knn_pcr_nn

November 29, 2025

1 HDB Resale Price Regression Models: KNN, PCR, and Neural Networks

Models implemented: 1. K-Nearest Neighbors (KNN) Regression 2. Principal Component Regression (PCR) 3. Neural Network (Multi-layer Perceptron)

Common settings: - 80/20 train-test split - 5-fold Cross-Validation (CV) for hypertuning - RMSE used as main metric - StandardScaler applied for KNN and NN (distance-based methods require scaling)

[17]:
```python
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import torch
import torch.nn as nn
import torch.optim as optim
from torch.utils.data import TensorDataset, DataLoader

from sklearn.model_selection import train_test_split, GridSearchCV, KFold
from sklearn.preprocessing import StandardScaler
from sklearn.neighbors import KNeighborsRegressor
from sklearn.decomposition import PCA
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_squared_error
from sklearn.pipeline import Pipeline

# Check if MPS (Apple GPU) is available
device = torch.device("mps" if torch.backends.mps.is_available() else "cpu")
print(f"Using device: {device}")
if device.type == "mps":
    print("  Apple GPU (MPS) is available and will be used for neural network␣
 ↪training")
else:
    print("  MPS not available, using CPU")
```

```
Using device: mps
  Apple GPU (MPS) is available and will be used for neural network training
```

1.1 Load and Prepare Data

```
[18]: DATA_PATH = "../data/HDB_data_2021_sample.xlsx"

      df = pd.read_excel(DATA_PATH)

      # drop rows with missing resale_price
      df = df.dropna(subset=["resale_price"])

      # define target: use log(price) for nicer regression properties
      df["log_resale_price"] = np.log(df["resale_price"])
```

1.1.1 Feature Selection for Models

```
[19]: # for KNN, PCR, and NN, we'll use all columns except the target and year (year␣
       ↪is constant 2021)
      drop_cols_full = ["resale_price", "log_resale_price", "year"]
      X_full = df.drop(columns=drop_cols_full)
      y = df["log_resale_price"].values

      feature_names_full = X_full.columns.tolist()
      print(f"Total number of features: {len(feature_names_full)}")
```

```
Total number of features: 228
```

1.2 Train-Test Split (80/20)

```
[20]: X_full_train, X_full_test, y_train, y_test = train_test_split(
          X_full, y, test_size=0.2, random_state=42
      )

      print(f"Training set size: {X_full_train.shape[0]}")
      print(f"Test set size: {X_full_test.shape[0]}")
```

```
Training set size: 4800
Test set size: 1200
```

1.3 Utility: Compute RMSE

```
[21]: def rmse(y_true, y_pred):
          return np.sqrt(mean_squared_error(y_true, y_pred))
```

1.4 K-Nearest Neighbors (KNN) Regression

KNN is a non-parametric method that predicts based on the average of the k nearest neighbors. It requires feature scaling since it uses distance metrics.

[22]:
```python
# Standardize features for KNN (distance-based method requires scaling)
scaler_knn = StandardScaler()
X_full_train_scaled_knn = scaler_knn.fit_transform(X_full_train)
X_full_test_scaled_knn = scaler_knn.transform(X_full_test)

# Baseline: KNN with default parameters (n_neighbors=5)
knn_baseline = KNeighborsRegressor()
knn_baseline.fit(X_full_train_scaled_knn, y_train)

y_pred_train_knn_base = knn_baseline.predict(X_full_train_scaled_knn)
y_pred_test_knn_base = knn_baseline.predict(X_full_test_scaled_knn)

print(f"KNN Baseline - Train RMSE: {rmse(y_train, y_pred_train_knn_base):.4f}")
print(f"KNN Baseline - Test  RMSE: {rmse(y_test, y_pred_test_knn_base):.4f}")
```

```
KNN Baseline - Train RMSE: 0.1081
KNN Baseline - Test  RMSE: 0.1423
```

[23]:
```python
# Hypertuned KNN with GridSearchCV
# Hyperparameters to tune: n_neighbors, weights, metric
knn_param_grid = {
    "n_neighbors": [3, 5, 7, 10, 15, 20, 25],
    "weights": ["uniform", "distance"],
    "metric": ["euclidean", "manhattan"],
}

knn_grid = GridSearchCV(
    estimator=KNeighborsRegressor(),
    param_grid=knn_param_grid,
    scoring="neg_mean_squared_error",
    cv=5,
    n_jobs=-1,
    verbose=1,
)

knn_grid.fit(X_full_train_scaled_knn, y_train)

best_knn = knn_grid.best_estimator_
y_pred_test_knn_tuned = best_knn.predict(X_full_test_scaled_knn)

print(f"\nKNN Tuned - Best Params: {knn_grid.best_params_}")
print(f"KNN Tuned - Test RMSE:  {rmse(y_test, y_pred_test_knn_tuned):.4f}")

# Also get train RMSE for comparison
y_pred_train_knn_tuned = best_knn.predict(X_full_train_scaled_knn)
print(f"KNN Tuned - Train RMSE: {rmse(y_train, y_pred_train_knn_tuned):.4f}")
```

