

# **AI for the Greater Good**

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## **Research Summary**

**Information Retrieval Machine Learning Data Mining High Performance Computing Data Analysis Methods and Applications** Improving Web search utility [WWWJ'13, IEEE IC'2013, ACM CIKM'09, DMIN'09] Clustering and pattern mining [IEEE BDS'19, IEEE MC'19, StatsRef'17, SIP'14, CRC'13, IEEE CIKM'11, IEEE SIGIR'11, COLING'10] Traffic analytics from video [IEEE CVPR'23, IEEE CVPR'22, IEEE CVPR'21, BDAT'20, IEEE CVPR'20, IEEE CVPR'19, IEEE SOSE'19, IEEE MC'19, IEEE CVPR'18, IEEE SmartWorld'17] Applications of machine learning and data mining [AAAI'24, IEEE BigData'23, AAAI'23, Bioinformatics'23, DataBrief'23, GHTC'22, ECTEL'22, Microbio'22, KDD-UC'22, iDSC'19, IEEE CIKM'18, GHC'18, IEEE SCI'17, IEEE ICDE'15] Fast nearest neighbors computation [JPDC'17, JDSA'17, iDSC'17, IEEE DSAA'16, IA3'16, ACM CIKM'15, IA3'15, IEEE ICDE'14] 2





## **Outline**

- AI Research for the Greater Good
- Hydrologic Flow Prediction
	- An Extreme-Adaptive Time Series Prediction Model Based on Probability-Enhanced LSTM Neural Networks
	- SEED: An Effective Model for Highly-Skewed Streamflow Time Series Data Forecasting
- Chronic Kidney Disease
	- On-Device Prediction for Chronic Kidney Disease
	- Color Constancy for Accurate CKD Prediction
- References



## AI Research for the Greater Good

## What drives your choice of projects?



## **Medical Analytics**

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[iDSC'19] A Data-Driven Approach for Detecting Autism Spectrum Disorders

**Autism Prediction** *w/ Megan C. Chang, SJSU*



- EKG and skin-conductance data collected during a sensory trial protocol.
- Multivariate time series analysis with very long series (~4M points per subject).

[FIM'22] Identification of Distinct Characteristics of Antibiofilm Peptides and Prospection of Diverse Sources for Efficacious

**Sequences** 

**Antibiofilm and Antithrombotic Peptide Prediction**

*w/ Anand K. Ramasubramanian, SJSU*

- Given a peptide's amino acid sequence
	- Determine its ability to prevent biofilm production or the clotting of the blood.
	- Determine whether the compound that is derived from the peptide is likely to have unintended side effects for the patient.

[GHTC'22] Alex Whelan, Soham Phadke & David C. Anastasiu. On-Device Prediction for Chronic Kidney Disease. In 2022 IEEE Global Humanitarian Technology Conference (GHTC) (GHTC 2022), 2022.

#### **Kidney Health Screening** *w/ Alessandro Bellofiore, SJSU*

 $T$  I  $S$  M

- Decide severity of kidney disease by taking a picture of a test strip
	- Deep Learning localization models for capture quality.
	- Machine Learning regression to translate picture to amount of creatinine.
	- Classify based on regression output.



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#### **Mass-Cytometry Screening**

*w/ Edgar A. Arriaga, University of Minnesota*

- Analyze large multidimensional single-cell datasets
	- Developed a graph-based clustering algorithm to identify related compounds
	- CosTaL transforms high-dimensional cells into a weighted k-NN graph; weights refined via Tanimoto; community detection via Leiden's algorithm

[Bioinformatics'23] Yijia Li, Jonathan Nguyen, David C. Anastasiu, Edgar A. Arriaga. CosTaL: an accurate and scalable graph-based clustering algorithm for high-dimensional single-cell data analysis. Briefings in Bioinformatics, 2023

#### **NVIDIA** Traffic Analytics

#### SANTA CLARA UNIVERSITY

[IEEE CVPR'19] CityFlow: A City-Scale Benchmark for Multi-Target Multi-Camera Vehicle Tracking and Re-Identification [IEEE CVPRW'23, '22, '21, '20, '19, IEEE SOSE'19, IEEE SOSE'19, IEEE MC'19, IEEE CVPRW'18, IEEE SmartWorld'17]

*w/ NVIDIA, Toyota, Johns Hopkins, Iowa State, Boston Univ., Univ. of Albany – SUNY, IIT Kanpur, Australian National Univ.*

