

# CONFORMAL PREDICTION

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# TOPICS

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## ***Motivations***

- *More efficient approach than Bayesian Estimation*
- *Learn from/Experiment with Valeriy Manokhin found on Social Media*

## ***Overview of Bayesian Estimation***

- *Introduction to Bayesian Estimation*
- *From Bayesian Estimation to Conformal Prediction*
- *Bayesian must go through prior to provide distribution*

## ***Overview of Conformal Prediction***

- *Nonconformity Scores*
- *Algorithmic Steps*
- *Complexity Analysis (compare using sentiment analysis)*
- *Applications of Conformal Prediction (Show CODE snippet)*

## ***Application Demo***

## ***Conclusion/Next steps***

# MOTIVATIONS

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**Both of us have motivations to find efficient classification algorithms**

- *Michael G – Works in data science*
- *Mike W – Interested in applications of classifiers in cybersecurity logs analysis*

**Both interested in finding an improvement over Bayesian methods**

**Learned of conformal prediction through interaction with Valeriy Manokhin on Social Media. (LinkedIn)**

- *Reviewed his papers & publications, including*  
Practical Guide to Applied Conformal Prediction in Python: Learn and apply the best uncertainty frameworks to your industry applications. (ISBN: 1805122762)

**Conformal Prediction was a suitable topic for investigation both for education, but also our existing careers.**



Valeriy Manokhin,  
PhD, MBA, CQF

# OVERVIEW OF BAYESIAN ESTIMATION

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**Bayes' Theorem** - The probability of event A, given that event B has occurred:

$$P(A|B) = \frac{P(A) \cdot P(B|A)}{[P(A) \cdot P(B|A)] + [P(\bar{A}) \cdot P(B|\bar{A})]}$$

**Key Concept** - Updates prior beliefs based on new evidence.

**Key Terms:**

- **Posterior Distribution:** Bayesian inference relies on updating beliefs through the posterior distribution, which combines the likelihood of the observed data with the prior distribution
- **Credible Intervals:** Unlike frequentist confidence intervals, Bayesian credible intervals offer a probability-based interpretation of parameter uncertainty

# PROS/CONS OF BAYESIAN ESTIMATION

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## Advantages of Bayesian Methods

- *Probabilistic framework for inference.*
- *Intuitive interpretation of uncertainty.*
- *Flexibility in model updating*

## Critiques of Bayesian Methods

- **Subjectivity in Prior Selection:** *Researcher intuition & common heuristics (e.g., principle of indifference).*
- **Computational Complexity:** *High-dimensional models require costly calculations.*
  - *Example: Use of Markov Chain Monte Carlo (MCMC) used to explore priors.*
- **Scalability Issues:** *High-dimensional Bayesian models struggle to scale efficiently for big data.*

# ALTERNATIVE – CONFORMAL PREDICTION (CP)

- **Key Idea:** Constructs prediction sets without requiring a full probability distribution,
  - Computes ***nonconformity scores*** to measure deviations.
  - Uses empirical quantiles to form ***prediction sets***.

Feature	Bayesian Inference	Conformal Prediction
Prior Knowledge	Required	Not Needed
Uncertainty Estimation	Posterior Distributions	Prediction Sets
Computational Cost	H (MCMC)	Efficient (Quartile Based)
Scalability	Limited for Big Data	Highly Scalable

# APPLICATIONS OF CONFORMAL PREDICTION

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- **Healthcare:** Medical diagnostics with uncertainty estimation
- **Finance:** Stock market risk assessment
- **Cybersecurity:** Anomaly detection in network traffic
- **Our Project:** Forecasting news article counts across:
  - Entertainment, Politics, Sports, Technology

# APPROACH AND COMPUTATIONAL COMPLEXITY

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1. Train a base model (linear regression).
2. Compute residuals (nonconformity scores).
3. Estimate threshold using empirical quantiles.
4. Construct prediction intervals.

