━━ **0s** 3ms/step

Y-Scrambled AUC: 0.4957 ± 0.0118

Y-Scrambled MCC: 0.0000 ± 0.0000

============================================================

📊 EVALUATING: MLP

============================================================

Fold 1/5:

**101/101** ━━━━━━━━━━━━━━━━━━━━ **1s** 4ms/step

Accuracy: 0.9708, AUC: 0.9926, MCC: 0.9419

Fold 2/5:

**101/101** ━━━━━━━━━━━━━━━━━━━━ **0s** 3ms/step

Accuracy: 0.9733, AUC: 0.9943, MCC: 0.9467

Fold 3/5:

**101/101** ━━━━━━━━━━━━━━━━━━━━ **0s** 3ms/step

Accuracy: 0.9764, AUC: 0.9954, MCC: 0.9529

Fold 4/5:

**101/101** ━━━━━━━━━━━━━━━━━━━━ **0s** 3ms/step

Accuracy: 0.9814, AUC: 0.9961, MCC: 0.9628

Fold 5/5:

**101/101** ━━━━━━━━━━━━━━━━━━━━ **0s** 3ms/step

Accuracy: 0.9628, AUC: 0.9910, MCC: 0.9259

MLP - 5-Fold CV Summary:

==================================================

MLP Average Metrics

==================================================

Accuracy: 0.9730

Sensitivity: 0.9770

Specificity: 0.9689

Precision: 0.9693

F1-Score: 0.9731

MCC: 0.9460

AUC-ROC: 0.9939

==================================================

🔀 Y-Scrambling Test for MLP:

**101/101** ━━━━━━━━━━━━━━━━━━━━ **0s** 3ms/step

**101/101** ━━━━━━━━━━━━━━━━━━━━ **0s** 3ms/step

**101/101** ━━━━━━━━━━━━━━━━━━━━ **0s** 3ms/step

Y-Scrambled AUC: 0.5015 ± 0.0039

Y-Scrambled MCC: 0.0065 ± 0.0185

============================================================

📊 EVALUATING: XGBoost

============================================================

Fold 1/5:

Accuracy: 0.9870, AUC: 0.9972, MCC: 0.9740

Fold 2/5:

Accuracy: 0.9848, AUC: 0.9983, MCC: 0.9696

Fold 3/5:

Accuracy: 0.9870, AUC: 0.9988, MCC: 0.9740

Fold 4/5:

Accuracy: 0.9851, AUC: 0.9983, MCC: 0.9702

Fold 5/5:

Accuracy: 0.9876, AUC: 0.9987, MCC: 0.9752

XGBoost - 5-Fold CV Summary:

==================================================

XGBoost Average Metrics

==================================================

Accuracy: 0.9863

Sensitivity: 0.9885

Specificity: 0.9841

Precision: 0.9842

F1-Score: 0.9863

MCC: 0.9726

AUC-ROC: 0.9983

==================================================

🔀 Y-Scrambling Test for XGBoost:

Y-Scrambled AUC: 0.5058 ± 0.0124

Y-Scrambled MCC: 0.0062 ± 0.0226

============================================================

🔧 HYPERPARAMETER TUNING: XGBoost

============================================================

Searching for best hyperparameters...

Fitting 3 folds for each of 50 candidates, totalling 150 fits

Best parameters found:

subsample: 0.9

n\_estimators: 400

min\_child\_weight: 1

max\_depth: 6

learning\_rate: 0.05

gamma: 0.1

colsample\_bytree: 1.0

Best CV score: 0.9943

============================================================

🎯 FINAL MODEL TRAINING AND TEST SET EVALUATION

============================================================

1️⃣ Training final CNN model...