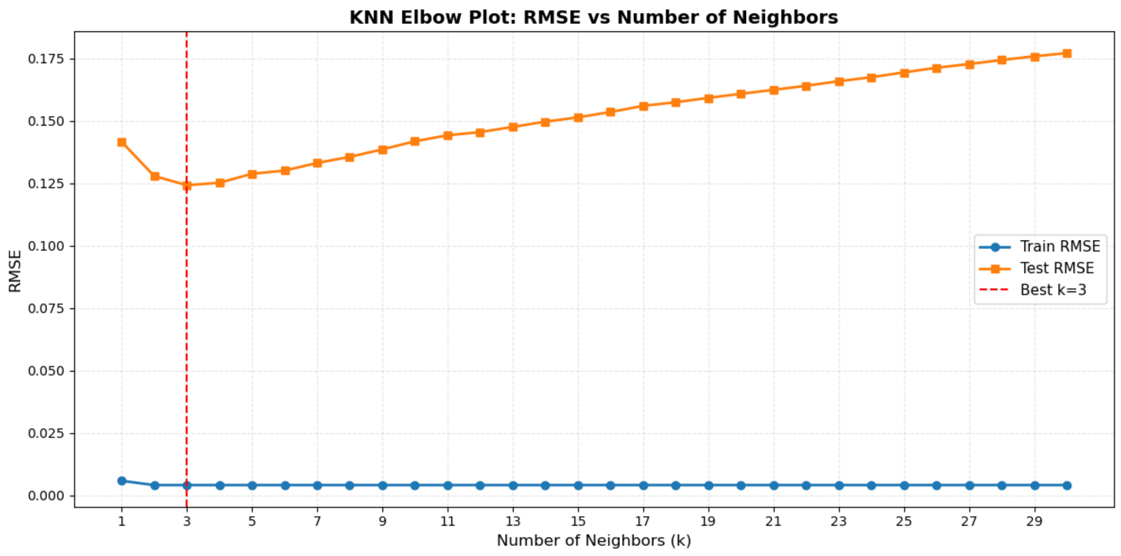
```
Fitting 5 folds for each of 28 candidates, totalling 140 fits
```

```
KNN Tuned - Best Params: {'metric': 'manhattan', 'n_neighbors': 3, 'weights':
'distance'}
KNN Tuned - Test RMSE:  0.1242
KNN Tuned - Train RMSE: 0.0041
```

1.4.1 KNN Visualizations

[24]:
```python
# 1. Elbow Plot: RMSE vs Number of Neighbors (k)
# This helps visualize the optimal k value
print("Creating elbow plot for KNN...")
k_values = range(1, 31)  # Test k from 1 to 30
train_rmse_scores = []
test_rmse_scores = []

for k in k_values:
    knn_temp = KNeighborsRegressor(n_neighbors=k, weights='distance',␣
 ↪metric='manhattan')
    knn_temp.fit(X_full_train_scaled_knn, y_train)

    y_pred_train_temp = knn_temp.predict(X_full_train_scaled_knn)
    y_pred_test_temp = knn_temp.predict(X_full_test_scaled_knn)

    train_rmse_scores.append(rmse(y_train, y_pred_train_temp))
    test_rmse_scores.append(rmse(y_test, y_pred_test_temp))

# Create elbow plot
fig, ax = plt.subplots(figsize=(12, 6))
ax.plot(k_values, train_rmse_scores, 'o-', label='Train RMSE', linewidth=2,␣
 ↪markersize=6)
ax.plot(k_values, test_rmse_scores, 's-', label='Test RMSE', linewidth=2,␣
 ↪markersize=6)
ax.axvline(x=best_knn.n_neighbors, color='r', linestyle='--', linewidth=1.5,
           label=f'Best k={best_knn.n_neighbors}')
ax.set_xlabel('Number of Neighbors (k)', fontsize=12)
ax.set_ylabel('RMSE', fontsize=12)
ax.set_title('KNN Elbow Plot: RMSE vs Number of Neighbors', fontsize=14,␣
 ↪fontweight='bold')
ax.legend(fontsize=11)
ax.grid(alpha=0.3, linestyle='--')
ax.set_xticks(range(1, 31, 2))
plt.tight_layout()
plt.show()

print(f"Best k from grid search: {best_knn.n_neighbors}")
print(f"Test RMSE at k={best_knn.n_neighbors}: {test_rmse_scores[best_knn.
 ↪n_neighbors-1]:.4f}")
```

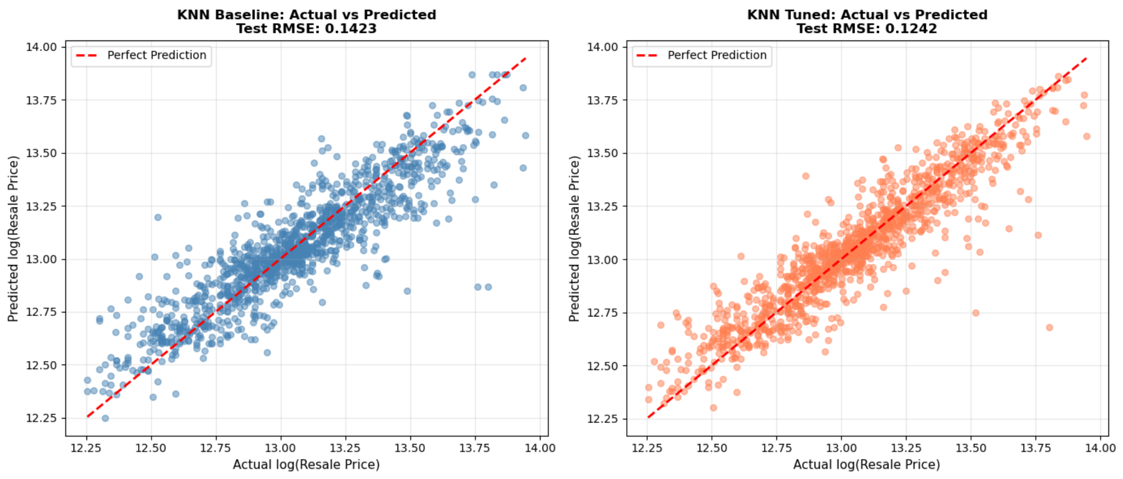
```
Creating elbow plot for KNN…
```



```
Best k from grid search: 3
Test RMSE at k=3: 0.1242
```