CP Method	Complexity	Pros	Cons
Inductive CP (ICP)	$O(n)$	Fast, Scalable	Wider Intervals
Transductive CP (TCP)	$O(nk)$	Tighter Intervals	Computationally Expensive
Mondrian CP	$O(n \log n)$	Efficient & adaptive	Assumes conditional independence



# EXAMPLE: CLASSIFICATION OF NEWS STORIES

```
> class ConformalCoverForest:--

# --- Generate Synthetic Data ---
np.random.seed(42)
subjects = ["Health", "Entertainment", "Sports", "Politics", "Technology"]
num_samples = 100

data = pd.DataFrame({
    "Subject": np.random.choice(subjects, num_samples),
    "Feature1": np.random.randn(num_samples) * 100 + 500,
    "Feature2": np.random.randn(num_samples) * 50 + 200,
    "Actual_Count": np.random.randint(3900, 4100, num_samples)
})

# --- Train Model ---
X = data.drop(columns=["Actual_Count", "Subject"])
y = data["Actual_Count"]
model = ConformalCoverForest(alpha=0.05)
model.fit(X, y)

# --- Predict and Evaluate ---
X_test = X[:10]
lower, upper = model.predict(X_test)

# --- Save Output CSV ---
output_df = pd.DataFrame({
    "Subject": data["Subject"][:10],
    "Actual_Count": y[:10],
    "Lower_Bound": lower,
    "Upper_Bound": upper,
    "Within": ((y[:10] >= lower) & (y[:10] <= upper)).astype(int) # One-hot encoding for correctness
})

output_csv = "COMP_4581_Project_Output.csv"
output_df.to_csv(output_csv, index=False)
print(f"Output saved to {output_csv}")

# --- Save Log File ---
log_file = "COMP_4581_Project_Log.txt"
with open(log_file, "w") as log:
    log.write(f"Model Execution Summary:\n")
