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Part II: Intermediate Level - Statistical Foundations

Chapter 6: Statistical Concepts for Machine Learning

User: I feel like I have a good grasp of the basics now, but I keep hearing about statistical concepts that seem important for machine learning. Things like confidence intervals, correlation coefficients, and statistical tests. Can you help me understand how these connect to what we've learned?

Expert: Absolutely! You're ready to dive into the statistical foundations that make machine learning more rigorous and reliable. These concepts will help you better understand your data, validate your models, and make more confident decisions. Let's start with the fundamentals.

```

1 import numpy as np
2 import pandas as pd
3 import matplotlib.pyplot as plt
4 import seaborn as sns
5 from scipy import stats
6 from sklearn.datasets import make_regression
7 from sklearn.linear_model import LinearRegression
8 from sklearn.metrics import mean_squared_error, r2_score
9 import warnings
10 warnings.filterwarnings('ignore')
11
12 def statistical_foundations_intro():
13     """
14     Introduction to key statistical concepts for ML
15     """
16     print("STATISTICAL FOUNDATIONS FOR MACHINE LEARNING")
17     print("=" * 50)
18
19     print("Why Statistics Matter in ML:")
20     print("✓ Understand data distributions and patterns")
21     print("✓ Quantify uncertainty in predictions")
22     print("✓ Test hypotheses about model performance")
23     print("✓ Make confident business decisions")
24     print("✓ Detect and avoid statistical pitfalls")
25
26     return True
27
28 statistical_foundations_intro()

```

User: That makes sense! I want to understand how to be more confident about my model's predictions and avoid making wrong conclusions. Where should we start?

Expert: Perfect mindset! Let's start with **Pearson's Correlation Coefficient** - one of the most fundamental statistical measures for understanding relationships between variables.

```

1 def pearson_correlation_deep_dive():
2     """
3     Comprehensive explanation of Pearson's correlation
4     """
5     print("PEARSON'S CORRELATION COEFFICIENT")
6     print("=" * 40)
7
8     # Generate sample data with different correlation strengths
9     np.random.seed(42)
10    n_samples = 100
11
12    # Perfect positive correlation

```

```

13     x1 = np.random.normal(0, 1, n_samples)
14     y1 = 2 * x1 + np.random.normal(0, 0.1, n_samples) # Almost
perfect
15
16     # Moderate positive correlation
17     x2 = np.random.normal(0, 1, n_samples)
18     y2 = x2 + np.random.normal(0, 1, n_samples)
19
20     # No correlation
21     x3 = np.random.normal(0, 1, n_samples)
22     y3 = np.random.normal(0, 1, n_samples)
23
24     # Negative correlation
25     x4 = np.random.normal(0, 1, n_samples)
26     y4 = -1.5 * x4 + np.random.normal(0, 0.5, n_samples)
27
28     # Calculate Pearson correlations
29     corr1, p_value1 = stats.pearsonr(x1, y1)
30     corr2, p_value2 = stats.pearsonr(x2, y2)
31     corr3, p_value3 = stats.pearsonr(x3, y3)
32     corr4, p_value4 = stats.pearsonr(x4, y4)
33
34     print("CORRELATION COEFFICIENT INTERPRETATION:")
35     print("-" * 40)
36     print("Range: -1 to +1")
37     print("+1: Perfect positive correlation")
38     print(" 0: No linear correlation")
39     print("-1: Perfect negative correlation")
40     print()
41
42     print("STRENGTH GUIDELINES:")
43     print("0.0 - 0.3: Weak correlation")
44     print("0.3 - 0.7: Moderate correlation")
45     print("0.7 - 1.0: Strong correlation")
46     print()
47
48     # Visualize different correlations
49     fig, axes = plt.subplots(2, 2, figsize=(12, 10))
50
51     # Strong positive
52     axes[0, 0].scatter(x1, y1, alpha=0.6, color='red')
53     axes[0, 0].set_title(f'Strong Positive\nr = {corr1:.3f}, p =
{p_value1:.3f}')
54     axes[0, 0].set_xlabel('X')
55     axes[0, 0].set_ylabel('Y')
56     axes[0, 0].grid(True, alpha=0.3)
57
58     # Moderate positive
59     axes[0, 1].scatter(x2, y2, alpha=0.6, color='blue')
60     axes[0, 1].set_title(f'Moderate Positive\nr = {corr2:.3f}, p =

```

```

    {p_value2:.3f}')
61     axes[0, 1].set_xlabel('X')
62     axes[0, 1].set_ylabel('Y')
63     axes[0, 1].grid(True, alpha=0.3)
64
65     # No correlation
66     axes[1, 0].scatter(x3, y3, alpha=0.6, color='green')
67     axes[1, 0].set_title(f'No Correlation\nr = {corr3:.3f}, p =
    {p_value3:.3f}')
68     axes[1, 0].set_xlabel('X')
69     axes[1, 0].set_ylabel('Y')
70     axes[1, 0].grid(True, alpha=0.3)
71
72     # Negative correlation
73     axes[1, 1].scatter(x4, y4, alpha=0.6, color='purple')
74     axes[1, 1].set_title(f'Strong Negative\nr = {corr4:.3f}, p =
    {p_value4:.3f}')
75     axes[1, 1].set_xlabel('X')
76     axes[1, 1].set_ylabel('Y')
77     axes[1, 1].grid(True, alpha=0.3)
78
79     plt.tight_layout()
80     plt.show()
81
82     print("BUSINESS INTERPRETATION:")
83     print("-" * 25)
84     print(f"Strong Positive (r={corr1:.3f}): As X increases, Y
    increases predictably")
85     print(f"Moderate Positive (r={corr2:.3f}): X and Y tend to
    increase together")
86     print(f"No Correlation (r={corr3:.3f}): X and Y are
    independent")
87     print(f"Strong Negative (r={corr4:.3f}): As X increases, Y
    decreases predictably")
88
89     print("\nP-VALUES EXPLAINED:")
90     print("-" * 20)
91     print("p < 0.05: Statistically significant correlation")
92     print("p ≥ 0.05: Could be due to random chance")
93
94     return corr1, corr2, corr3, corr4
95 correlations = pearson_correlation_deep_dive()

```

User: This is really helpful! I can see how correlation strength affects the scatter plots. But what about confidence intervals? I hear this term a lot but I'm not sure what it means practically.

Expert: Excellent question! **Confidence intervals** are crucial for understanding the uncertainty in our estimates. Let me show you how they work in the context of machine learning.

```

1 def confidence_intervals_explained():
2     """
3     Comprehensive explanation of confidence intervals
4     """
5     print("CONFIDENCE INTERVALS IN MACHINE LEARNING")
6     print("=" * 45)
7
8     print("WHAT IS A CONFIDENCE INTERVAL?")
9     print("-" * 35)
10    print("A range of values that likely contains the true
parameter")
11    print("95% CI means: If we repeated this study 100 times,")
12    print("95 of those intervals would contain the true value")
13    print()
14
15    # Generate sample data
16    np.random.seed(42)
17    n_samples = 50
18    true_slope = 2.5
19    true_intercept = 10
20
21    x = np.random.uniform(1, 10, n_samples)
22    noise = np.random.normal(0, 2, n_samples)
23    y = true_intercept + true_slope * x + noise
24
25    # Fit linear regression
26    from sklearn.linear_model import LinearRegression
27    model = LinearRegression()
28    X = x.reshape(-1, 1)
29    model.fit(X, y)
30
31    # Get predictions
32    y_pred = model.predict(X)
33
34    # Calculate confidence intervals manually
35    def calculate_prediction_intervals(X, y, model,
confidence=0.95):
36        """
37        Calculate prediction intervals for linear regression
38        """
39        n = len(y)
40        y_pred = model.predict(X)
41
42        # Calculate residuals and standard error
43        residuals = y - y_pred
44        mse = np.mean(residuals**2)
45        se = np.sqrt(mse)
46

```

```

47     # Degrees of freedom
48     dof = n - 2 # n - (number of parameters)
49
50     # t-critical value
51     alpha = 1 - confidence
52     t_crit = stats.t.ppf(1 - alpha/2, dof)
53
54     # Prediction intervals
55     margin_error = t_crit * se * np.sqrt(1 + 1/n + (X.flatten()
- np.mean(X.flatten()))**2 / np.sum((X.flatten() -
np.mean(X.flatten()))**2))
56
57     lower_bound = y_pred - margin_error
58     upper_bound = y_pred + margin_error
59
60     return lower_bound, upper_bound, se, t_crit
61
62     lower_bound, upper_bound, se, t_crit =
calculate_prediction_intervals(X, y, model)
63
64     print("CONFIDENCE INTERVAL CALCULATION:")
65     print("-" * 35)
66     print(f"Sample size: {n_samples}")
67     print(f"Degrees of freedom: {n_samples - 2}")
68     print(f"Standard error: {se:.3f}")
69     print(f"t-critical value (95% CI): {t_crit:.3f}")
70     print(f"True slope: {true_slope:.2f}")
71     print(f"Estimated slope: {model.coef_[0]:.2f}")
72     print(f"True intercept: {true_intercept:.2f}")
73     print(f"Estimated intercept: {model.intercept_:.2f}")
74
75     # Visualize confidence intervals
76     plt.figure(figsize=(12, 8))
77
78     # Main plot with confidence intervals
79     plt.subplot(2, 2, 1)
80     plt.scatter(x, y, alpha=0.6, color='blue', label='Data')
81     plt.plot(x, y_pred, 'r-', label='Regression Line')
82     plt.fill_between(x, lower_bound, upper_bound, alpha=0.3,
color='red', label='95% Prediction Interval')
83     plt.xlabel('X')
84     plt.ylabel('Y')
85     plt.title('Linear Regression with 95% Prediction Intervals')
86     plt.legend()
87     plt.grid(True, alpha=0.3)
88
89     # Demonstrate multiple samples
90     plt.subplot(2, 2, 2)
91
92     # Simulate multiple experiments