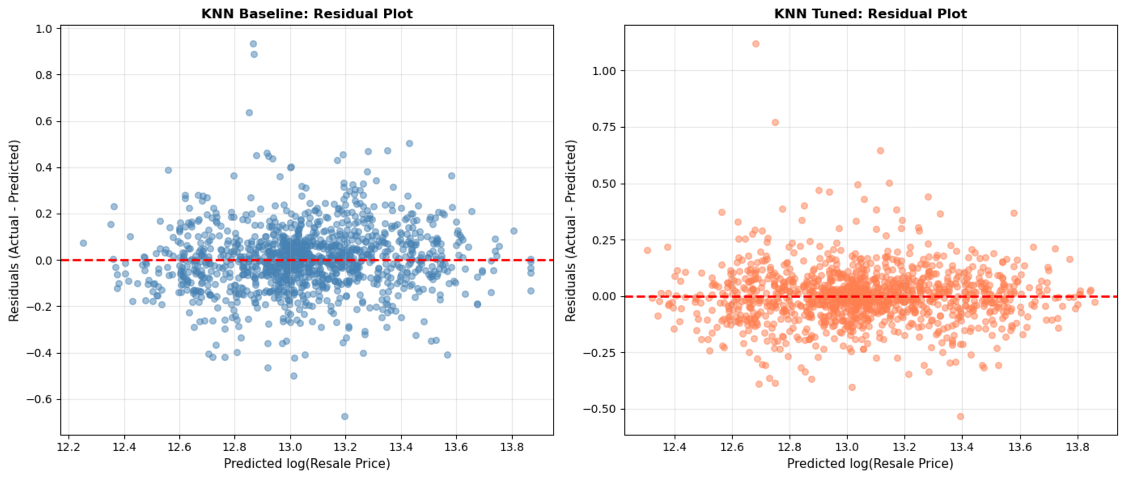
[27]:
```
# 2. Actual vs Predicted Scatter Plot (Test Set)
# Shows how well predictions match actual values
fig, axes = plt.subplots(1, 2, figsize=(14, 6))

# Baseline model
axes[0].scatter(y_test, y_pred_test_knn_base, alpha=0.5, s=30,␣
 ↪color='steelblue')
axes[0].plot([y_test.min(), y_test.max()], [y_test.min(), y_test.max()],
             'r--', linewidth=2, label='Perfect Prediction')
axes[0].set_xlabel('Actual log(Resale Price)', fontsize=11)
axes[0].set_ylabel('Predicted log(Resale Price)', fontsize=11)
axes[0].set_title(f'KNN Baseline: Actual vs Predicted\nTest RMSE: {rmse(y_test,␣
 ↪y_pred_test_knn_base):.4f}',
                    fontsize=12, fontweight='bold')
axes[0].legend()
axes[0].grid(alpha=0.3)

# Tuned model
axes[1].scatter(y_test, y_pred_test_knn_tuned, alpha=0.5, s=30, color='coral')
axes[1].plot([y_test.min(), y_test.max()], [y_test.min(), y_test.max()],
             'r--', linewidth=2, label='Perfect Prediction')
axes[1].set_xlabel('Actual log(Resale Price)', fontsize=11)
axes[1].set_ylabel('Predicted log(Resale Price)', fontsize=11)
```

```
axes[1].set_title(f'KNN Tuned: Actual vs Predicted\nTest RMSE: {rmse(y_test,␣
↪y_pred_test_knn_tuned):.4f}',
                    fontsize=12, fontweight='bold')
axes[1].legend()
axes[1].grid(alpha=0.3)

plt.tight_layout()
plt.show()
```



[28]:
```
# 3. Residual Plot (Test Set)
# Shows prediction errors - helps identify patterns in residuals
fig, axes = plt.subplots(1, 2, figsize=(14, 6))

# Baseline residuals
residuals_baseline = y_test - y_pred_test_knn_base
axes[0].scatter(y_pred_test_knn_base, residuals_baseline, alpha=0.5, s=30,␣
↪color='steelblue')
axes[0].axhline(y=0, color='r', linestyle='--', linewidth=2)
axes[0].set_xlabel('Predicted log(Resale Price)', fontsize=11)
axes[0].set_ylabel('Residuals (Actual - Predicted)', fontsize=11)
axes[0].set_title('KNN Baseline: Residual Plot', fontsize=12, fontweight='bold')
axes[0].grid(alpha=0.3)

# Tuned residuals
residuals_tuned = y_test - y_pred_test_knn_tuned
axes[1].scatter(y_pred_test_knn_tuned, residuals_tuned, alpha=0.5, s=30,␣
↪color='coral')
axes[1].axhline(y=0, color='r', linestyle='--', linewidth=2)
axes[1].set_xlabel('Predicted log(Resale Price)', fontsize=11)
axes[1].set_ylabel('Residuals (Actual - Predicted)', fontsize=11)
```