    log.write(f"Training Time: {model.train_time:.4f} seconds\n")
    log.write(f"Prediction Time: {model.predict_time:.4f} seconds\n")
    log.write(f"Total Run Time: {model.train_time + model.predict_time:.4f} seconds\n")

print(f"Log saved to {log_file}")
```

```
# --- Generate and Save Plot, Aggregate Data, and Ensure One Entry Per Category ---
output_df_grouped = output_df.groupby("Subject", as_index=False).mean()

plt.figure(figsize=(12, 6))
categories = output_df_grouped["Subject"]
actual_counts = output_df_grouped["Actual_Count"]
lower_bounds = output_df_grouped["Lower_Bound"]
upper_bounds = output_df_grouped["Upper_Bound"]

# Compute error bar range
errorBars = [actual_counts - lower_bounds, upper_bounds - actual_counts]

# Scatter plot for actual counts
plt.scatter(categories, actual_counts, color="black", label="Actual Count", zorder=3)

# Error bars for prediction intervals
plt.errorbar(categories, actual_counts, yerr=errorBars, fmt="o", color="blue", label="Prediction Interval")

plt.xlabel("News Subject")
plt.ylabel("Article Count")
plt.title("Conformal Prediction Intervals for News Subjects")

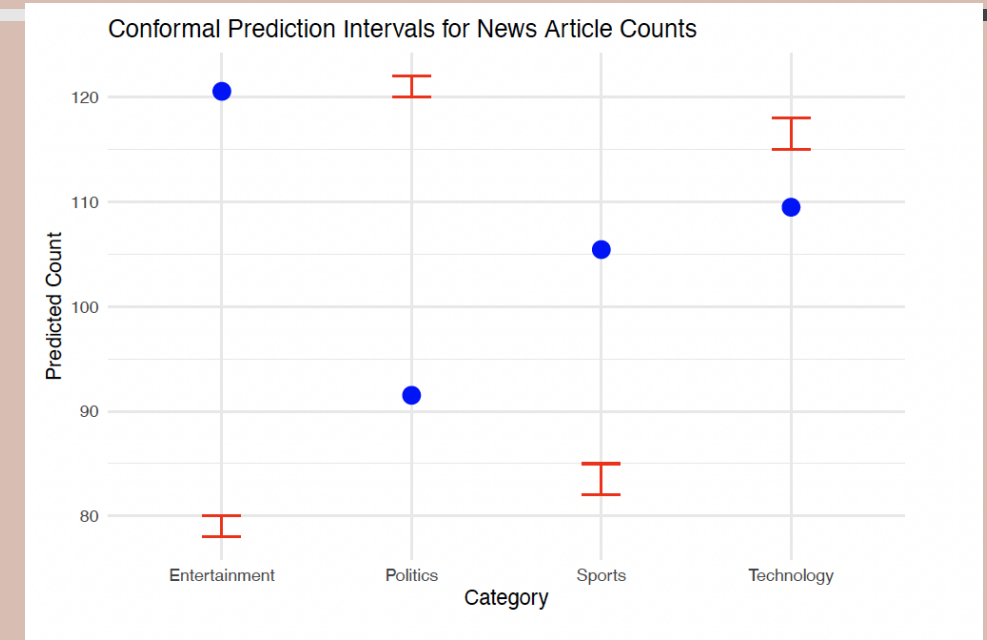
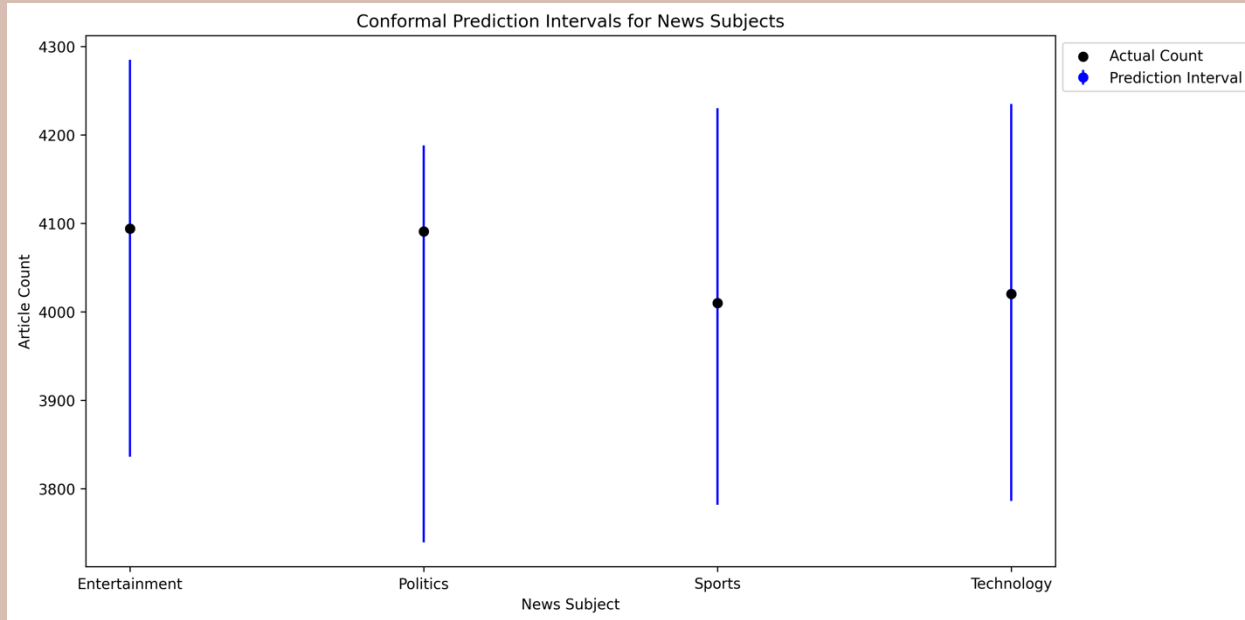
# Move legend outside the plot
plt.legend(loc='upper left', bbox_to_anchor=(1, 1))

# Adjust layout and save
plt.tight_layout()
plt.savefig("COMP_4581_Project_Plot.png", bbox_inches="tight", dpi=300)

print("Plot saved as COMP_4581_Project_Plot.png")

##
# Note:
# Completion, debugging, and validation of the code was assisted by GenAI/LLMs.
##
```