- Organizing member and Evaluation Chair for the **AI City Challenge**.
- Address challenges in traffic analysis from video, including:
	- Multi-camera vehicle tracking and multi-movement counting
	- Speed estimation from video
	- Anomaly detection
	- Accident description
	- Driver activity recognition







## AI Models for Hydrologic Flow Prediction

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[AAAI 2024: Learning from Polar Representation: An Extreme-Adaptive Model for Long-Term Time Series Forecasting [IEEE BigData'23: SEED: An Effective Model for Highly-Skewed Streamflow Time Series Data Forecasting] [AAAI 2023: An Extreme-Adaptive Time Series Prediction Model Based on Probability-Enhanced LSTM Neural Networks]



- Data have extreme events that are hard to distinguish from base levels
- Proposed several models for reservoir level and stream flow prediction











# KDD Undergraduate Consortium

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- Expand and enhance the participation of undergraduate students of diverse backgrounds in research pertaining to knowledge discovery from data.
- What to expect
	- Feedback on current research
	- Paper/poster presentations
	- Academic and industry mentors
	- Keynote talks about research careers and funding
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- How to apply
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## An Extreme-Adaptive Time Series Prediction Model Based on Probability-Enhanced LSTM Neural Networks

## Yanhong Li, Jack Xu, David C. Anastasiu

AAAI 2023



## Problem: Univariate Time Series with Extreme Events Forecasting

 $[X_1, X_2, \ldots, X_T] \in R^T \to [X_{T+1}, \ldots, X_{T+H}], \in R^H$ 

#### **Challenges:**

- A majority of normal values that significantly contribute to the overall prediction performance.
- A minority of extreme values that must be precisely forecasted to avoid disastrous events.

#### **Goal:**

- A model concurrently learns extreme and normal prediction functions.
- Long sequence forecasting.
- Good generalization.

#### **Dataset:**

• We evaluate the proposed model on the difficult 3-day ahead hourly water level prediction task applied to 9 reservoirs in California.





#### Extreme Events



**GEV (**Generalized Extreme Value) distribution provides a better fit, showing the presence of extreme values in our data,

$$
F(x; \mu, \sigma, \xi) = \exp\left\{-\left[1 + \xi \left(\frac{x-\mu}{\sigma}\right)\right]^{-1/\xi}\right\}, \quad (1)
$$

where  $μ ∈ R$ ,  $σ > 0$ , and ξ are the location, scale, and shape parameters, respectively, conditioned on 1+ξ(x-μ)/σ > 0.



Motivation: achieving the best overall prediction performance, without sacrificing either the quality of normal or of extreme predictions.

Root Mean Square Error *(RMSE)*

Mean Absolute Percentage Error *(MAPE)*

## Proposed Methods:

**GMM Indicator:** an unsupervised clustering approach to dynamically produce distribution indicators, which improves the model's robustness to the occurrence of severe events.

**NEC framework:** a framework to account for the distribution shift between normal and extreme values in the time series.

**Selected Backpropagation:** to help the models learn the positions and values of appropriate normal or extreme data better.

**Parameterized Loss Function:** a model concurrently learns extreme and normal prediction functions.







A Gaussian mixture model (GMM) is a weighted sum of M component Gaussian densities,

 $p(x|\lambda) = \sum_{i=1}^{M} w_i g(x|\mu_i, \sum i)$ ,

where x is a D-dimensional continuous-valued vector,  $w_i$   $\forall i = 1, \ldots, M$  are the mixture weights, and

 $g(x|\mu_i, \Sigma i)$  are the component Gaussian densities.

We compute an indicator feature as the weighted sum of all component probabilities, given the weights learned when fitting the GMM model.



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NEC is composed of three separate models, which can be trained in parallel:

- $\triangleright$  The Normal (N) model is trained to best fit normal values in the time series.
- $\triangleright$  The Extreme (E) model is trained to best fit extreme time series values.
- $\triangleright$  The Classifier (C) model is trained to detect when a certain value may be categorized as normal or extreme.





#### Two-stage sampling policy:

1. Randomly sample subsections of length h + f from the series as samples to use in training our models. 2. Perform stratified sampling of regions with and without extreme values, allowing the E and C models to oversample up to OS% samples with at least 1 extreme value in the prediction zone.

#### Selected Backpropagation:

N model: only normal values add to the loss.

E model: only extreme values add to the loss.