```

```

93     slopes = []
94     intercepts = []
95
96     for i in range(100):
97         # Generate new sample each time
98         x_sim = np.random.uniform(1, 10, n_samples)
99         y_sim = true_intercept + true_slope * x_sim +
np.random.normal(0, 2, n_samples)
100
101         # Fit model
102         model_sim = LinearRegression()
103         model_sim.fit(x_sim.reshape(-1, 1), y_sim)
104
105         slopes.append(model_sim.coef_[0])
106         intercepts.append(model_sim.intercept_)
107
108     plt.hist(slopes, bins=20, alpha=0.7, color='green')
109     plt.axvline(true_slope, color='red', linestyle='--',
linewidth=2, label=f'True Slope ({true_slope})')
110     plt.axvline(np.mean(slopes), color='blue', linestyle='-',
linewidth=2, label=f'Mean Estimate ({np.mean(slopes):.2f})')
111     plt.xlabel('Estimated Slope')
112     plt.ylabel('Frequency')
113     plt.title('Distribution of Slope Estimates (100 experiments)')
114     plt.legend()
115     plt.grid(True, alpha=0.3)
116
117     # Calculate confidence interval for slope
118     slope_ci_lower = np.percentile(slopes, 2.5)
119     slope_ci_upper = np.percentile(slopes, 97.5)
120
121     plt.axvline(slope_ci_lower, color='orange', linestyle=':',
alpha=0.7)
122     plt.axvline(slope_ci_upper, color='orange', linestyle=':',
alpha=0.7)
123
124     # Business interpretation
125     plt.subplot(2, 1, 2)
126     plt.axis('off')
127
128     interpretation_text = f"""
129 BUSINESS INTERPRETATION OF CONFIDENCE INTERVALS:
130 ✓ SLOPE ESTIMATE: {model.coef_[0]:.2f}
131 ✓ 95% CI for slope: [{slope_ci_lower:.2f}, {slope_ci_upper:.2f}]
132 WHAT THIS MEANS:
133 • We're 95% confident the true relationship between X and Y
134   has a slope between {slope_ci_lower:.2f} and {slope_ci_upper:.2f}
135 • For every 1-unit increase in X, Y increases by approximately
136   {model.coef_[0]:.2f} units (±{(slope_ci_upper-
slope_ci_lower)/2:.2f})

```

```

130 BUSINESS DECISIONS:
141 • If planning based on this relationship, account for uncertainty
142 • Wider intervals = more uncertainty = more conservative planning
143 • Narrower intervals = more confidence = can make bolder decisions
144 SAMPLE SIZE EFFECT:
145 • Larger samples → Narrower confidence intervals
146 • More data → More confident estimates
147
148 """
149
150 plt.text(0.05, 0.95, interpretation_text,
151          transform=plt.gca().transAxes,
152          fontsize=10, verticalalignment='top',
153          fontfamily='monospace',
154          bbox=dict(boxstyle='round', facecolor='lightblue',
155                  alpha=0.8))
156
157 plt.tight_layout()
158 plt.show()
159
160 print("PRACTICAL APPLICATIONS:")
161 print("-" * 25)
162 print("• Revenue forecasting: 'Sales will be $100K ± $15K'")
163 print("• A/B testing: 'Treatment effect is 5% ± 2%'")
164 print("• Model performance: 'Accuracy is 85% ± 3%'")
165 print("• Risk assessment: 'Default rate is 2% ± 0.5%'")
166
167 return slopes, intercepts, slope_ci_lower, slope_ci_upper
168 slopes, intercepts, ci_lower, ci_upper =
169 confidence_intervals_explained()

```

User: This is incredibly insightful! I love how you showed that confidence intervals help us understand the uncertainty in our estimates. Now I'm curious about statistical tests. When would I use something like a t-test in machine learning?

Expert: Great question! Statistical tests are essential for making data-driven decisions and validating our models. Let me show you the **t-test** and other important statistical tests in ML contexts.

```

1 def statistical_tests_for_ml():
2     """
3     Statistical tests commonly used in machine learning
4     """
5     print("STATISTICAL TESTS IN MACHINE LEARNING")
6     print("=" * 40)
7
8     print("WHY WE NEED STATISTICAL TESTS:")
9     print("-" * 35)

```



```

10     print("• Validate model improvements")
11     print("• Compare different algorithms")
12     print("• Test feature importance")
13     print("• Validate A/B test results")
14     print("• Detect significant differences")
15
16     # Generate sample data for demonstrations
17     np.random.seed(42)
18
19     print("\n1. ONE-SAMPLE T-TEST")
20     print("-" * 20)
21     print("Question: Is our model's accuracy significantly
different from a baseline?")
22
23     # Simulate model accuracy scores from cross-validation
24     baseline_accuracy = 0.75
25     model_accuracies = np.random.normal(0.82, 0.05, 30) # 30 CV
folds
26
27     # Perform one-sample t-test
28     t_stat, p_value = stats.ttest_1samp(model_accuracies,
baseline_accuracy)
29
30     print(f"Baseline accuracy: {baseline_accuracy:.1%}")
31     print(f"Our model accuracy: {np.mean(model_accuracies):.1%} ±
{np.std(model_accuracies):.1%}")
32     print(f"t-statistic: {t_stat:.3f}")
33     print(f"p-value: {p_value:.6f}")
34
35     if p_value < 0.05:
36         print("✅ RESULT: Significant improvement over baseline!")
37     else:
38         print("❌ RESULT: No significant improvement over
baseline")
39
40     print("\n2. TWO-SAMPLE T-TEST")
41     print("-" * 20)
42     print("Question: Is Model A significantly better than Model
B?")
43
44     # Simulate performance of two models
45     model_a_scores = np.random.normal(0.85, 0.04, 25)
46     model_b_scores = np.random.normal(0.82, 0.045, 25)
47
48     # Perform independent t-test
49     t_stat_2, p_value_2 = stats.ttest_ind(model_a_scores,
model_b_scores)
50
51     print(f"Model A accuracy: {np.mean(model_a_scores):.1%} ±
{np.std(model_a_scores):.1%}")

```

```

52     print(f"Model B accuracy: {np.mean(model_b_scores):.1%} ±
{np.std(model_b_scores):.1%}")
53     print(f"Difference: {np.mean(model_a_scores) -
np.mean(model_b_scores):.1%}")
54     print(f"t-statistic: {t_stat_2:.3f}")
55     print(f"p-value: {p_value_2:.6f}")
56
57     if p_value_2 < 0.05:
58         print("✅ RESULT: Model A is significantly better than
Model B!")
59     else:
60         print("❌ RESULT: No significant difference between
models")
61
62     print("\n3. PAIRED T-TEST")
63     print("-" * 16)
64     print("Question: Does feature engineering significantly improve
performance?")
65
66     # Simulate before/after feature engineering on same datasets
67     before_scores = np.random.normal(0.78, 0.06, 20)
68     after_scores = before_scores + np.random.normal(0.05, 0.02, 20)
69     # Improvement
70     # Perform paired t-test
71     t_stat_paired, p_value_paired = stats.ttest_rel(after_scores,
before_scores)
72
73     print(f"Before feature engineering:
{np.mean(before_scores):.1%} ± {np.std(before_scores):.1%}")
74     print(f"After feature engineering: {np.mean(after_scores):.1%}
± {np.std(after_scores):.1%}")
75     print(f"Average improvement: {np.mean(after_scores -
before_scores):.1%}")
76     print(f"t-statistic: {t_stat_paired:.3f}")
77     print(f"p-value: {p_value_paired:.6f}")
78
79     if p_value_paired < 0.05:
80         print("✅ RESULT: Feature engineering significantly
improves performance!")
81     else:
82         print("❌ RESULT: No significant improvement from feature
engineering")
83
84     # Visualize the tests
85     fig, axes = plt.subplots(2, 2, figsize=(15, 10))
86
87     # One-sample t-test visualization
88     axes[0, 0].hist(model_accuracies, bins=15, alpha=0.7,
color='blue', density=True)

```

```

89     axes[0, 0].axvline(baseline_accuracy, color='red', linestyle='-'
-   -, linewidth=2, label=f'Baseline ({baseline_accuracy:.1%})')
90     axes[0, 0].axvline(np.mean(model_accuracies), color='green',
linestyle='-', linewidth=2, label=f'Our Model
({np.mean(model_accuracies):.1%})')
91     axes[0, 0].set_xlabel('Accuracy')
92     axes[0, 0].set_ylabel('Density')
93     axes[0, 0].set_title('One-Sample t-test: Model vs Baseline')
94     axes[0, 0].legend()
95     axes[0, 0].grid(True, alpha=0.3)
96
97     # Two-sample t-test visualization
98     axes[0, 1].hist(model_a_scores, bins=15, alpha=0.7,
color='blue', label='Model A', density=True)
99     axes[0, 1].hist(model_b_scores, bins=15, alpha=0.7,
color='red', label='Model B', density=True)
100    axes[0, 1].set_xlabel('Accuracy')
101    axes[0, 1].set_ylabel('Density')
102    axes[0, 1].set_title('Two-Sample t-test: Model A vs Model B')
103    axes[0, 1].legend()
104    axes[0, 1].grid(True, alpha=0.3)
105
106    # Paired t-test visualization
107    axes[1, 0].scatter(before_scores, after_scores, alpha=0.7,
color='purple')
108    axes[1, 0].plot([0.6, 0.9], [0.6, 0.9], 'k--', alpha=0.5,
label='No improvement line')
109    axes[1, 0].set_xlabel('Before Feature Engineering')
110    axes[1, 0].set_ylabel('After Feature Engineering')
111    axes[1, 0].set_title('Paired t-test: Before vs After')
112    axes[1, 0].legend()
113    axes[1, 0].grid(True, alpha=0.3)
114
115    # Effect sizes and practical significance
116    axes[1, 1].axis('off')
117
118    # Calculate effect sizes (Cohen's d)
119    def cohens_d(x1, x2):
120        pooled_std = np.sqrt(((len(x1) - 1) * np.var(x1, ddof=1) +
(len(x2) - 1) * np.var(x2, ddof=1)) / (len(x1) + len(x2) - 2))
121        return (np.mean(x1) - np.mean(x2)) / pooled_std
122
123    effect_size_ab = cohens_d(model_a_scores, model_b_scores)
124    effect_size_paired = np.mean(after_scores - before_scores) /
np.std(after_scores - before_scores)
125
126    effect_text = f"""
127    EFFECT SIZES & PRACTICAL SIGNIFICANCE:
128    Cohen's d interpretation:
129    • Small effect: d = 0.2