# EXAMPLE: CLASSIFICATION OF NEWS STORIES



Model Execution Summary:  
Training Time: 0.1065 seconds  
Prediction Time: 0.0063 seconds  
Total Run Time: 0.1129 seconds

# CONCLUSION/NEXT STEPS

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- **Conclusion**
  - *Conformal Prediction (CP) ensures reliable prediction sets with finite-sample validity*
  - *Advancements have made CP feasible for large-scale applications despite computational challenges.*
  - *See github repo for practical example*
- **Future Considerations:**
  - *Improving Interval Tightness: Adaptive nonconformity scores.*
  - *Comparing CP with Bayesian Methods: Performance trade-offs.*
  - *Scaling CP for Big Data: Efficient parallel processing.*

# THANK YOU

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# CLASS DEFINITION

```
class ConformalCoverForest:
    """
    Conformal Prediction using Random Forest for classification-based uncertainty estimation.
    This version improves residual estimation to prevent overfitting and enhances generalization.

    Attributes:
    - alpha: Significance level (1 - confidence level).
    - base_model: The base regression model (default is RandomForestRegressor).
    - residuals: Stores the absolute residuals from calibration.
    - train_time: Tracks model training time.
    - predict_time: Tracks prediction interval computation time.
    - label_encoder: Encodes categorical target labels.
    """

    def __init__(self, alpha=0.05, base_model=None):
        """
        Initializes the Conformal Cover Forest model with a specified confidence level.

        Parameters:
        - alpha (float): Significance level (e.g., 0.05 means 95% confidence).
        - base_model: The base regression model (default: RandomForestRegressor with better hyperparameters).
        """
        self.alpha = alpha
        self.base_model = base_model if base_model else RandomForestRegressor(
            n_estimators=300, max_depth=10, bootstrap=True, random_state=42
        )
        self.residuals = None
        self.train_time = 0.0
        self.predict_time = 0.0
        self.is_fitted = False # Track if model is fitted
        self.label_encoder = None # For encoding categorical target labels

    def preprocess_data(self, X, y):
        """
        Converts categorical features and target labels into numeric format.

        Parameters:
        - X (DataFrame or array-like): Feature matrix (may contain categorical columns).
        - y (Series or array-like): Target labels (categorical or numerical).

        Returns:
        - X_processed: Numeric feature matrix.
        - y_processed: Encoded numeric target variable.
        """
        X = pd.DataFrame(X) # Ensure X is a DataFrame

        # Convert categorical features to numerical (One-Hot Encoding)
        for col in X.select_dtypes(include=['object']).columns:
            one_hot = pd.get_dummies(X[col], prefix=col)
            X = X.drop(col, axis=1)
            X = pd.concat([X, one_hot], axis=1)

        # Encode target labels if they are categorical
        if isinstance(y, pd.Series) and y.dtype == 'object':
            self.label_encoder = LabelEncoder()
            y = self.label_encoder.fit_transform(y)

        return X.values, y
```

```
    def fit(self, X, y):
        """
        Trains the model on provided data and calculates residuals for conformal prediction.

        Parameters:
        - X (array-like): Feature matrix.
        - y (array-like): Target variable (discrete class labels).

        Steps:
        1. Preprocesses categorical data into numeric format.
        2. Splits data into training (80%) and calibration (20%) sets.
        3. Fits the RandomForest model on the training set.
        4. Predicts on the calibration set and computes residuals using MAD + noise.
        """
        X, y = self.preprocess_data(X, y) # Convert categorical data

        # Increase calibration set size for better generalization (80-20 split)
        X_train, X_calib, y_train, y_calib = train_test_split(X, y, test_size=0.2, random_state=42)

        print("Training model...")
        start_time = time.time()
        for _ in trange(1, desc="Training Progress"):
            self.base_model.fit(X_train, y_train)
        self.train_time = time.time() - start_time
        self.is_fitted = True

        print("Computing residuals on calibration set...")
        y_pred_calib = self.base_model.predict(X_calib)

        # Compute residuals using Median Absolute Deviation (MAD) and Gaussian noise
        self.residuals = np.abs(y_calib - y_pred_calib)
        mad = median_absolute_error(y_calib, y_pred_calib)

        # FIX: Reduce excess variability by scaling noise contribution
        self.residuals += mad + np.random.normal(0, mad * 0.5, size=self.residuals.shape)

    def predict(self, X_test):
        """
        Generates conformal prediction intervals.

        Parameters:
        - X_test (array-like): Feature matrix for predictions.

        Returns:
        - lower_bounds: Lower bound predictions.
        - upper_bounds: Upper bound predictions.
        """
        if not self.is_fitted:
            raise NotFittedError("Model must be fitted before predicting. Call 'fit()' first.")

        print("Generating predictions...")
        X_test, _ = self.preprocess_data(X_test, np.zeros(len(X_test))) # Encode test features

        start_time = time.time()
        y_pred = self.base_model.predict(X_test)
        q_alpha = np.quantile(self.residuals, 1 - self.alpha)

        lower_bounds = np.floor(y_pred - q_alpha) # Rounded to discrete labels
        upper_bounds = np.ceil(y_pred + q_alpha)
        self.predict_time = time.time() - start_time

        return lower_bounds, upper_bounds
```