Epoch 1/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **6s** 7ms/step - accuracy: 0.5875 - loss: 0.6884 - val\_accuracy: 0.0000e+00 - val\_loss: 0.9443

Epoch 2/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **2s** 6ms/step - accuracy: 0.6201 - loss: 0.6648 - val\_accuracy: 0.0828 - val\_loss: 0.8775

Epoch 3/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **2s** 6ms/step - accuracy: 0.6388 - loss: 0.6476 - val\_accuracy: 0.2646 - val\_loss: 0.7979

Epoch 4/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **3s** 6ms/step - accuracy: 0.6688 - loss: 0.6138 - val\_accuracy: 0.3756 - val\_loss: 0.7555

Epoch 5/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **3s** 7ms/step - accuracy: 0.6841 - loss: 0.5921 - val\_accuracy: 0.4755 - val\_loss: 0.6998

Epoch 6/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **2s** 6ms/step - accuracy: 0.6991 - loss: 0.5677 - val\_accuracy: 0.5282 - val\_loss: 0.6837

Epoch 7/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **2s** 6ms/step - accuracy: 0.7115 - loss: 0.5463 - val\_accuracy: 0.6520 - val\_loss: 0.6250

Epoch 8/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **2s** 6ms/step - accuracy: 0.7253 - loss: 0.5325 - val\_accuracy: 0.6607 - val\_loss: 0.6335

Epoch 9/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **3s** 6ms/step - accuracy: 0.7300 - loss: 0.5182 - val\_accuracy: 0.6411 - val\_loss: 0.6678

Epoch 10/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **3s** 6ms/step - accuracy: 0.7384 - loss: 0.5104 - val\_accuracy: 0.7162 - val\_loss: 0.6019

Epoch 11/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **5s** 6ms/step - accuracy: 0.7482 - loss: 0.5037 - val\_accuracy: 0.7736 - val\_loss: 0.5507

Epoch 12/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **2s** 6ms/step - accuracy: 0.7495 - loss: 0.5033 - val\_accuracy: 0.7280 - val\_loss: 0.6012

Epoch 13/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **3s** 6ms/step - accuracy: 0.7632 - loss: 0.4910 - val\_accuracy: 0.6858 - val\_loss: 0.6435

Epoch 14/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **3s** 6ms/step - accuracy: 0.7619 - loss: 0.4853 - val\_accuracy: 0.7438 - val\_loss: 0.5756

Epoch 15/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **5s** 6ms/step - accuracy: 0.7632 - loss: 0.4813 - val\_accuracy: 0.7075 - val\_loss: 0.6251

Epoch 16/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **2s** 5ms/step - accuracy: 0.7712 - loss: 0.4720 - val\_accuracy: 0.7208 - val\_loss: 0.6055

Epoch 17/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **3s** 5ms/step - accuracy: 0.7674 - loss: 0.4746 - val\_accuracy: 0.6917 - val\_loss: 0.6225

Epoch 18/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **2s** 6ms/step - accuracy: 0.7717 - loss: 0.4706 - val\_accuracy: 0.7516 - val\_loss: 0.5674

Epoch 19/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **3s** 7ms/step - accuracy: 0.7718 - loss: 0.4634 - val\_accuracy: 0.7134 - val\_loss: 0.6026

Epoch 20/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **5s** 6ms/step - accuracy: 0.7743 - loss: 0.4676 - val\_accuracy: 0.6951 - val\_loss: 0.6279

Epoch 21/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **2s** 5ms/step - accuracy: 0.7697 - loss: 0.4689 - val\_accuracy: 0.7320 - val\_loss: 0.5799

**126/126** ━━━━━━━━━━━━━━━━━━━━ **1s** 3ms/step

2️⃣ Training final MLP model...

Epoch 1/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **6s** 5ms/step - accuracy: 0.8730 - loss: 0.2782 - val\_accuracy: 0.9736 - val\_loss: 0.0941

Epoch 2/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **2s** 3ms/step - accuracy: 0.9642 - loss: 0.1100 - val\_accuracy: 0.9746 - val\_loss: 0.0866

Epoch 3/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **1s** 3ms/step - accuracy: 0.9704 - loss: 0.0917 - val\_accuracy: 0.9780 - val\_loss: 0.0708

Epoch 4/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **1s** 3ms/step - accuracy: 0.9749 - loss: 0.0758 - val\_accuracy: 0.9755 - val\_loss: 0.0849

Epoch 5/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **1s** 3ms/step - accuracy: 0.9799 - loss: 0.0632 - val\_accuracy: 0.9764 - val\_loss: 0.0869

Epoch 6/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **3s** 3ms/step - accuracy: 0.9821 - loss: 0.0560 - val\_accuracy: 0.9755 - val\_loss: 0.1007

Epoch 7/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **2s** 4ms/step - accuracy: 0.9860 - loss: 0.0515 - val\_accuracy: 0.9764 - val\_loss: 0.0990