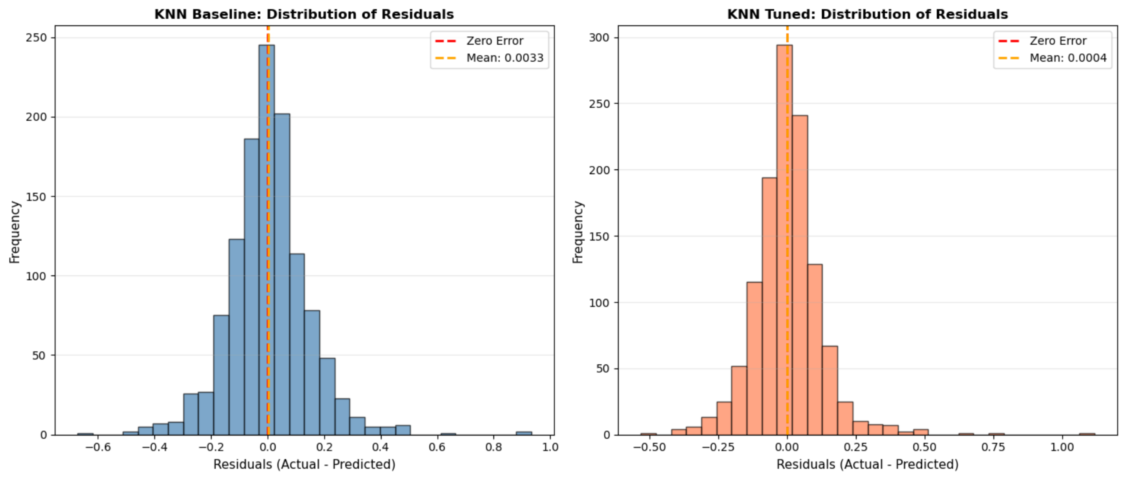
```
axes[1].set_title('KNN Tuned: Residual Plot', fontsize=12, fontweight='bold')
axes[1].grid(alpha=0.3)

plt.tight_layout()
plt.show()

# Print residual statistics
print("Residual Statistics (Test Set):")
print(f"Baseline - Mean: {np.mean(residuals_baseline):.6f}, Std: {np.
 ↪std(residuals_baseline):.4f}")
print(f"Tuned    - Mean: {np.mean(residuals_tuned):.6f}, Std: {np.
 ↪std(residuals_tuned):.4f}")
print(f"\nIdeal residuals should be centered around 0 with constant variance.")
```



```
Residual Statistics (Test Set):
Baseline - Mean: 0.003313, Std: 0.1423
Tuned    - Mean: 0.000374, Std: 0.1242

Ideal residuals should be centered around 0 with constant variance.
```

[29]:
```
# 4. Distribution of Prediction Errors
# Shows the distribution of residuals to check for normality
fig, axes = plt.subplots(1, 2, figsize=(14, 6))

# Baseline error distribution
axes[0].hist(residuals_baseline, bins=30, alpha=0.7, color='steelblue',␣
 ↪edgecolor='black')
axes[0].axvline(x=0, color='r', linestyle='--', linewidth=2, label='Zero Error')
axes[0].axvline(x=np.mean(residuals_baseline), color='orange', linestyle='--',␣
 ↪linewidth=2,
                label=f'Mean: {np.mean(residuals_baseline):.4f}')
```

```
axes[0].set_xlabel('Residuals (Actual - Predicted)', fontsize=11)
axes[0].set_ylabel('Frequency', fontsize=11)
axes[0].set_title('KNN Baseline: Distribution of Residuals', fontsize=12,␣
 ↪fontweight='bold')
axes[0].legend()
axes[0].grid(alpha=0.3, axis='y')

# Tuned error distribution
axes[1].hist(residuals_tuned, bins=30, alpha=0.7, color='coral',␣
 ↪edgecolor='black')
axes[1].axvline(x=0, color='r', linestyle='--', linewidth=2, label='Zero Error')
axes[1].axvline(x=np.mean(residuals_tuned), color='orange', linestyle='--',␣
 ↪linewidth=2,
                label=f'Mean: {np.mean(residuals_tuned):.4f}')
axes[1].set_xlabel('Residuals (Actual - Predicted)', fontsize=11)
axes[1].set_ylabel('Frequency', fontsize=11)
axes[1].set_title('KNN Tuned: Distribution of Residuals', fontsize=12,␣
 ↪fontweight='bold')
axes[1].legend()
axes[1].grid(alpha=0.3, axis='y')

plt.tight_layout()
plt.show()
```



1.5 Principal Component Regression (PCR)

PCR combines Principal Component Analysis (PCA) with linear regression. It reduces dimensionality by projecting features onto principal components, which can help with multicollinearity and overfitting.

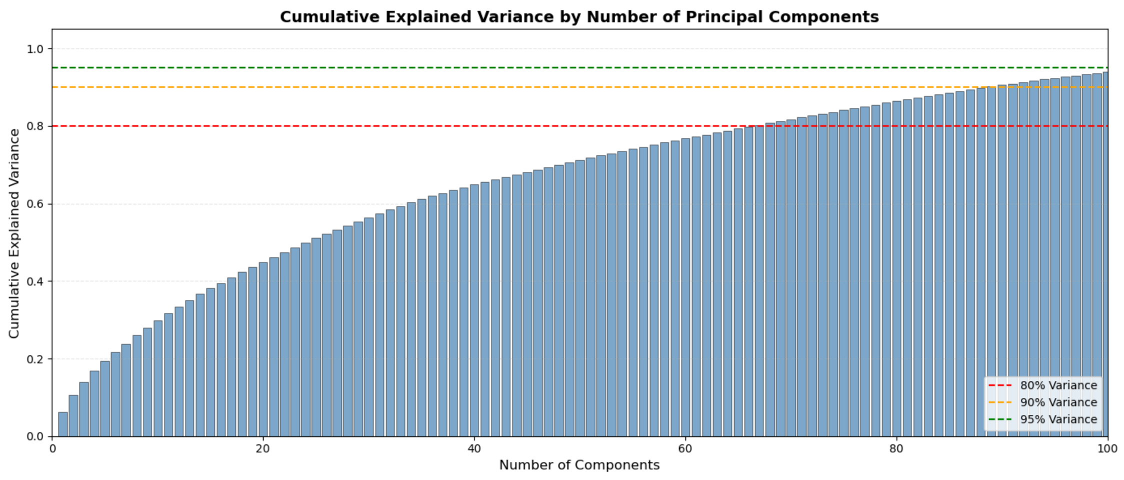
[8]:
```
# Standardize features for PCR (PCA is sensitive to scale)
scaler_pcr = StandardScaler()
X_full_train_scaled_pcr = scaler_pcr.fit_transform(X_full_train)
X_full_test_scaled_pcr = scaler_pcr.transform(X_full_test)

# Baseline: PCR with a fixed number of components (e.g., 10)
# We'll use 10 components as a reasonable baseline
n_components_baseline = 10
pca_baseline = PCA(n_components=n_components_baseline)
X_pca_train_base = pca_baseline.fit_transform(X_full_train_scaled_pcr)
X_pca_test_base = pca_baseline.transform(X_full_test_scaled_pcr)

pcr_baseline = LinearRegression()
pcr_baseline.fit(X_pca_train_base, y_train)

y_pred_train_pcr_base = pcr_baseline.predict(X_pca_train_base)
y_pred_test_pcr_base = pcr_baseline.predict(X_pca_test_base)

print(f"PCR Baseline (n_components={n_components_baseline}) - Train RMSE:␣
 ↪{rmse(y_train, y_pred_train_pcr_base):.4f}")
print(f"PCR Baseline (n_components={n_components_baseline}) - Test  RMSE:␣
 ↪{rmse(y_test, y_pred_test_pcr_base):.4f}")

# Check explained variance
explained_var = np.sum(pca_baseline.explained_variance_ratio_)
print(f"\nExplained variance ratio (first {n_components_baseline} components):␣
 ↪{explained_var:.4f}")
```

```
PCR Baseline (n_components=10) - Train RMSE: 0.2419
PCR Baseline (n_components=10) - Test  RMSE: 0.2434

Explained variance ratio (first 10 components): 0.2991
```

