Summary of Personal Computational Project

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[1] Kaggle RNA 3D Folding Challenge: A Computational Approach to Structural Prediction

• The Challenge: RNA's 3D Puzzle

- RNA plays a vital role in biological processes (e.g., gene expression, catalytic reactions).
- Core challenge: Predicting RNA's 3D structure accurately and efficiently remains a key hurdle in computational biology.
- Our Goal: To precisely predict the three-dimensional coordinates of RNA sequences using advanced deep learning models.
- My Role:
 - Computational pipeline setup and data preprocessing.
 - Integration and optimization of multi-model prediction results.

[1] Kaggle RNA 3D Folding Challenge: A Computational Approach to Structural Prediction

Our Core Strategy

- Recognizing the limitations of a single model, we adopted a dual-model parallel prediction strategy, integrating two leading Diffusion Models: Boltz-1 and Protenix.
- Briefly on Diffusion Models: Imagine starting with a random "point cloud" (disordered structure); the model refines it step-by-step through a multi-stage "denoising" process into a clear, meaningful 3D structure.

[1] Kaggle RNA 3D Folding Challenge: A Computational Approach to Structural Prediction

Data Flow & My Contributions

- Input Data Standardization: I was responsible for converting raw RNA sequence text files into the specific structured YAML format required by the models. This ensured data could be accurately read and processed by deep learning models, serving as the foundation for model inference.
- Merging & Optimization: I developed post-processing scripts to precisely extract the 3D coordinates of the C1' atom for each nucleotide from the raw outputs of both models.
- An intelligent merging strategy was implemented: the effective prediction results of Boltz-1 were prioritized, while Protenix's predictions were utilized to fill in any potential prediction gaps of Boltz-1, significantly enhancing the robustness and completeness of the final outcome.

YAML Configuration Generation Script

Python script for generating YAML configs

```
1 import pandas as pd
2 import os
4 # Ensure the output directory exists
5 os.makedirs('/kaggle/working/inputs_prediction', exist_ok=True)
7 # Loop through target IDs and sequences from your test data
8 # 'names' and 'sequences' would typically come from loading
     test_sequences.csv'
9 for tmp_id, tmp_sequence in zip(names, sequences):
     with open(f'/kaggle/working/inputs_prediction/{tmp_id}.yaml
     ', 'w') as f:
         f.write("constraints: []\n")
11
         f.write("sequences:\n")
12
         f.write("- rna:\n")
       f.write(" id:\n")
14
      f.write(" - A1\n")
         f.write(f" sequence: {tmp sequence}")
16
```

Summary of Personal Computational Project

[II] Research on Three-Factor Return Modeling and Hedging Strategies of Crude Oil Futures

Data Engineering Innovation

Dynamic Splicing Technology for Futures Main Contracts (High-Frequency Data Processing)

Convenient Proxy Variable Design for Returns:

$$\widetilde{CY}_t = \frac{F_t^{\text{close}} - F_t^{\text{settle}}}{F_t^{\text{settle}}} - r_t$$

Dynamic Modeling of Volatility GARCH(1,1):

$$\sigma_t^2 = \omega + \alpha \epsilon_{t-1}^2 + \beta \sigma_{t-1}^2$$

Calibration Process through Maximum Likelihood Estimation (MLE) Technical Highlights: Capturing Volatility Clustering Effects and Asymmetric Market Effects

[II] Research on Three-Factor Return Modeling and Hedging Strategies of Crude Oil Futures

Three-factor model calculation implementation

Multi-factor regression architecture — OLS model:

$$R_t = \alpha + \beta_1 C Y_t + \beta_2 \sigma_t + \beta_3 r_t + \epsilon_t$$

Robustness analysis: There was no significant multicollinearity. The Bruchy-pagan test showed that the model residuals did not have significant heteroscedasticity. And residual autocorrelation diagnosis.



[II] Research on Three-Factor Return Modeling and Hedging Strategies of Crude Oil Futures

Dynamic Hedging Algorithm and Backtesting

• Dynamic Hedging Algorithm: alculation of Hedging Ratio:

$$h_t^* = \frac{\mathsf{Cov}(R_t^s, \widehat{R_t^f})}{\mathsf{Var}(\widehat{R_t^f})}$$

Real-time Prediction Framework: Daily update of three factors \rightarrow Prediction of return rate \rightarrow Dynamic portfolio adjustment

- Backtesting System Design:
 Performance Indicators: Hedging Effectiveness (HE) = 46.92%,
 Volatility Compression from 1.94% to 1.42%, Sharpe Ratio
 Optimization
- Technology Stack: R Language

【III】 Analysis of the Impact of Meteorological Factors on Urban Air Quality

Research Framework & Technical Approach

- Scientific Question
 - Quantify nonlinear impact of meteorological factors on pollutants
 - Reveal synergistic mechanisms of temperature-precipitation-wind
- ullet Technical Pathway: Data Integration o Feature Engineering o Random Forest Modeling o Policy Optimization
- Technology Stack: R Language (randomForest(ntree=100), ggplot2, car)

【III】 Analysis of the Impact of Meteorological Factors on Urban Air Quality

Model Architecture & Key Findings

- Model Architecture
 - Six independent RF regressions

Air Quality =
$$RF(X_1, X_2, \cdots, X_k) + \epsilon$$

Among them, Air Quality represents the six pollutants: PM2.5, PM10, SO2, NO2, CO, and O3.