Epoch 8/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **2s** 3ms/step - accuracy: 0.9870 - loss: 0.0446 - val\_accuracy: 0.9805 - val\_loss: 0.0762

Epoch 9/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **1s** 3ms/step - accuracy: 0.9877 - loss: 0.0392 - val\_accuracy: 0.9814 - val\_loss: 0.0857

Epoch 10/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **2s** 3ms/step - accuracy: 0.9889 - loss: 0.0391 - val\_accuracy: 0.9817 - val\_loss: 0.0849

Epoch 11/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **1s** 3ms/step - accuracy: 0.9905 - loss: 0.0315 - val\_accuracy: 0.9770 - val\_loss: 0.1113

Epoch 12/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **1s** 3ms/step - accuracy: 0.9919 - loss: 0.0309 - val\_accuracy: 0.9820 - val\_loss: 0.0919

Epoch 13/100

**403/403** ━━━━━━━━━━━━━━━━━━━━ **1s** 3ms/step - accuracy: 0.9914 - loss: 0.0281 - val\_accuracy: 0.9823 - val\_loss: 0.0921

**126/126** ━━━━━━━━━━━━━━━━━━━━ **1s** 4ms/step

3️⃣ Training final XGBoost model...

4️⃣ Creating ensemble predictions...

============================================================

📊 FINAL TEST SET RESULTS

============================================================

==================================================

CNN - Test Set

==================================================

Accuracy: 0.6883

Sensitivity: 0.6035

Specificity: 0.7732

Precision: 0.7268

F1-Score: 0.6594

MCC: 0.3822

AUC-ROC: 0.7441

==================================================

==================================================

MLP - Test Set

==================================================

Accuracy: 0.8906

Sensitivity: 0.7965

Specificity: 0.9846

Precision: 0.9811

F1-Score: 0.8792

MCC: 0.7953

AUC-ROC: 0.9785

==================================================

==================================================

XGBoost - Test Set

==================================================

Accuracy: 0.8739

Sensitivity: 0.7583

Specificity: 0.9896

Precision: 0.9864

F1-Score: 0.8575

MCC: 0.7687

AUC-ROC: 0.9812

==================================================

==================================================

Ensemble - Test Set

==================================================

Accuracy: 0.8826

Sensitivity: 0.7777

Specificity: 0.9876

Precision: 0.9843

F1-Score: 0.8689

MCC: 0.7827

AUC-ROC: 0.9811

==================================================

============================================================

📈 GENERATING VISUALIZATIONS

============================================================

A graph of a curve

AI-generated content may be incorrect.

A green and yellow bar chart

AI-generated content may be incorrect.

A graph with lines and dots

AI-generated content may be incorrect.

A graph of a number of people

AI-generated content may be incorrect.

WARNING:absl:You are saving your model as an HDF5 file via `model.save()` or `keras.saving.save\_model(model)`. This file format is considered legacy. We recommend using instead the native Keras format, e.g. `model.save('my\_model.keras')` or `keras.saving.save\_model(model, 'my\_model.keras')`.

WARNING:absl:You are saving your model as an HDF5 file via `model.save()` or `keras.saving.save\_model(model)`. This file format is considered legacy. We recommend using instead the native Keras format, e.g. `model.save('my\_model.keras')` or `keras.saving.save\_model(model, 'my\_model.keras')`.

============================================================

💾 SAVING RESULTS

============================================================

Saving models...

============================================================

📋 FINAL SUMMARY REPORT

============================================================

Dataset Information:

Training samples: 16120 (8060 positive)

Test samples: 4030 (2015 positive)

Feature dimension: 1280

Best Model Performance (Test Set):

Model: XGBoost

AUC-ROC: 0.9812

MCC: 0.7687

Accuracy: 0.8739

Sensitivity: 0.7583

Specificity: 0.9896

Y-Scrambling Control:

All models showed AUC ~0.50 with scrambled labels

This confirms models learned real patterns

Files saved to: /content/drive/MyDrive/AllergenAI-new/results

- Models: /content/drive/MyDrive/AllergenAI-new/results/models

- Results: /content/drive/MyDrive/AllergenAI-new/results/metrics

- Plots: /content/drive/MyDrive/AllergenAI-new/results/plots

✅ Pipeline completed successfully!