```

```

131 • Medium effect: d = 0.5
132 • Large effect: d = 0.8
133 Model A vs B: d = {effect_size_ab:.2f}
134 Before vs After: d = {effect_size_paired:.2f}
135 REMEMBER:
136 ✓ Statistical significance ≠ Practical significance
137 ✓ Large samples can make tiny differences "significant"
138 ✓ Always consider business impact
139 ✓ Effect size matters more than p-value for decisions
140 BUSINESS DECISION FRAMEWORK:
141 1. Is the difference statistically significant? (p < 0.05)
142 2. Is the effect size meaningful? (d > 0.2)
143 3. Is the business impact worth the cost?
144 """
145
146 axes[1, 1].text(0.05, 0.95, effect_text, transform=axes[1,
147 1].transAxes,
148
149                 fontsize=9, verticalalignment='top',
150                 fontfamily='monospace',
151                 bbox=dict(boxstyle='round',
152                 facecolor='lightyellow', alpha=0.8))
153
154 plt.tight_layout()
155 plt.show()
156
157 return {
158     'one_sample': (t_stat, p_value),
159     'two_sample': (t_stat_2, p_value_2),
160     'paired': (t_stat_paired, p_value_paired),
161     'effect_sizes': (effect_size_ab, effect_size_paired)
162 }
163 test_results = statistical_tests_for_ml()

```

User: This is fantastic! I can see how statistical tests help us make confident decisions about model improvements. But I'm also curious about the error metrics we use. I know about MSE and RMSE, but can you explain the differences and when to use each one?

Expert: Excellent question! Understanding different error metrics is crucial for choosing the right evaluation approach. Let me show you **MSE, RMSE, and MAE** with their practical implications.

```

1 def error_metrics_comprehensive():
2     """
3     Comprehensive explanation of regression error metrics
4     """
5     print("REGRESSION ERROR METRICS: MSE, RMSE, MAE")
6     print("=" * 45)
7

```

```

8     # Generate sample data with different error patterns
9     np.random.seed(42)
10    n_samples = 100
11
12    # True values
13    y_true = np.random.uniform(10, 100, n_samples)
14
15    # Different prediction scenarios
16    # Scenario 1: Good predictions with small errors
17    y_pred_good = y_true + np.random.normal(0, 5, n_samples)
18
19    # Scenario 2: Predictions with some outliers
20    y_pred_outliers = y_true + np.random.normal(0, 3, n_samples)
21    outlier_indices = np.random.choice(n_samples, 5, replace=False)
22    y_pred_outliers[outlier_indices] += np.random.choice([-30, 30],
5)
23
24    # Scenario 3: Consistently biased predictions
25    y_pred_biased = y_true * 1.2 + np.random.normal(0, 2,
n_samples)
26
27    def calculate_all_metrics(y_true, y_pred):
28        """Calculate all error metrics"""
29        mse = np.mean((y_true - y_pred) ** 2)
30        rmse = np.sqrt(mse)
31        mae = np.mean(np.abs(y_true - y_pred))
32
33        # Additional metrics
34        mape = np.mean(np.abs((y_true - y_pred) / y_true)) * 100
35        max_error = np.max(np.abs(y_true - y_pred))
36
37        return {
38            'MSE': mse,
39            'RMSE': rmse,
40            'MAE': mae,
41            'MAPE': mape,
42            'Max_Error': max_error
43        }
44
45    # Calculate metrics for all scenarios
46    metrics_good = calculate_all_metrics(y_true, y_pred_good)
47    metrics_outliers = calculate_all_metrics(y_true,
y_pred_outliers)
48    metrics_biased = calculate_all_metrics(y_true, y_pred_biased)
49
50    print("METRIC DEFINITIONS:")
51    print("-" * 20)
52    print("MSE (Mean Squared Error): Average of squared
differences")
53    print("    • Formula: (1/n) Σ(actual - predicted)²")

```

```

54     print(" • Units: Original units squared")
55     print(" • Heavily penalizes large errors")
56     print()
57     print("RMSE (Root Mean Squared Error): Square root of MSE")
58     print(" • Formula:  $\sqrt{\text{MSE}}$ ")
59     print(" • Units: Same as original data")
60     print(" • Interpretable scale, penalizes large errors")
61     print()
62     print("MAE (Mean Absolute Error): Average of absolute
differences")
63     print(" • Formula:  $(1/n) \sum |\text{actual} - \text{predicted}|$ ")
64     print(" • Units: Same as original data")
65     print(" • Robust to outliers")
66
67     # Create comparison table
68     print(f"\nMETRIC COMPARISON:")
69     print("-" * 18)
70     print(f"{'Scenario':<15} {'MSE':<8} {'RMSE':<8} {'MAE':<8}
{'MAPE':<8} {'Max_Err':<8}")
71     print("-" * 65)
72     print(f"{'Good Model':<15} {metrics_good['MSE']:<8.1f}
{metrics_good['RMSE']:<8.1f} {metrics_good['MAE']:<8.1f}
{metrics_good['MAPE']:<8.1f}% {metrics_good['Max_Error']:<8.1f}")
73     print(f"{'With Outliers':<15} {metrics_outliers['MSE']:<8.1f}
{metrics_outliers['RMSE']:<8.1f} {metrics_outliers['MAE']:<8.1f}
{metrics_outliers['MAPE']:<8.1f}% {metrics_outliers['Max_Error']:<8.1f}")
74     print(f"{'Biased Model':<15} {metrics_biased['MSE']:<8.1f}
{metrics_biased['RMSE']:<8.1f} {metrics_biased['MAE']:<8.1f}
{metrics_biased['MAPE']:<8.1f}% {metrics_biased['Max_Error']:<8.1f}")
75
76     # Visualize the differences
77     fig, axes = plt.subplots(2, 3, figsize=(18, 12))
78
79     scenarios = [
80         (y_pred_good, 'Good Model', 'green'),
81         (y_pred_outliers, 'With Outliers', 'red'),
82         (y_pred_biased, 'Biased Model', 'blue')
83     ]
84
85     for i, (y_pred, title, color) in enumerate(scenarios):
86         # Scatter plot
87         axes[0, i].scatter(y_true, y_pred, alpha=0.6, color=color)
88         axes[0, i].plot([y_true.min(), y_true.max()],
[y_true.min(), y_true.max()], 'k--', alpha=0.7)
89         axes[0, i].set_xlabel('True Values')
90         axes[0, i].set_ylabel('Predicted Values')
91         axes[0, i].set_title(f'{title}\nRMSE:
{np.sqrt(np.mean((y_true - y_pred)**2)).1f}, MAE:

```

```

100 {np.mean(np.abs(y_true - y_pred)).1f}')
101 axes[0, i].grid(True, alpha=0.3)
102
103 # Residual plot
104 residuals = y_true - y_pred
105 axes[1, i].scatter(y_pred, residuals, alpha=0.6,
106 color=color)
107 axes[1, i].axhline(y=0, color='k', linestyle='--',
108 alpha=0.7)
109 axes[1, i].set_xlabel('Predicted Values')
110 axes[1, i].set_ylabel('Residuals')
111 axes[1, i].set_title(f'Residuals - {title}')
112 axes[1, i].grid(True, alpha=0.3)
113
114 plt.tight_layout()
115 plt.show()
116
117 print("\nWHEN TO USE EACH METRIC:")
118 print("-" * 27)
119 print("USE MSE WHEN:")
120 print("  ✓ You want to heavily penalize large errors")
121 print("  ✓ Optimizing model parameters (differentiable)")
122 print("  ✓ Mathematical convenience in algorithms")
123 print()
124 print("USE RM
125 <user>: continue
126 <Claude Sonnet 4>: ```python
127 print("USE RMSE WHEN:")
128 print("  ✓ You want interpretable error in original units")
129 print("  ✓ Large errors are more costly than small ones")
130 print("  ✓ Reporting to stakeholders (easier to understand)")
131 print("  ✓ Comparing models on the same scale as your data")
132 print()
133 print("USE MAE WHEN:")
134 print("  ✓ You want equal weight for all errors")
135 print("  ✓ Data has outliers that shouldn't dominate")
136 print("  ✓ Robust evaluation is more important")
137 print("  ✓ All errors have similar business impact")
138
139 # Demonstrate sensitivity to outliers
140 print(f"\nOUTLIER SENSITIVITY ANALYSIS:")
141 print("-" * 32)
142
143 # Compare metrics with and without outliers
144 y_clean = y_true[:95] # Remove outlier points
145 y_pred_clean = y_pred_outliers[:95]
146 y_pred_with_outliers = y_pred_outliers
147
148 metrics_clean = calculate_all_metrics(y_clean, y_pred_clean)
149 metrics_with_outliers = calculate_all_metrics(y_true,

```

```

y_pred_with_outliers)
139
140     print("Impact of 5 outliers on metrics:")
141     print(f"RMSE: {metrics_clean['RMSE']:.1f} →
{metrics_with_outliers['RMSE']:.1f}
({((metrics_with_outliers['RMSE']/metrics_clean['RMSE'])-1)*100:+.0f}%)")
142     print(f"MAE: {metrics_clean['MAE']:.1f} →
{metrics_with_outliers['MAE']:.1f}
({((metrics_with_outliers['MAE']/metrics_clean['MAE'])-1)*100:+.0f}%)")
143     print("→ RMSE is more sensitive to outliers than MAE")
144
145     return {
146         'good': metrics_good,
147         'outliers': metrics_outliers,
148         'biased': metrics_biased
149     }
150 error_metrics = error_metrics_comprehensive()

```

User: This comparison really helps me understand when to use each metric! Now I'm curious about something I keep hearing about - sensitivity and recall. Are these the same thing? And how do they relate to the precision and recall we learned about earlier?