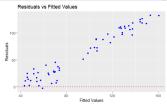
- ullet High temp o photochemical O3 generation
- ullet Low temp o PM accumulation
- Limited rain cleansing effect
- Strong temperature correlation



【III】 Analysis of the Impact of Meteorological Factors on Urban Air Quality

Statistical Validation

ullet Residuals reject normality (p=0.000138) o Uncaptured key factors



VIF confirms temperature collinearity

Policy Recommendations

- High-temp O early warning system
- Low-temp mobile source control
- Meteorology-pollution coordinated response

Research Framework & Technical Approach

- Scientific Objective
 - Build sustainable catastrophe insurance: Balance insurer profitability and policyholder affordability
 - Minimize coverage gaps: Reduce uninsured risk exposure
- ullet Technical Pathway: Multi-source Data Integration o Risk Prediction o Insurance Pricing o Payment Capacity Assessment o Profit and Loss Decision

Core ML Tech

- ARIMA Time Series Forecasting: Dynamic Modeling of Disaster Frequency (Optimization of p, d, q Parameters)
- Random Forest Regression: Prediction of Disaster Loss Magnitude (Feature Importance Analysis)
- Fuzzy Comprehensive Evaluation (FCE): Multi-dimensional Quantification of Engineering Risks

Technology Stack:

- R language, Python, SPSS
- forecast(ARIMA), randomForest, AHP

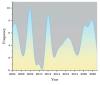


Data Analysis and Visualization

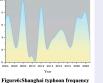


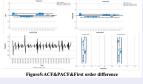
Figure4:Florida Hurricane Frequency

(a)

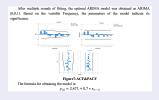


(c)





(b)



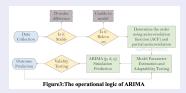
Core Models & Empirical Findings

Actuarial Pricing Model:

$$C = X + Y = np \times \left(\frac{1}{1+i}\right)^{t} \times (1 + \alpha + \beta + \gamma)$$

ML Prediction Engine: ARIMA(1,0,0)

$$\widehat{y}_t = \mu + \emptyset_1 y_{t-1} + \ldots + \emptyset_p y_{t-p} + \theta_1 e_{t-1} + \ldots + \theta_q e_{t-q}$$



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Loss degree model

Multiple linear regression model

$$y = 5.684 \times 10^{-16} + 0.3827x_1 + 0.5682x_2 + 0.3828x_3 + 0.6852x_4$$

Table2: Clustering centers								
Cluster	DAMAGE	INJURIES	DEATHS	INJURIES	Count	DEATHS		
types	PROPERTY	INDIRECT	INDIRECT	DIRECT	Count	DIRECT		
1	142118455.690	1.457	0.199	78.371	94.80	5.057		
2	2687065009.366	2.333	0.999	1090.666	225	96		
3	5111544738.749	12.333	5	1984.666	392	194.333		
4	1302903562.679	18.125	1.75	521.25	256.875	41.75		

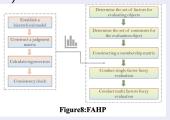
K-means Model

Table3:Model evaluation effect						
	MSE	RMSE	MAE	MAPE	R ²	
Training set	0.047	0.216	0.113	5.783	0.939	
Test set	0.431	0.657	0.281	13.311	-1.205	

Random Forest Loss Prediction:

From Insurance to Heritage Preservation

 Fuzzy Comprehensive Evaluation Method(FCE) and Analytic Hierarchy Process(AHP)



Construct a judgment matrix to implement AHP analysis

$$A = \left[\begin{array}{ccc} \frac{W_1}{W_1} & \cdots & \frac{W_1}{W_n} \\ \vdots & \ddots & \vdots \\ \frac{W_n}{W_1} & \cdots & \frac{W_n}{W_n} \end{array} \right]$$

calculate the eigenvectors

$$\begin{cases} M_{i} = \prod_{j=1}^{n} a_{ij} & (i = 1, 2, \dots, n) \\ \overline{W_{i}} = \sqrt[n]{W_{i}} & (i = 1, 2, \dots, n) \\ W_{i} = \overline{W_{i}} / \sum_{i=1}^{n} \overline{W_{i}} & (i = 1, 2, \dots, n) \\ W = (W_{1}, W_{2}, \dots, W_{n})^{T} \end{cases}$$

Table 7:index weight

Primary indicators	Weight	Secondary indicators	Weight
		Extreme weather frequency	0.276
Natural factors	0.405	Extreme weather damage level	0.431
		Geographic location	0.292
	0.384	Per Capita Disposable Income	0.380
		Urban supporting facilities	0.251
Social factors		Market supply and demand relationship	0.257
		Macroeconomic policies	0.112
Engineering	0.211	Construction cost	0.594
factors		Project quality	0.406

Thanks!