[9]:
```
# First, let's check how many components explain different amounts of variance
pca_full = PCA()
pca_full.fit(X_full_train_scaled_pcr)

cumulative_var = np.cumsum(pca_full.explained_variance_ratio_)
n_components = len(cumulative_var)

print("Cumulative explained variance by number of components:")
for n in [5, 10, 15, 20, 25, 30, min(50, n_components)]:
    if n <= n_components:
        print(f"  {n:2d} components: {cumulative_var[n-1]:.4f}")

# Create bar chart showing cumulative explained variance for all components
plt.figure(figsize=(14, 6))
```

```python
component_numbers = np.arange(1, n_components + 1)
plt.bar(component_numbers, cumulative_var, alpha=0.7, color='steelblue', edgecolor='black', linewidth=0.5)
plt.xlabel('Number of Components', fontsize=12)
plt.ylabel('Cumulative Explained Variance', fontsize=12)
plt.title('Cumulative Explained Variance by Number of Principal Components', fontsize=14, fontweight='bold')
plt.grid(axis='y', alpha=0.3, linestyle='--')
plt.axhline(y=0.8, color='r', linestyle='--', linewidth=1.5, label='80% Variance')
plt.axhline(y=0.9, color='orange', linestyle='--', linewidth=1.5, label='90% Variance')
plt.axhline(y=0.95, color='green', linestyle='--', linewidth=1.5, label='95% Variance')
plt.legend(loc='lower right')
plt.xlim(0, min(n_components + 5, 100))  # Show up to 100 components or all if less
plt.tight_layout()
plt.show()

# Print summary statistics
print(f"\nSummary:")
print(f"  Total number of components: {n_components}")
print(f"  Components needed for 80% variance: {np.argmax(cumulative_var >= 0.8) + 1}")
print(f"  Components needed for 90% variance: {np.argmax(cumulative_var >= 0.9) + 1}")
print(f"  Components needed for 95% variance: {np.argmax(cumulative_var >= 0.95) + 1}")
```

```
Cumulative explained variance by number of components:
   5 components: 0.1931
  10 components: 0.2991
  15 components: 0.3811
  20 components: 0.4496
  25 components: 0.5106
  30 components: 0.5644
  50 components: 0.7123
```



```
Summary:
  Total number of components: 228
  Components needed for 80% variance: 67
  Components needed for 90% variance: 89
  Components needed for 95% variance: 105
```

[10]:
```
# Hypertuned PCR: tune number of components using GridSearchCV
# We'll search over a range of component numbers
max_components = min(50, X_full_train_scaled_pcr.shape[1],␣
 ↪X_full_train_scaled_pcr.shape[0] - 1)
component_range = list(range(5, max_components + 1, 5))  # Try 5, 10, 15, ...,␣
 ↪up to max

# Create a pipeline for PCR
pcr_pipeline = Pipeline([
    ("scaler", StandardScaler()),
    ("pca", PCA()),
    ("regression", LinearRegression())
])

pcr_param_grid = {
    "pca__n_components": component_range
}

pcr_grid = GridSearchCV(
    estimator=pcr_pipeline,
    param_grid=pcr_param_grid,
    scoring="neg_mean_squared_error",
    cv=5,
    n_jobs=-1,
    verbose=1
)

pcr_grid.fit(X_full_train, y_train)

best_pcr = pcr_grid.best_estimator_
y_pred_test_pcr_tuned = best_pcr.predict(X_full_test)

print(f"\nPCR Tuned - Best n_components: {pcr_grid.
 ↪best_params_['pca__n_components']}")
print(f"PCR Tuned - Test RMSE:  {rmse(y_test, y_pred_test_pcr_tuned):.4f}")

# Also get train RMSE for comparison
y_pred_train_pcr_tuned = best_pcr.predict(X_full_train)
print(f"PCR Tuned - Train RMSE: {rmse(y_train, y_pred_train_pcr_tuned):.4f}")

# Get explained variance for best model
best_n_components = pcr_grid.best_params_['pca__n_components']
pca_best = best_pcr.named_steps['pca']
explained_var_best = np.sum(pca_best.explained_variance_ratio_)
print(f"\nExplained variance ratio (best {best_n_components} components):␣
 ↪{explained_var_best:.4f}")
```

```
Fitting 5 folds for each of 10 candidates, totalling 50 fits

PCR Tuned - Best n_components: 50
PCR Tuned - Test RMSE:  0.1322
PCR Tuned - Train RMSE: 0.1323

Explained variance ratio (best 50 components): 0.7123
```

1.6 Neural Network (Multi-layer Perceptron)

Neural networks can capture complex non-linear relationships. We'll use sklearn's MLPRegressor, which is a feedforward neural network.