Expert: Great question! **Sensitivity and recall are actually the same thing** - just different names used in different contexts. Let me clarify this and show you the complete picture of classification metrics.

```

1 def sensitivity_recall_comprehensive():
2     """
3     Comprehensive explanation of sensitivity, recall, and related
4     metrics
5     """
6     print("SENSITIVITY, RECALL, AND CLASSIFICATION METRICS")
7     print("=" * 50)
8
9     print("TERMINOLOGY CLARIFICATION:")
10    print("-" * 28)
11    print("SENSITIVITY = RECALL = TRUE POSITIVE RATE")
12    print("• Medical/Scientific context: 'Sensitivity'")
13    print("• Machine Learning context: 'Recall'")
14    print("• Signal Detection context: 'True Positive Rate'")
15    print("• Same formula: TP / (TP + FN)")
16    print()
17
18    # Generate sample medical diagnosis data
19    np.random.seed(42)
20    n_patients = 1000

```



```

21     # True disease status (1 = has disease, 0 = healthy)
22     true_disease = np.random.choice([0, 1], n_patients, p=[0.9,
0.1]) # 10% have disease
23
24     # Simulate test results with realistic performance
25     predicted_disease = []
26     for i in range(n_patients):
27         if true_disease[i] == 1: # Actually has disease
28             # 85% chance test detects it (sensitivity = 0.85)
29             pred = np.random.choice([0, 1], p=[0.15, 0.85])
30         else: # Actually healthy
31             # 90% chance test correctly identifies healthy
(specificity = 0.90)
32             pred = np.random.choice([0, 1], p=[0.90, 0.10])
33             predicted_disease.append(pred)
34
35     predicted_disease = np.array(predicted_disease)
36
37     # Calculate confusion matrix
38     from sklearn.metrics import confusion_matrix,
classification_report
39     cm = confusion_matrix(true_disease, predicted_disease)
40     tn, fp, fn, tp = cm.ravel()
41
42     # Calculate all metrics
43     sensitivity_recall = tp / (tp + fn) # Same as recall
44     specificity = tn / (tn + fp)
45     precision_ppv = tp / (tp + fp) # Positive Predictive Value
46     npv = tn / (tn + fn) # Negative Predictive Value
47     accuracy = (tp + tn) / (tp + tn + fp + fn)
48     f1_score = 2 * (precision_ppv * sensitivity_recall) /
(precision_ppv + sensitivity_recall)
49
50     print("COMPLETE METRICS BREAKDOWN:")
51     print("-" * 30)
52     print(f"True Positives (TP): {tp:3d} - Correctly identified
disease")
53     print(f"True Negatives (TN): {tn:3d} - Correctly identified
healthy")
54     print(f"False Positives (FP): {fp:3d} - Incorrectly flagged as
disease")
55     print(f"False Negatives (FN): {fn:3d} - Missed disease cases")
56     print()
57
58     print("SENSITIVITY/RECALL FAMILY:")
59     print("-" * 28)
60     print(f"Sensitivity/Recall: {sensitivity_recall:.3f} - Of
diseased patients, % correctly identified")
61     print(f"Specificity: {specificity:.3f} - Of healthy
patients, % correctly identified")

```

```

62     print(f"Precision/PPV:           {precision_ppv:.3f} - Of
positive tests, % actually have disease")
63     print(f"Negative Pred. Value:    {npv:.3f} - Of negative tests,
% actually healthy")
64     print(f"Accuracy:                {accuracy:.3f} - Overall
correct predictions")
65     print(f"F1-Score:                {f1_score:.3f} - Harmonic mean
of precision & recall")
66
67     # Visualize the confusion matrix and metrics
68     fig, axes = plt.subplots(2, 3, figsize=(18, 12))
69
70     # Confusion Matrix
71     im = axes[0, 0].imshow(cm, interpolation='nearest',
cmap='Blues')
72     axes[0, 0].set_title('Confusion Matrix\n(Medical Test
Example)')
73
74     # Add text annotations
75     thresh = cm.max() / 2.
76     for i in range(2):
77         for j in range(2):
78             axes[0, 0].text(j, i, f'{cm[i, j]}\n({cm[i,
j]/n_patients:.1%})',
79                             ha="center", va="center",
80                             color="white" if cm[i, j] > thresh else
"black",
81                             fontsize=12, fontweight='bold')
82
83     axes[0, 0].set_ylabel('True Label')
84     axes[0, 0].set_xlabel('Predicted Label')
85     axes[0, 0].set_xticks([0, 1])
86     axes[0, 0].set_xticklabels(['Healthy', 'Disease'])
87     axes[0, 0].set_yticks([0, 1])
88     axes[0, 0].set_yticklabels(['Healthy', 'Disease'])
89
90     # Sensitivity vs Specificity Trade-off
91     # Simulate different threshold values
92     thresholds = np.linspace(0, 1, 100)
93     sensitivities = []
94     specificities = []
95
96     for threshold in thresholds:
97         # Simulate how changing threshold affects predictions
98         sens = 1 - threshold * 0.8 # As threshold increases,
sensitivity decreases
99         spec = threshold * 0.9     # As threshold increases,
specificity increases
100         sensitivities.append(max(0, min(1, sens)))
101         specificities.append(max(0, min(1, spec)))

```

```

102
103     axes[0, 1].plot(1 - np.array(specificities), sensitivities, 'b-
', linewidth=2)
104     axes[0, 1].plot([0, 1], [0, 1], 'k--', alpha=0.5)
105     axes[0, 1].scatter(1 - specificity, sensitivity_recall,
color='red', s=100, zorder=5)
106     axes[0, 1].set_xlabel('1 - Specificity (False Positive Rate)')
107     axes[0, 1].set_ylabel('Sensitivity (True Positive Rate)')
108     axes[0, 1].set_title('ROC Curve\n(Receiver Operating
Characteristic)')
109     axes[0, 1].grid(True, alpha=0.3)
110     axes[0, 1].annotate(f'Current Test\n(Sens=
{sensitivity_recall:.2f}, Spec={specificity:.2f})',
111                        xy=(1-specificity, sensitivity_recall),
xytext=(0.6, 0.3),
112                        arrowprops=dict(arrowstyle='->',
color='red'))
113
114     # Precision-Recall Trade-off
115     precisions = []
116     recalls = []
117
118     for threshold in thresholds:
119         # Simulate precision-recall trade-off
120         recall = 1 - threshold * 0.8
121         precision = 0.3 + threshold * 0.6 # Higher threshold →
higher precision
122         recalls.append(max(0, min(1, recall)))
123         precisions.append(max(0, min(1, precision)))
124
125     axes[0, 2].plot(recalls, precisions, 'g-', linewidth=2)
126     axes[0, 2].scatter(sensitivity_recall, precision_ppv,
color='red', s=100, zorder=5)
127     axes[0, 2].set_xlabel('Recall (Sensitivity)')
128     axes[0, 2].set_ylabel('Precision (PPV)')
129     axes[0, 2].set_title('Precision-Recall Curve')
130     axes[0, 2].grid(True, alpha=0.3)
131     axes[0, 2].annotate(f'Current Test\n(Prec={precision_ppv:.2f},
Rec={sensitivity_recall:.2f})',
132                        xy=(sensitivity_recall, precision_ppv),
xytext=(0.3, 0.8),
133                        arrowprops=dict(arrowstyle='->',
color='red'))
134
135     # Context-specific interpretations
136     contexts = [
137         ('Medical Screening', 'High Sensitivity', 'Don\'t miss any
diseases'),
138         ('Spam Detection', 'High Precision', 'Don\'t block
important emails'),

```

```

139         ('Fraud Detection', 'Balanced F1', 'Balance catching fraud
vs false alarms')
140     ]
141
142     context_colors = ['red', 'blue', 'green']
143
144     axes[1, 0].axis('off')
145     axes[1, 0].set_title('Context-Specific Priorities',
fontweight='bold')
146
147     for i, (context, priority, reason) in enumerate(contexts):
148         y_pos = 0.8 - i * 0.25
149         axes[1, 0].text(0.1, y_pos, f"{context}:",
fontweight='bold', fontsize=12, color=context_colors[i])
150         axes[1, 0].text(0.1, y_pos-0.05, f"Priority: {priority}",
fontsize=10)
151         axes[1, 0].text(0.1, y_pos-0.10, f"Reason: {reason}",
fontsize=10, style='italic')
152
153     # Metrics comparison chart
154     metrics_names = ['Sensitivity\n(Recall)', 'Specificity',
'Precision\n(PPV)', 'NPV', 'Accuracy', 'F1-Score']
155     metrics_values = [sensitivity_recall, specificity,
precision_ppv, npv, accuracy, f1_score]
156
157     bars = axes[1, 1].bar(metrics_names, metrics_values,
158                           color=['red', 'blue', 'green', 'orange',
'purple', 'brown'],
159                               alpha=0.7)
160     axes[1, 1].set_ylabel('Score')
161     axes[1, 1].set_title('All Classification Metrics')
162     axes[1, 1].set_ylim(0, 1)
163     axes[1, 1].tick_params(axis='x', rotation=45)
164     axes[1, 1].grid(True, alpha=0.3)
165
166     # Add value labels on bars
167     for bar, value in zip(bars, metrics_values):
168         axes[1, 1].text(bar.get_x() + bar.get_width()/2,
bar.get_height() + 0.01,
169                         f'{value:.3f}', ha='center', va='bottom',
fontweight='bold')
170
171     # Business decision framework
172     axes[1, 2].axis('off')
173
174     decision_text = f"""
175 BUSINESS DECISION FRAMEWORK:
176 MEDICAL DIAGNOSIS:
177 ✓ High Sensitivity (Recall): {sensitivity_recall:.1%}
178 → Catch most disease cases

```

```

180 ✓ Accept lower Specificity: {specificity:.1%}
181   → Some false alarms OK
182 SPAM DETECTION:
184 ✓ High Precision: Minimize false positives
185 ✓ Accept lower Recall: Some spam gets through
186   → Better than blocking important emails
188 FRAUD DETECTION:
189 ✓ Balance Sensitivity & Precision
190 ✓ Use F1-Score: {f1_score:.1%}
191   → Optimize overall performance
192 KEY INSIGHT:
193 The "best" metric depends on the cost of
194 different types of errors in your specific
195 business context.
196 """
197
198
199     axes[1, 2].text(0.05, 0.95, decision_text, transform=axes[1,
200 2].transAxes,
201                    fontsize=10, verticalalignment='top',
202                    fontfamily='monospace',
203                    bbox=dict(boxstyle='round',
204                             facecolor='lightcyan', alpha=0.8))
205
206     plt.tight_layout()
207     plt.show()
208
209     print("\nPRACTICAL GUIDELINES:")
210     print("-" * 22)
211     print("PRIORITIZE SENSITIVITY/RECALL WHEN:")
212     print("    • Missing positives is very costly (medical
213 diagnosis)")
214     print("    • You want to catch as many cases as possible")
215     print("    • False negatives are worse than false positives")
216     print()
217     print("PRIORITIZE SPECIFICITY WHEN:")
218     print("    • False positives are very costly")
219     print("    • You need to be sure about negative cases")
220     print("    • Resources for follow-up are limited")
221     print()
222     print("PRIORITIZE PRECISION WHEN:")
223     print("    • Acting on positive predictions is expensive")
224     print("    • You need high confidence in positive predictions")
225     print("    • False alarms cause significant problems")
226
227     return {
228         'confusion_matrix': cm,
229         'sensitivity': sensitivity_recall,
230         'specificity': specificity,
231         'precision': precision_ppv,
232         'npv': npv,

```

```

229         'accuracy': accuracy,
230         'f1_score': f1_score
231     }
232 classification_metrics = sensitivity_recall_comprehensive()

```

User: This is incredibly comprehensive! I love how you showed that sensitivity and recall are the same thing, just used in different contexts. Now I'm really curious about ROC curves - I see them mentioned a lot but I'm not sure how to interpret them properly.

Expert: Excellent! **ROC curves** (Receiver Operating Characteristic) are one of the most important tools for evaluating classification models. Let me give you a complete understanding of how to create, interpret, and use them effectively.

```

1 def roc_curve_comprehensive():
2     """
3     Comprehensive explanation of ROC curves and AUC
4     """
5     print("ROC CURVES AND AUC: COMPLETE GUIDE")
6     print("=" * 40)
7
8     print("WHAT IS A ROC CURVE?")
9     print("-" * 22)
10    print("• Plots True Positive Rate (Sensitivity) vs False
    Positive Rate (1-Specificity)")
11    print("• Shows performance across all classification
    thresholds")
12    print("• Helps choose optimal threshold for your business
    needs")
13    print("• AUC (Area Under Curve) summarizes overall
    performance")
14    print()
15
16    # Generate sample data with different model qualities
17    np.random.seed(42)
18    n_samples = 1000
19
20    # True labels (20% positive class)
21    y_true = np.random.choice([0, 1], n_samples, p=[0.8, 0.2])
22
23    # Simulate different model prediction probabilities
24
25    # Model 1: Excellent model
26    y_prob_excellent = []
27    for label in y_true:
28        if label == 1:
29            prob = np.random.beta(8, 2) # High probabilities for
    positive class

```

```

30         else:
31             prob = np.random.beta(2, 8) # Low probabilities for
negative class
32             y_prob_excellent.append(prob)
33             y_prob_excellent = np.array(y_prob_excellent)
34
35         # Model 2: Good model
36         y_prob_good = []
37         for label in y_true:
38             if label == 1:
39                 prob = np.random.beta(5, 3)
40             else:
41                 prob = np.random.beta(3, 5)
42             y_prob_good.append(prob)
43             y_prob_good = np.array(y_prob_good)
44
45         # Model 3: Poor model
46         y_prob_poor = []
47         for label in y_true:
48             if label == 1:
49                 prob = np.random.beta(3, 4)
50             else:
51                 prob = np.random.beta(4, 3)
52             y_prob_poor.append(prob)
53             y_prob_poor = np.array(y_prob_poor)
54
55         # Model 4: Random model
56         y_prob_random = np.random.uniform(0, 1, n_samples)
57
58         # Calculate ROC curves
59         from sklearn.metrics import roc_curve, auc
60
61         models = {
62             'Excellent Model': y_prob_excellent,
63             'Good Model': y_prob_good,
64             'Poor Model': y_prob_poor,
65             'Random Model': y_prob_random
66         }
67
68         colors = ['green', 'blue', 'orange', 'red']
69
70         fig, axes = plt.subplots(2, 3, figsize=(18, 12))
71
72         # Plot ROC curves
73         axes[0, 0].plot([0, 1], [0, 1], 'k--', alpha=0.5, label='Random
Classifier')
74
75         roc_data = {}
76
77         for i, (model_name, y_prob) in enumerate(models.items()):

```

```

78     fpr, tpr, thresholds = roc_curve(y_true, y_prob)
79     roc_auc = auc(fpr, tpr)
80
81     axes[0, 0].plot(fpr, tpr, color=colors[i], linewidth=2,
82                     label=f'{model_name} (AUC = {roc_auc:.3f})')
83
84     roc_data[model_name] = {
85         'fpr': fpr,
86         'tpr': tpr,
87         'thresholds': thresholds,
88         'auc': roc_auc
89     }
90
91     axes[0, 0].set_xlabel('False Positive Rate (1 - Specificity)')
92     axes[0, 0].set_ylabel('True Positive Rate (Sensitivity)')
93     axes[0, 0].set_title('ROC Curves Comparison')
94     axes[0, 0].legend(loc='lower right')
95     axes[0, 0].grid(True, alpha=0.3)
96
97     # Show probability distributions
98     axes[0, 1].hist(y_prob_excellent[y_true == 0], bins=30,
99                    label='Negative Class', color='red',
100                   density=True)
101     axes[0, 1].hist(y_prob_excellent[y_true == 1], bins=30,
102                    label='Positive Class', color='green',
103                   density=True)
104     axes[0, 1].axvline(0.5, color='black', linestyle='--',
105                       alpha=0.7, label='Threshold = 0.5')
106     axes[0, 1].set_xlabel('Predicted Probability')
107     axes[0, 1].set_ylabel('Density')
108     axes[0, 1].set_title('Excellent Model: Probability
109                          Distributions')
110     axes[0, 1].legend()
111     axes[0, 1].grid(True, alpha=0.3)
112
113     # Show threshold selection
114     excellent_fpr = roc_data['Excellent Model']['fpr']
115     excellent_tpr = roc_data['Excellent Model']['tpr']
116     excellent_thresholds = roc_data['Excellent Model']
117     ['thresholds']
118
119     # Find optimal threshold (closest to top-left corner)
120     distances = np.sqrt((excellent_fpr - 0)**2 + (excellent_tpr -
121     1)**2)
122     optimal_idx = np.argmin(distances)
123     optimal_threshold = excellent_thresholds[optimal_idx]
124     optimal_fpr = excellent_fpr[optimal_idx]
125     optimal_tpr = excellent_tpr[optimal_idx]

```



```

120
121     axes[0, 2].plot(excellent_fpr, excellent_tpr, 'g-',
122                     linewidth=2, label='ROC Curve')
123     axes[0, 2].scatter(optimal_fpr, optimal_tpr, color='red',
124                         s=100, zorder=5,
125                         label=f'Optimal Threshold =
126                             {optimal_threshold:.3f}')
127     axes[0, 2].plot([0, 1], [0, 1], 'k--', alpha=0.5)
128     axes[0, 2].set_xlabel('False Positive Rate')
129     axes[0, 2].set_ylabel('True Positive Rate')
130     axes[0, 2].set_title('Threshold Selection')
131     axes[0, 2].legend()
132     axes[0, 2].grid(True, alpha=0.3)
133
134     # AUC interpretation
135     axes[1, 0].axis('off')
136
137     auc_text = f"""
138     AUC INTERPRETATION GUIDE:
139     AUC = 1.0: Perfect classifier
140     AUC = 0.9-1.0: Excellent
141     AUC = 0.8-0.9: Good
142     AUC = 0.7-0.8: Fair
143     AUC = 0.6-0.7: Poor
144     AUC = 0.5: Random (no skill)
145     AUC < 0.5: Worse than random
146     OUR MODELS:
147     • Excellent: {roc_data['Excellent Model']['auc']:.3f}
148     • Good: {roc_data['Good Model']['auc']:.3f}
149     • Poor: {roc_data['Poor Model']['auc']:.3f}
150     • Random: {roc_data['Random Model']['auc']:.3f}
151     BUSINESS MEANING:
152     AUC = Probability that model ranks
153     a random positive example higher
154     than a random negative example.
155     """
156
157     axes[1, 0].text(0.05, 0.95, auc_text, transform=axes[1,
158                     0].transAxes,
159                     fontsize=11, verticalalignment='top',
160                     fontfamily='monospace',
161                     bbox=dict(boxstyle='round',
162                             facecolor='lightgreen', alpha=0.8))
163
164     # Threshold analysis table
165     axes[1, 1].axis('off')
166
167     # Calculate metrics at different thresholds for excellent model
168     thresholds_to_analyze = [0.3, 0.5, 0.7, optimal_threshold]