[14]:
```
# Define PyTorch neural network model and training functions
class MLPRegressor(nn.Module):
    def __init__(self, input_size, hidden_sizes=(100,), activation='relu',␣
 ↪alpha=0.0001):
        super(MLPRegressor, self).__init__()

        # Build layers
        layers = []
        prev_size = input_size

        for hidden_size in hidden_sizes:
            layers.append(nn.Linear(prev_size, hidden_size))
            if activation == 'relu':
                layers.append(nn.ReLU())
            elif activation == 'leaky_relu':
                layers.append(nn.LeakyReLU(negative_slope=0.01))
            elif activation == 'tanh':
                layers.append(nn.Tanh())
            prev_size = hidden_size

        # Output layer (single value for regression)
        layers.append(nn.Linear(prev_size, 1))

        self.network = nn.Sequential(*layers)
        self.alpha = alpha  # L2 regularization (weight decay)

    def forward(self, x):
        return self.network(x).squeeze()

# Training function
def train_pytorch_nn(X_train, y_train, X_val, y_val, hidden_sizes=(100,),
                     activation='relu', alpha=0.001, learning_rate=0.001,
                     epochs=300, batch_size=64, patience=30, device=device):
    """
    Train a PyTorch neural network with early stopping.
    Returns: trained model, training history
    """
    # Convert to tensors
    X_train_tensor = torch.FloatTensor(X_train).to(device)
    y_train_tensor = torch.FloatTensor(y_train).to(device)
    X_val_tensor = torch.FloatTensor(X_val).to(device)
    y_val_tensor = torch.FloatTensor(y_val).to(device)

    # Create model
    model = MLPRegressor(
        input_size=X_train.shape[1],
        hidden_sizes=hidden_sizes,
        activation=activation,
        alpha=alpha
    ).to(device)

    # Loss and optimizer (Adam with weight decay for L2 regularization)
    criterion = nn.MSELoss()
    optimizer = optim.Adam(model.parameters(), lr=learning_rate,␣
 ↪weight_decay=alpha)

    # Training with early stopping
    train_losses = []
    val_losses = []
```

```python
    best_val_loss = float('inf')
    patience_counter = 0
    best_model_state = None

    train_loader = DataLoader(TensorDataset(X_train_tensor, y_train_tensor),
                              batch_size=batch_size, shuffle=True)

    for epoch in range(epochs):
        # Training
        model.train()
        train_loss = 0.0
        for X_batch, y_batch in train_loader:
            optimizer.zero_grad()
            y_pred = model(X_batch)
            loss = criterion(y_pred, y_batch)
            loss.backward()
            optimizer.step()
            train_loss += loss.item()

        train_loss /= len(train_loader)

        # Validation
        model.eval()
        with torch.no_grad():
            y_val_pred = model(X_val_tensor)
            val_loss = criterion(y_val_pred, y_val_tensor).item()

        train_losses.append(train_loss)
        val_losses.append(val_loss)

        # Early stopping
        if val_loss < best_val_loss:
            best_val_loss = val_loss
            patience_counter = 0
            best_model_state = model.state_dict().copy()
        else:
            patience_counter += 1
            if patience_counter >= patience:
                break

    # Load best model
    if best_model_state is not None:
        model.load_state_dict(best_model_state)

    return model, {'train_losses': train_losses, 'val_losses': val_losses}

# Prediction function
```

```python
def predict_pytorch_nn(model, X, device=device):
    """Make predictions with PyTorch model"""
    model.eval()
    X_tensor = torch.FloatTensor(X).to(device)
    with torch.no_grad():
        y_pred = model(X_tensor).cpu().numpy()
    return y_pred
```