```

```

167     threshold_analysis = []
168     for thresh in thresholds_to_analyze:
169         y_pred = (y_prob_excellent >= thresh).astype(int)
170
171         from sklearn.metrics import confusion_matrix,
precision_score, recall_score
172         cm = confusion_matrix(y_true, y_pred)
173         tn, fp, fn, tp = cm.ravel()
174
175         precision = precision_score(y_true, y_pred)
176         recall = recall_score(y_true, y_pred)
177         specificity = tn / (tn + fp)
178
179         threshold_analysis.append({
180             'threshold': thresh,
181             'precision': precision,
182             'recall': recall,
183             'specificity': specificity,
184             'fpr': 1 - specificity
185         })
186
187     # Create table
188     table_data = []
189     table_data.append(['Threshold', 'Precision', 'Recall',
'Specificity', 'FPR'])
190
191     for analysis in threshold_analysis:
192         row = [
193             f"{analysis['threshold']:.3f}",
194             f"{analysis['precision']:.3f}",
195             f"{analysis['recall']:.3f}",
196             f"{analysis['specificity']:.3f}",
197             f"{analysis['fpr']:.3f}"
198         ]
199         table_data.append(row)
200
201     table = axes[1, 1].table(cellText=table_data[1:],
202                             colLabels=table_data[0],
203                             cellLoc='center',
204                             loc='center',
205                             bbox=[0, 0.3, 1, 0.6])
206
207     table.auto_set_font_size(False)
208     table.set_fontsize(10)
209     table.scale(1, 2)
210
211     # Color code the header and optimal row
212     for i in range(5):
213         table[(0, i)].set_facecolor('#4CAF50')
214         table[(0, i)].set_text_props(weight='bold', color='white')

```

```

215
216     # Highlight optimal threshold row
217     optimal_row = 4 # Last row is optimal
218     for i in range(5):
219         table[(optimal_row, i)].set_facecolor('#FFE082')
220
221     axes[1, 1].set_title('Threshold Analysis for Excellent Model',
222 pad=20, fontweight='bold')
223
224     # Business decision guide
225     axes[1, 2].axis('off')
226
227     decision_guide = f"""
228 BUSINESS DECISION GUIDE:
229 CHOOSE THRESHOLD BASED ON:
230 1. COST OF FALSE POSITIVES:
231     High cost → Higher threshold
232     Low cost → Lower threshold
233 2. COST OF FALSE NEGATIVES:
234     High cost → Lower threshold
235     Low cost → Higher threshold
236 3. BUSINESS CONTEXT:
237 MEDICAL SCREENING:
238     • Low threshold (0.3)
239     • High sensitivity, catch all cases
240     • Accept more false alarms
241 SPAM DETECTION:
242     • High threshold (0.7)
243     • High precision, avoid blocking
244     • Accept some spam getting through
245 FRAUD DETECTION:
246     • Optimal threshold ({optimal_threshold:.3f})
247     • Balance sensitivity & precision
248     • Minimize total cost
249 REMEMBER:
250 ROC curve shows ALL possible
251 trade-offs. Choose the point
252 that best fits your business needs!
253 """
254
255     axes[1, 2].text(0.05, 0.95, decision_guide, transform=axes[1,
256 2].transAxes,
257                     fontsize=9, verticalalignment='top',
258                     fontfamily='monospace',
259                     bbox=dict(boxstyle='round',
260 facecolor='lightblue', alpha=0.8))
261
262     plt.tight_layout()
263     plt.show()
264

```

```

269     print("KEY INSIGHTS:")
270     print("-" * 15)
271     print("✓ ROC curve shows performance across all thresholds")
272     print("✓ AUC summarizes overall discriminative ability")
273     print("✓ Closer to top-left corner = better performance")
274     print("✓ Diagonal line = random performance")
275     print("✓ Choose threshold based on business costs")
276     print("✓ ROC curves are threshold-independent evaluation")
277
278     return roc_data, threshold_analysis
280 roc_results, threshold_results = roc_curve_comprehensive()

```

Chapter 7: Advanced Evaluation Metrics and Techniques

User: The ROC curves really helped me understand model evaluation better! But I feel like there are still some advanced techniques I should know about. What about cross-validation? And are there other important evaluation methods I should be aware of?

Expert: Absolutely! You're ready for the advanced evaluation techniques that separate good data scientists from great ones. Let's dive into **cross-validation**, **bootstrap sampling**, and other sophisticated evaluation methods.

```

1  def cross_validation_comprehensive():
2      """
3      Comprehensive guide to cross-validation techniques
4      """
5      print("CROSS-VALIDATION: ADVANCED MODEL EVALUATION")
6      print("=" * 50)
7
8      print("WHY CROSS-VALIDATION?")
9      print("-" * 23)
10     print("• Single train/test split can be misleading")
11     print("• Results depend on which data points end up in test
    set")
12     print("• Cross-validation gives more robust performance
    estimates")
13     print("• Helps detect overfitting and model instability")
14     print()
15
16     # Generate sample data
17     from sklearn.datasets import make_classification
18     from sklearn.model_selection import cross_val_score,
    StratifiedKFold, TimeSeriesSplit
19     from sklearn.linear_model import LogisticRegression
20     from sklearn.ensemble import RandomForestClassifier

```



```

label='Testing')
63 <user>: continue
64 <Claude Sonnet 4>: ```python
65     else:
66         axes[0, 0].scatter(x_pos[:len(train_idx)],
        y_pos[:len(train_idx)],
67                             c='blue', alpha=0.6, s=1)
68         axes[0, 0].scatter(x_pos[len(train_idx):],
        y_pos[len(train_idx):],
69                             c='red', alpha=0.6, s=1)
70
71     axes[0, 0].set_xlabel('Sample Index')
72     axes[0, 0].set_ylabel('Fold Number')
73     axes[0, 0].set_title('5-Fold Cross-Validation Splits')
74     axes[0, 0].legend()
75     axes[0, 0].grid(True, alpha=0.3)
76
77     # Perform cross-validation for all models
78     cv_results = {}
79
80     for model_name, model in models.items():
81         scores = cross_val_score(model, X, y, cv=5,
        scoring='accuracy')
82         cv_results[model_name] = {
83             'scores': scores,
84             'mean': scores.mean(),
85             'std': scores.std()
86         }
87
88     # Plot cross-validation results
89     model_names = list(cv_results.keys())
90     means = [cv_results[name]['mean'] for name in model_names]
91     stds = [cv_results[name]['std'] for name in model_names]
92
93     bars = axes[0, 1].bar(model_names, means, yerr=stds, capsize=5,
94                           alpha=0.7, color=['blue', 'green'])
95     axes[0, 1].set_ylabel('Accuracy')
96     axes[0, 1].set_title('Cross-Validation Results (5-Fold)')
97     axes[0, 1].grid(True, alpha=0.3)
98
99     # Add value labels
100    for i, (bar, mean, std) in enumerate(zip(bars, means, stds)):
101        axes[0, 1].text(bar.get_x() + bar.get_width()/2,
        bar.get_height() + std + 0.01,
102                        f'{mean:.3f}±{std:.3f}', ha='center',
        va='bottom', fontweight='bold')
103
104    print(f"5-Fold CV Results:")
105    for name in model_names:
106        mean_acc = cv_results[name]['mean']

```

```

107         std_acc = cv_results[name]['std']
108         print(f"    {name}: {mean_acc:.3f} ± {std_acc:.3f}")
109
110     # 2. Stratified K-Fold
111     print(f"\n2. STRATIFIED K-FOLD CROSS-VALIDATION")
112     print("    • Maintains class distribution in each fold")
113     print("    • Important for imbalanced datasets")
114     print("    • Ensures each fold is representative")
115     print()
116
117     skf = StratifiedKFold(n_splits=5, shuffle=True,
random_state=42)
118
119     # Compare class distributions
120     fold_distributions = []
121     for i, (train_idx, test_idx) in enumerate(skf.split(X, y)):
122         train_dist = np.bincount(y[train_idx]) / len(train_idx)
123         test_dist = np.bincount(y[test_idx]) / len(test_idx)
124         fold_distributions.append({
125             'fold': i+1,
126             'train_class_0': train_dist[0],
127             'train_class_1': train_dist[1],
128             'test_class_0': test_dist[0],
129             'test_class_1': test_dist[1]
130         })
131
132     # Visualize class distributions
133     folds = [d['fold'] for d in fold_distributions]
134     train_0 = [d['train_class_0'] for d in fold_distributions]
135     train_1 = [d['train_class_1'] for d in fold_distributions]
136     test_0 = [d['test_class_0'] for d in fold_distributions]
137     test_1 = [d['test_class_1'] for d in fold_distributions]
138
139     x = np.arange(len(folds))
140     width = 0.35
141
142     axes[1, 0].bar(x - width/2, train_0, width, label='Train Class
0', alpha=0.7, color='lightblue')
143     axes[1, 0].bar(x - width/2, train_1, width, bottom=train_0,
label='Train Class 1', alpha=0.7, color='lightcoral')
144     axes[1, 0].bar(x + width/2, test_0, width, label='Test Class
0', alpha=0.7, color='blue')
145     axes[1, 0].bar(x + width/2, test_1, width, bottom=test_0,
label='Test Class 1', alpha=0.7, color='red')
146
147     axes[1, 0].set_xlabel('Fold')
148     axes[1, 0].set_ylabel('Class Proportion')
149     axes[1, 0].set_title('Stratified K-Fold: Class Distribution')
150     axes[1, 0].set_xticks(x)
151     axes[1, 0].set_xticklabels([f'Fold {i}' for i in folds])

```

```

152 axes[1, 0].legend()
153 axes[1, 0].grid(True, alpha=0.3)
154
155 # 3. Time Series Cross-Validation
156 print("3. TIME SERIES CROSS-VALIDATION")
157 print("    • Respects temporal order of data")
158 print("    • No future data leakage")
159 print("    • Expanding or sliding window approach")
160 print()
161
162 # Generate time series data
163 np.random.seed(42)
164 n_time_points = 100
165 time_X = np.random.randn(n_time_points, 5)
166 time_y = np.random.randn(n_time_points)
167
168 tscv = TimeSeriesSplit(n_splits=5)
169
170 # Visualize time series splits
171 for i, (train_idx, test_idx) in enumerate(tscv.split(time_X)):
172     y_pos = [i] * len(range(n_time_points))
173     colors = ['lightgray'] * n_time_points
174
175     for idx in train_idx:
176         colors[idx] = 'blue'
177     for idx in test_idx:
178         colors[idx] = 'red'
179
180     axes[1, 1].scatter(range(n_time_points), y_pos, c=colors,
181 alpha=0.7, s=10)
182
183 axes[1, 1].set_xlabel('Time Point')
184 axes[1, 1].set_ylabel('Fold Number')
185 axes[1, 1].set_title('Time Series Cross-Validation')
186
187 # Add legend
188 from matplotlib.patches import Patch
189 legend_elements = [Patch(facecolor='blue', label='Training'),
190 Patch(facecolor='red', label='Testing'),
191 Patch(facecolor='lightgray', label='Not
Used')]
192 axes[1, 1].legend(handles=legend_elements)
193 axes[1, 1].grid(True, alpha=0.3)
194
195 # 4. Leave-One-Out Cross-Validation (LOOCV)
196 print("4. LEAVE-ONE-OUT CROSS-VALIDATION (LOOCV)")
197 print("    • Each sample is test set once")
198 print("    • n-fold CV where n = number of samples")
199 print("    • Maximum use of data, but computationally
expensive")

```



```

199     print()
200
201     # Demonstrate with smaller dataset
202     from sklearn.model_selection import LeaveOneOut
203
204     # Use smaller subset for LOOCV demonstration
205     X_small = X[:50]
206     y_small = y[:50]
207
208     loo = LeaveOneOut()
209     loo_scores =
cross_val_score(LogisticRegression(random_state=42), X_small,
y_small, cv=loo)
210
211     print(f"LOOCV Results on 50 samples:")
212     print(f"    Mean Accuracy: {loo_scores.mean():.3f}")
213     print(f"    Std Accuracy: {loo_scores.std():.3f}")
214     print(f"    Number of folds: {len(loo_scores)}")
215
216     # 5. Nested Cross-Validation
217     print(f"\n5. NESTED CROSS-VALIDATION")
218     print("    • Outer loop: Model evaluation")
219     print("    • Inner loop: Hyperparameter tuning")
220     print("    • Unbiased estimate of model performance")
221     print()
222
223     from sklearn.model_selection import GridSearchCV
224
225     # Nested CV example
226     def nested_cross_validation(X, y, model, param_grid,
outer_cv=5, inner_cv=3):
227         outer_scores = []
228
229         outer_kf = StratifiedKFold(n_splits=outer_cv, shuffle=True,
random_state=42)
230
231         for train_idx, test_idx in outer_kf.split(X, y):
232             X_train, X_test = X[train_idx], X[test_idx]
233             y_train, y_test = y[train_idx], y[test_idx]
234
235             # Inner CV for hyperparameter tuning
236             inner_cv = StratifiedKFold(n_splits=inner_cv,
shuffle=True, random_state=42)
237             grid_search = GridSearchCV(model, param_grid,
cv=inner_cv, scoring='accuracy')
238             grid_search.fit(X_train, y_train)
239
240             # Test best model on outer test set
241             best_model = grid_search.best_estimator_
242             score = best_model.score(X_test, y_test)

```

```

243         outer_scores.append(score)
244
245     return np.array(outer_scores)
246
247     # Perform nested CV
248     param_grid = {'C': [0.1, 1, 10], 'max_iter': [100, 1000]}
249     nested_scores = nested_cross_validation(X, y,
        LogisticRegression(random_state=42), param_grid)
250
251     print(f"Nested CV Results:")
252     print(f"    Mean Accuracy: {nested_scores.mean():.3f}")
253     print(f"    Std Accuracy: {nested_scores.std():.3f}")
254
255     # Visualize different CV methods comparison
256     cv_methods = ['5-Fold', 'Stratified 5-Fold', 'LOOCV (50
        samples)', 'Nested CV']
257     cv_means = [
258         cv_results['Logistic Regression']['mean'],
259         cv_results['Logistic Regression']['mean'], # Similar for
        stratified
260         loo_scores.mean(),
261         nested_scores.mean()
262     ]
263     cv_stds = [
264         cv_results['Logistic Regression']['std'],
265         cv_results['Logistic Regression']['std'],
266         loo_scores.std(),
267         nested_scores.std()
268     ]
269
270     bars = axes[2, 0].bar(cv_methods, cv_means, yerr=cv_stds,
        capsize=5,
271         alpha=0.7, color=['blue', 'green',
        'orange', 'red'])
272     axes[2, 0].set_ylabel('Accuracy')
273     axes[2, 0].set_title('Cross-Validation Methods Comparison')
274     axes[2, 0].tick_params(axis='x', rotation=45)
275     axes[2, 0].grid(True, alpha=0.3)
276
277     # Add value labels
278     for bar, mean, std in zip(bars, cv_means, cv_stds):
279         axes[2, 0].text(bar.get_x() + bar.get_width()/2,
        bar.get_height() + std + 0.01,
280             f'{mean:.3f}±{std:.3f}', ha='center',
        va='bottom', fontweight='bold', fontsize=9)
281
282     # Cross-validation best practices
283     axes[2, 1].axis('off')
284
285     best_practices = """

```

```

286 CROSS-VALIDATION BEST PRACTICES:
287 ✓ CHOOSE THE RIGHT METHOD:
289     • Standard: K-Fold (k=5 or k=10)
290     • Imbalanced data: Stratified K-Fold
291     • Time series: TimeSeriesSplit
292     • Small datasets: LOOCV
293     • Hyperparameter tuning: Nested CV
294 ✓ CONSIDERATIONS:
296     • More folds = less bias, more variance
297     • Fewer folds = more bias, less variance
298     • Computational cost increases with folds
299 ✓ COMMON MISTAKES TO AVOID:
301     • Data leakage between folds
302     • Not stratifying imbalanced data
303     • Using future data in time series
304     • Tuning hyperparameters on test set
305 ✓ REPORTING RESULTS:
307     • Always report mean ± standard deviation
308     • Consider confidence intervals
309     • Test statistical significance of differences
310     • Validate on truly held-out test set
311     """
312
313     axes[2, 1].text(0.05, 0.95, best_practices, transform=axes[2,
314     1].transAxes,
315                     fontsize=10, verticalalignment='top',
316                     fontfamily='monospace',
317                     bbox=dict(boxstyle='round',
318                             facecolor='lightcyan', alpha=0.8))
319
320     plt.tight_layout()
321     plt.show()
322
323     return cv_results, nested_scores
324 cv_results, nested_scores = cross_validation_comprehensive()

```

User: Cross-validation makes so much sense now! I can see how it gives us much more confidence in our model evaluation. But what about bootstrap sampling? I've heard it's another important technique for understanding uncertainty.

Expert: Excellent question! **Bootstrap sampling** is a powerful statistical technique that complements cross-validation beautifully. It's particularly useful for estimating confidence intervals and understanding the stability of your model performance.

```

1 def bootstrap_sampling_comprehensive():
2     """
3     Comprehensive guide to bootstrap sampling for model evaluation

```

```

4      """
5      print("BOOTSTRAP SAMPLING FOR MODEL EVALUATION")
6      print("=" * 45)
7
8      print("WHAT IS BOOTSTRAP SAMPLING?")
9      print("-" * 32)
10     print("• Sampling WITH replacement from your dataset")
11     print("• Creates multiple 'bootstrap samples' of same size as
original")
12     print("• Each sample is slightly different due to random
sampling")
13     print("• Estimates sampling distribution of any statistic")
14     print("• Provides confidence intervals without assumptions")
15     print()
16
17     # Generate sample data
18     from sklearn.datasets import make_regression
19     from sklearn.linear_model import LinearRegression
20     from sklearn.metrics import mean_squared_error, r2_score
21
22     np.random.seed(42)
23     X, y = make_regression(n_samples=200, n_features=5, noise=10,
random_state=42)
24
25     # Original model performance
26     model = LinearRegression()
27     model.fit(X, y)
28     y_pred = model.predict(X)
29     original_r2 = r2_score(y, y_pred)
30     original_mse = mean_squared_error(y, y_pred)
31
32     print("BOOTSTRAP PROCEDURE:")
33     print("-" * 21)
34     print("1. Sample n observations WITH replacement")
35     print("2. Train model on bootstrap sample")
36     print("3. Evaluate model performance")
37     print("4. Repeat B times (typically B = 1000)")
38     print("5. Analyze distribution of performance metrics")
39     print()
40
41     # Perform bootstrap sampling
42     def bootstrap_model_evaluation(X, y, model, n_bootstrap=1000):
43         """
44         Perform bootstrap evaluation of model performance
45         """
46         n_samples = len(X)
47         bootstrap_scores = {
48             'r2_scores': [],
49             'mse_scores': [],
50             'coefficients': [],

```

```

51         'intercepts': []
52     }
53
54     for i in range(n_bootstrap):
55         # Bootstrap sample
56         bootstrap_indices = np.random.choice(n_samples,
size=n_samples, replace=True)
57         X_bootstrap = X[bootstrap_indices]
58         y_bootstrap = y[bootstrap_indices]
59
60         # Train model on bootstrap sample
61         bootstrap_model = LinearRegression()
62         bootstrap_model.fit(X_bootstrap, y_bootstrap)
63
64         # Evaluate on bootstrap sample
65         y_pred_bootstrap = bootstrap_model.predict(X_bootstrap)
66         r2_bootstrap = r2_score(y_bootstrap, y_pred_bootstrap)
67         mse_bootstrap = mean_squared_error(y_bootstrap,
y_pred_bootstrap)
68
69         # Store results
70         bootstrap_scores['r2_scores'].append(r2_bootstrap)
71         bootstrap_scores['mse_scores'].append(mse_bootstrap)
72
73         bootstrap_scores['coefficients'].append(bootstrap_model.coef_)
74
75         bootstrap_scores['intercepts'].append(bootstrap_model.intercept_)
76
77     return bootstrap_scores
78
79     print("Performing 1000 bootstrap samples...")
80     bootstrap_results = bootstrap_model_evaluation(X, y, model,
n_bootstrap=1000)
81
82     # Convert to numpy arrays for easier analysis
83     r2_scores = np.array(bootstrap_results['r2_scores'])
84     mse_scores = np.array(bootstrap_results['mse_scores'])
85     coefficients = np.array(bootstrap_results['coefficients'])
86     intercepts = np.array(bootstrap_results['intercepts'])
87
88     # Calculate confidence intervals
89     def calculate_confidence_intervals(data,
confidence_level=0.95):
90         """
91         Calculate confidence intervals using percentile method
92         """
93         alpha = 1 - confidence_level
94         lower_percentile = (alpha/2) * 100
95         upper_percentile = (1 - alpha/2) * 100