[ ]:
```python
# Standardize features for Neural Network (required for convergence)
scaler_nn = StandardScaler()
X_full_train_scaled_nn = scaler_nn.fit_transform(X_full_train)
X_full_test_scaled_nn = scaler_nn.transform(X_full_test)

# Baseline: Simple MLP with default parameters
print("Training baseline neural network...")
print("Parameters: hidden_sizes=(100,), activation='relu', lr=0.001")

# Split training data for validation (10% for early stopping)
X_nn_train, X_nn_val, y_nn_train, y_nn_val = train_test_split(
    X_full_train_scaled_nn, y_train, test_size=0.1, random_state=42
)

nn_baseline, baseline_history = train_pytorch_nn(
    X_nn_train, y_nn_train, X_nn_val, y_nn_val,
    hidden_sizes=(100,),
    activation='relu',
    learning_rate=0.001,
    epochs=300,
    device=device
)

y_pred_train_nn_base = predict_pytorch_nn(nn_baseline, X_full_train_scaled_nn,␣
 ↪device)
y_pred_test_nn_base = predict_pytorch_nn(nn_baseline, X_full_test_scaled_nn,␣
 ↪device)

print(f"\nNN Baseline - Train RMSE: {rmse(y_train, y_pred_train_nn_base):.4f}")
print(f"NN Baseline - Test  RMSE: {rmse(y_test, y_pred_test_nn_base):.4f}")
print(f"NN Baseline - Training epochs: {len(baseline_history['train_losses'])}")
```

```
Training baseline neural network…
Parameters: hidden_sizes=(100,), activation='relu', lr=0.001

NN Baseline - Train RMSE: 0.1704
NN Baseline - Test  RMSE: 0.2033
NN Baseline - Training epochs: 159
NN Baseline - Final train loss: 0.034670
NN Baseline - Final val loss: 0.083216
```

```
[16]: print("Starting hyperparameter tuning with 5-fold CV...")
      kf = KFold(n_splits=5, shuffle=True, random_state=42)

      param_combinations = []
      for hidden_sizes in [(50,), (100,), (150,), (100, 50)]:
          for activation in ["relu", "leaky_relu", "tanh"]:
              for lr in [0.001, 0.01, 0.1]:
                  param_combinations.append(
                      {
                          "hidden_sizes": hidden_sizes,
                          "activation": activation,
                          "learning_rate": lr,
                      }
                  )

      print(f"Testing {len(param_combinations)} parameter combinations\n")

      best_score = float("inf")
      best_params = None

      # Grid search with cross-validation
      for i, params in enumerate(param_combinations):
          print(f"Testing {i+1}/{len(param_combinations)}: {params}")

          cv_rmse_scores = []

          for fold, (train_idx, val_idx) in enumerate(kf.
       ↪split(X_full_train_scaled_nn)):
              X_tr, X_val = X_full_train_scaled_nn[train_idx],␣
       ↪X_full_train_scaled_nn[val_idx]
              y_tr, y_val = y_train[train_idx], y_train[val_idx]

              # Use the CV validation fold for early stopping
              model, _ = train_pytorch_nn(
                  X_tr,
                  y_tr,
                  X_val,
                  y_val,
                  hidden_sizes=params["hidden_sizes"],
                  activation=params["activation"],
                  learning_rate=params["learning_rate"],
                  epochs=500,
                  device=device,
              )

              # Evaluate on the CV validation fold
              y_val_pred = predict_pytorch_nn(model, X_val, device)
```

```
        cv_rmse_scores.append(rmse(y_val, y_val_pred))

    mean_cv_rmse = np.mean(cv_rmse_scores)
    print(f"  Mean CV RMSE: {mean_cv_rmse:.4f}\n")

    if mean_cv_rmse < best_score:
        best_score = mean_cv_rmse
        best_params = params.copy()

print("=" * 60)
print("HYPERPARAMETER TUNING COMPLETE")
print("=" * 60)
print(f"Best parameters: {best_params}")
print(f"Best CV RMSE: {best_score:.4f}")

# Retrain on FULL training set with best hyperparameters
# Split training data for validation (10% for early stopping)
X_tr_inner, X_val_inner, y_tr_inner, y_val_inner = train_test_split(
    X_full_train_scaled_nn, y_train, test_size=0.1, random_state=42
)

final_model, _ = train_pytorch_nn(
    X_tr_inner,
    y_tr_inner,
    X_val_inner,
    y_val_inner,
    hidden_sizes=best_params["hidden_sizes"],
    activation=best_params["activation"],
    learning_rate=best_params["learning_rate"],
    epochs=500,
    device=device,
)

# Evaluate final model
y_pred_test_nn_tuned = predict_pytorch_nn(final_model, X_full_test_scaled_nn,␣
↪device)
y_pred_train_nn_tuned = predict_pytorch_nn(final_model, X_full_train_scaled_nn,␣
↪device)

print(f"\nNN Tuned - Test RMSE:  {rmse(y_test, y_pred_test_nn_tuned):.4f}")
print(f"NN Tuned - Train RMSE: {rmse(y_train, y_pred_train_nn_tuned):.4f}")
```

```
Starting hyperparameter tuning with 5-fold CV…
Testing 36 parameter combinations

Testing 1/36: {'hidden_sizes': (50,), 'activation': 'relu', 'learning_rate':
0.001}
```

```
  Mean CV RMSE: 0.2163

Testing 2/36: {'hidden_sizes': (50,), 'activation': 'relu', 'learning_rate':
0.01}
  Mean CV RMSE: 0.2881

Testing 3/36: {'hidden_sizes': (50,), 'activation': 'relu', 'learning_rate':
0.1}
  Mean CV RMSE: 31.7597

Testing 4/36: {'hidden_sizes': (50,), 'activation': 'leaky_relu',
'learning_rate': 0.001}
  Mean CV RMSE: 0.2045

Testing 5/36: {'hidden_sizes': (50,), 'activation': 'leaky_relu',
'learning_rate': 0.01}
  Mean CV RMSE: 0.3384

Testing 6/36: {'hidden_sizes': (50,), 'activation': 'leaky_relu',
'learning_rate': 0.1}
  Mean CV RMSE: 71.1036

Testing 7/36: {'hidden_sizes': (50,), 'activation': 'tanh', 'learning_rate':
0.001}
  Mean CV RMSE: 0.3976

Testing 8/36: {'hidden_sizes': (50,), 'activation': 'tanh', 'learning_rate':
0.01}
  Mean CV RMSE: 0.3716

Testing 9/36: {'hidden_sizes': (50,), 'activation': 'tanh', 'learning_rate':
0.1}
  Mean CV RMSE: 0.2049

Testing 10/36: {'hidden_sizes': (100,), 'activation': 'relu', 'learning_rate':
0.001}
  Mean CV RMSE: 0.2085

Testing 11/36: {'hidden_sizes': (100,), 'activation': 'relu', 'learning_rate':
0.01}
  Mean CV RMSE: 0.3774

Testing 12/36: {'hidden_sizes': (100,), 'activation': 'relu', 'learning_rate':
0.1}
  Mean CV RMSE: 65.0246

Testing 13/36: {'hidden_sizes': (100,), 'activation': 'leaky_relu',
'learning_rate': 0.001}
```

```
  Mean CV RMSE: 0.2061

Testing 14/36: {'hidden_sizes': (100,), 'activation': 'leaky_relu',
'learning_rate': 0.01}
  Mean CV RMSE: 1.4130

Testing 15/36: {'hidden_sizes': (100,), 'activation': 'leaky_relu',
'learning_rate': 0.1}
  Mean CV RMSE: 35.8707

Testing 16/36: {'hidden_sizes': (100,), 'activation': 'tanh', 'learning_rate':
0.001}
  Mean CV RMSE: 0.3738

Testing 17/36: {'hidden_sizes': (100,), 'activation': 'tanh', 'learning_rate':
0.01}
  Mean CV RMSE: 0.3300

Testing 18/36: {'hidden_sizes': (100,), 'activation': 'tanh', 'learning_rate':
0.1}
  Mean CV RMSE: 0.3850

Testing 19/36: {'hidden_sizes': (150,), 'activation': 'relu', 'learning_rate':
0.001}
  Mean CV RMSE: 0.2077

Testing 20/36: {'hidden_sizes': (150,), 'activation': 'relu', 'learning_rate':
0.01}
  Mean CV RMSE: 0.3530

Testing 21/36: {'hidden_sizes': (150,), 'activation': 'relu', 'learning_rate':
0.1}
  Mean CV RMSE: 73.4876

Testing 22/36: {'hidden_sizes': (150,), 'activation': 'leaky_relu',
'learning_rate': 0.001}
  Mean CV RMSE: 0.2376

Testing 23/36: {'hidden_sizes': (150,), 'activation': 'leaky_relu',
'learning_rate': 0.01}
  Mean CV RMSE: 0.5990

Testing 24/36: {'hidden_sizes': (150,), 'activation': 'leaky_relu',
'learning_rate': 0.1}
  Mean CV RMSE: 167.1990

Testing 25/36: {'hidden_sizes': (150,), 'activation': 'tanh', 'learning_rate':
0.001}
```

```
  Mean CV RMSE: 0.3769

Testing 26/36: {'hidden_sizes': (150,), 'activation': 'tanh', 'learning_rate':
0.01}
  Mean CV RMSE: 0.3307

Testing 27/36: {'hidden_sizes': (150,), 'activation': 'tanh', 'learning_rate':
0.1}
  Mean CV RMSE: 0.4918

Testing 28/36: {'hidden_sizes': (100, 50), 'activation': 'relu',
'learning_rate': 0.001}
  Mean CV RMSE: 0.2252

Testing 29/36: {'hidden_sizes': (100, 50), 'activation': 'relu',
'learning_rate': 0.01}
  Mean CV RMSE: 0.3102

Testing 30/36: {'hidden_sizes': (100, 50), 'activation': 'relu',
'learning_rate': 0.1}
  Mean CV RMSE: 0.2997

Testing 31/36: {'hidden_sizes': (100, 50), 'activation': 'leaky_relu',
'learning_rate': 0.001}
  Mean CV RMSE: 0.2050

Testing 32/36: {'hidden_sizes': (100, 50), 'activation': 'leaky_relu',
'learning_rate': 0.01}
  Mean CV RMSE: 0.2808

Testing 33/36: {'hidden_sizes': (100, 50), 'activation': 'leaky_relu',
'learning_rate': 0.1}
  Mean CV RMSE: 7.3626

Testing 34/36: {'hidden_sizes': (100, 50), 'activation': 'tanh',
'learning_rate': 0.001}
  Mean CV RMSE: 0.2141

Testing 35/36: {'hidden_sizes': (100, 50), 'activation': 'tanh',
'learning_rate': 0.01}
  Mean CV RMSE: 0.2566

Testing 36/36: {'hidden_sizes': (100, 50), 'activation': 'tanh',
'learning_rate': 0.1}
  Mean CV RMSE: 0.1127

============================================================
HYPERPARAMETER TUNING COMPLETE
```

```
============================================================
Best parameters: {'hidden_sizes': (100, 50), 'activation': 'tanh',
'learning_rate': 0.1}
Best CV RMSE: 0.1127

NN Tuned - Test RMSE:  0.1620
NN Tuned - Train RMSE: 0.1537
```