```

```

95         lower_bound = np.percentile(data, lower_percentile)
96         upper_bound = np.percentile(data, upper_percentile)
97
98         return lower_bound, upper_bound
99
100     # Calculate CIs for performance metrics
101     r2_ci_lower, r2_ci_upper =
calculate_confidence_intervals(r2_scores)
102     mse_ci_lower, mse_ci_upper =
calculate_confidence_intervals(mse_scores)
103
104     print("BOOTSTRAP RESULTS:")
105     print("-" * 18)
106     print(f"Original R2 Score: {original_r2:.4f}")
107     print(f"Bootstrap R2 Mean: {np.mean(r2_scores):.4f}")
108     print(f"Bootstrap R2 Std: {np.std(r2_scores):.4f}")
109     print(f"95% CI for R2:      [{r2_ci_lower:.4f},
{r2_ci_upper:.4f}]")
110     print()
111     print(f"Original MSE:      {original_mse:.2f}")
112     print(f"Bootstrap MSE Mean: {np.mean(mse_scores):.2f}")
113     print(f"Bootstrap MSE Std: {np.std(mse_scores):.2f}")
114     print(f"95% CI for MSE:      [{mse_ci_lower:.2f},
{mse_ci_upper:.2f}]")
115
116     # Visualize bootstrap results
117     fig, axes = plt.subplots(3, 2, figsize=(15, 18))
118
119     # R2 distribution
120     axes[0, 0].hist(r2_scores, bins=50, alpha=0.7, color='blue',
density=True)
121     axes[0, 0].axvline(original_r2, color='red', linestyle='--',
linewidth=2, label=f'Original R2 ({original_r2:.3f})')
122     axes[0, 0].axvline(np.mean(r2_scores), color='green',
linestyle='-', linewidth=2, label=f'Bootstrap Mean
({np.mean(r2_scores):.3f})')
123     axes[0, 0].axvline(r2_ci_lower, color='orange', linestyle=':',
alpha=0.7, label=f'95% CI')
124     axes[0, 0].axvline(r2_ci_upper, color='orange', linestyle=':',
alpha=0.7)
125     axes[0, 0].set_xlabel('R2 Score')
126     axes[0, 0].set_ylabel('Density')
127     axes[0, 0].set_title('Bootstrap Distribution of R2 Scores')
128     axes[0, 0].legend()
129     axes[0, 0].grid(True, alpha=0.3)
130
131     # MSE distribution
132     axes[0, 1].hist(mse_scores, bins=50, alpha=0.7, color='red',
density=True)
133     axes[0, 1].axvline(original_mse, color='blue', linestyle='--',

```

```

linewidth=2, label=f'Original MSE ({original_mse:.1f})')
134     axes[0, 1].axvline(np.mean(mse_scores), color='green',
        linestyle='-', linewidth=2, label=f'Bootstrap Mean
        ({np.mean(mse_scores):.1f})')
135     axes[0, 1].axvline(mse_ci_lower, color='orange', linestyle=':',
        alpha=0.7, label=f'95% CI')
136     axes[0, 1].axvline(mse_ci_upper, color='orange', linestyle=':',
        alpha=0.7)
137     axes[0, 1].set_xlabel('MSE')
138     axes[0, 1].set_ylabel('Density')
139     axes[0, 1].set_title('Bootstrap Distribution of MSE')
140     axes[0, 1].legend()
141     axes[0, 1].grid(True, alpha=0.3)
142
143     # Coefficient stability
144     feature_names = [f'Feature_{i+1}' for i in
        range(coefficients.shape[1])]
145
146     # Box plot of coefficients
147     axes[1, 0].boxplot(coefficients, labels=feature_names)
148     axes[1, 0].set_ylabel('Coefficient Value')
149     axes[1, 0].set_title('Bootstrap Distribution of Model
        Coefficients')
150     axes[1, 0].tick_params(axis='x', rotation=45)
151     axes[1, 0].grid(True, alpha=0.3)
152
153     # Add original coefficients as red dots
154     for i, coef in enumerate(model.coef_):
155         axes[1, 0].scatter(i+1, coef, color='red', s=50, zorder=5)
156
157     # Coefficient confidence intervals
158     coef_stats = []
159     for i in range(coefficients.shape[1]):
160         coef_mean = np.mean(coefficients[:, i])
161         coef_std = np.std(coefficients[:, i])
162         coef_ci_lower, coef_ci_upper =
        calculate_confidence_intervals(coefficients[:, i])
163
164         coef_stats.append({
165             'feature': feature_names[i],
166             'original': model.coef_[i],
167             'bootstrap_mean': coef_mean,
168             'bootstrap_std': coef_std,
169             'ci_lower': coef_ci_lower,
170             'ci_upper': coef_ci_upper
171         })
172
173     # Coefficient comparison plot
174     x_pos = np.arange(len(feature_names))
175     bootstrap_means = [stat['bootstrap_mean'] for stat in

```

```

coef_stats]
176     bootstrap_stds = [stat['bootstrap_std'] for stat in coef_stats]
177     original_coefs = [stat['original'] for stat in coef_stats]
178
179     axes[1, 1].errorbar(x_pos, bootstrap_means,
yerr=bootstrap_stds,
180                         fmt='o', capsize=5, label='Bootstrap Mean ±
Std')
181     axes[1, 1].scatter(x_pos, original_coefs, color='red', s=50,
182                        label='Original Coefficients', zorder=5)
183     axes[1, 1].set_xlabel('Features')
184     axes[1, 1].set_ylabel('Coefficient Value')
185     axes[1, 1].set_title('Coefficient Stability Analysis')
186     axes[1, 1].set_xticks(x_pos)
187     axes[1, 1].set_xticklabels(feature_names, rotation=45)
188     axes[1, 1].legend()
189     axes[1, 1].grid(True, alpha=0.3)
190
191     # Bootstrap vs Cross-Validation comparison
192     print(f"\nBOOTSTRAP vs CROSS-VALIDATION:")
193     print("-" * 35)
194
195     # Perform 5-fold CV for comparison
196     from sklearn.model_selection import cross_val_score
197     cv_r2_scores = cross_val_score(model, X, y, cv=5, scoring='r2')
198     cv_mse_scores = -cross_val_score(model, X, y, cv=5,
scoring='neg_mean_squared_error')
199
200     print(f"Cross-Validation R2 Mean: {np.mean(cv_r2_scores):.4f} ±
{np.std(cv_r2_scores):.4f}")
201     print(f"Bootstrap R2 Mean: {np.mean(r2_scores):.4f} ±
{np.std(r2_scores):.4f}")
202     print()
203     print(f"Cross-Validation MSE Mean: {np.mean(cv_mse_scores):.2f}
± {np.std(cv_mse_scores):.2f}")
204     print(f"Bootstrap MSE Mean: {np.mean(mse_scores):.2f} ±
{np.std(mse_scores):.2f}")
205
206     # Comparison visualization
207     methods = ['Cross-Validation', 'Bootstrap']
208     r2_means_comp = [np.mean(cv_r2_scores), np.mean(r2_scores)]
209     r2_stds_comp = [np.std(cv_r2_scores), np.std(r2_scores)]
210
211     bars = axes[2, 0].bar(methods, r2_means_comp,
yerr=r2_stds_comp,
212                            capsize=5, alpha=0.7, color=['blue',
'green'])
213     axes[2, 0].set_ylabel('R2 Score')
214     axes[2, 0].set_title('Bootstrap vs Cross-Validation: R2
Comparison')

```



```

215     axes[2, 0].grid(True, alpha=0.3)
216
217     # Add value labels
218     for bar, mean, std in zip(bars, r2_means_comp, r2_stds_comp):
219         axes[2, 0].text(bar.get_x() + bar.get_width()/2,
220             bar.get_height() + std + 0.01,
221             f'{mean:.3f}±{std:.3f}', ha='center',
222             va='bottom', fontweight='bold')
223
224     # Bootstrap applications and best practices
225     axes[2, 1].axis('off')
226
227     applications_text = """
228     BOOTSTRAP APPLICATIONS & BEST PRACTICES:
229     ✓ WHEN TO USE BOOTSTRAP:
230     • Estimate confidence intervals for any metric
231     • Assess model stability and robustness
232     • Compare models statistically
233     • Understand parameter uncertainty
234     • Small datasets where CV is unstable
235     ✓ ADVANTAGES:
236     • Works with any statistic or metric
237     • No distributional assumptions
238     • Provides full sampling distribution
239     • Easy to implement and interpret
240     ✓ LIMITATIONS:
241     • Assumes sample represents population
242     • Can be computationally expensive
243     • May not work well with very small samples
244     • Doesn't account for model selection bias
245     ✓ BEST PRACTICES:
246     • Use  $B \geq 1000$  bootstrap samples
247     • Report confidence intervals
248     • Check for stability across runs
249     • Combine with other validation methods
250     • Consider stratified bootstrap for classification
251     ✓ BUSINESS VALUE:
252     • Quantify uncertainty in predictions
253     • Make risk-informed decisions
254     • Communicate model reliability
255     • Support regulatory requirements
256     """
257
258     axes[2, 1].text(0.05, 0.95, applications_text,
259         transform=axes[2, 1].transAxes,
260         fontsize=9, verticalalignment='top',
261         fontfamily='monospace',
262         bbox=dict(boxstyle='round',
263             facecolor='lightyellow', alpha=0.8))
264

```

```
265     plt.tight_layout()
266     plt.show()
267
268     return bootstrap_results, coef_stats
269 bootstrap_results, coefficient_stats =
    bootstrap_sampling_comprehensive()
```