1.7 Model Comparison Summary

[17]:
```python
# Create a summary comparison table
results_summary = pd.DataFrame({
    "Model": ["KNN Baseline", "KNN Tuned",
              "PCR Baseline", "PCR Tuned",
              "NN Baseline", "NN Tuned"],
    "Train RMSE": [
        rmse(y_train, y_pred_train_knn_base),
        rmse(y_train, y_pred_train_knn_tuned),
        rmse(y_train, y_pred_train_pcr_base),
        rmse(y_train, y_pred_train_pcr_tuned),
        rmse(y_train, y_pred_train_nn_base),
        rmse(y_train, y_pred_train_nn_tuned)
    ],
    "Test RMSE": [
        rmse(y_test, y_pred_test_knn_base),
        rmse(y_test, y_pred_test_knn_tuned),
        rmse(y_test, y_pred_test_pcr_base),
        rmse(y_test, y_pred_test_pcr_tuned),
        rmse(y_test, y_pred_test_nn_base),
        rmse(y_test, y_pred_test_nn_tuned)
    ]
})

print("\n" + "="*60)
print("MODEL COMPARISON SUMMARY")
print("="*60)
print(results_summary.to_string(index=False))
print("="*60)

# Find best model by test RMSE
best_test_rmse_idx = results_summary["Test RMSE"].idxmin()
best_model_name = results_summary.loc[best_test_rmse_idx, "Model"]
best_test_rmse = results_summary.loc[best_test_rmse_idx, "Test RMSE"]

print(f"\nBest model (by Test RMSE): {best_model_name}")
print(f"Best Test RMSE: {best_test_rmse:.4f}")
```

```
============================================================
MODEL COMPARISON SUMMARY
============================================================
       Model  Train RMSE  Test RMSE
KNN Baseline    0.108149   0.142297
   KNN Tuned    0.004133   0.124174
PCR Baseline    0.241927   0.243392
   PCR Tuned    0.132263   0.132157
 NN Baseline    0.170382   0.203317
    NN Tuned    0.153715   0.162027
============================================================

Best model (by Test RMSE): KNN Tuned
Best Test RMSE: 0.1242
```