#### Parameterized Loss Function

$$
BCE(t, p) = -(t \times log (p) + (1 - t) \times log (1 - p))
$$

 $L = \beta \times BCE(t, p^{\alpha}) + (1 - \beta) \times RMSE(t, p)$ 

*where α and β are parameters that can be tuned. Values α > 1 cause the model to predict p values that are higher in general in order to minimize the distance between t and*  $p^{\alpha}$ *.* 

#### Problem: for datasets with a high imbalance between the two classes, BCE will favor the prominent class.

- $\triangleright$  The BCE part: can be thought of as a blunt instrument that grossly exaggerates all miss-classifications in order to more accurately predict the obscure class.
- $\triangleright$  The RMSE part: allows for a more gentle penalty based on the distance between t and p.



1. What is the effect of adding the GMM indicator to a model?

2. What is the effect of introducing exogenous features?

3. How do the loss function parameters affect performance?

4. How does NEC+ compare against state-of-the-art baselines?

### Baselines:

- ARIMA
- Prophet
- LSTM
- DNN-U: univariate LSTM-based encoder-decoder hydrologic model.
- Attention-LSTM: a state-of-the-art hydrologic model used to predict stream-flow.

• N-BEATS: a state-of-the-art time series prediction method that outperformed all competitors on the standard M3, M4 and TOURISM datasets.



## Research Questions:

- 1. What is the effect of adding the GMM indicator to a model?
- 2. What is the effect of introducing exogenous features?









### Research Questions:

3. How do the loss function parameters affect performance?





### Research Questions:

4. How does NEC+ compare against state-of-the-art baselines?





### Overall Evaluation:



Effectiveness Comparison (RMSE) of NEC+ Against Baselines for 9 Reservoirs

#### MAPE of NEC+ vs. Baselines for 9 Reservoirs







SEED: An Effective Model for Highly-Skewed Streamflow Time Series Data Forecasting

## Yanhong Li, Jack Xu, David C. Anastasiu

IEEE BigData 2023



## Problem: predicting long-term streamflow values with rain off data

$$
[x_1, x_2, \dots, x_T] \in \mathbb{R}^T \to [x_{T+1}, \dots, x_{T+H}] \in \mathbb{R}^H,
$$

 $x_1$  to  $x_T$ : the input sequence

 $x_{T+1}$  to  $x_{T+H}$  : the output sequence

*In our research: H = 3 \* 24 \* 4 = 288, with majority of normal values and much fewer extreme values which cause the data skewness to one side.*

#### **Challenges:**

- Long-range dependencies.
- Rare but important extreme values; very imbalanced data.

#### **Goal:**

- An end-to-end extreme-adaptive model.
- Long sequence forecasting *(predicted length = 288)*.

#### **Dataset:**

- Four groups of hydrologic datasets from Santa Clara County, CA.
- Namely Ross, Saratoga, UpperPen, and SFC, named after their respective locations.



### Dataset with high skewness and kurtosis scores:



*Four streams: Ross, Saratoga, UpperPen, and SFC. Hydro year: from September to May.*

*High skewness and kurtosis scores indicate that there is significant deviation from a normal distribution in our data!*





Motivation: achieving the best overall prediction performance, without sacrificing either the quality of normal or of extreme predictions.

> Root Mean Square Error *(RMSE)* Mean Absolute Percentage Error *(MAPE)*

## Proposed Methods:

**Framework:** Segment-Expandable Encoder-Decoder (SEED) model, which is the first to integrate segment

representation learning with a multi-tiered encoder-decoder framework.

**Importance-enhanced sampling strategy:** embedded within the SEED model, allowing it to skillfully identify key features and trends in datasets.

**Representation Learning:** A unique regularization strategy that incorporates a Kullback-Leibler divergence regularization loss term across multiple stacked layers, thereby increasing the model's robustness against anomalous events with divergent distributions.



## Background: Piecewise Linear Representation (PLR)



- $\triangleright$  PLR splits a series into several segments such that the maximum error of each segment does not exceed a threshold.
- **Prior work**: PLR describes the **linear** relationship of the multi-segment representation, mainly works as a preprocessing step to reduce both the space and computational cost of storing and transmitting time series.
- **Our work**: inspired by PLR, SEED learns **nonlinear segment representations** for heavily skewed long term time series.



#### SEED framework



- $\triangleright$  Comprises three core components: embedding, encoder, and decoder.
- $\triangleright$  The encoder generates a unique hidden state and a cell state which serve as the initial values for the corresponding layers in the decoder.
- $\triangleright$  Each decoder layer is assigned a distinct task, as they represent the mean value distribution of different lengths of subsegments in the predicted sequence.



### Convolutional Embedding Layers



#### CNN Layers :

- different kernel sizes to extract features at different spatial scales.
- subsequent tanh activation function.
- lower level: larger kernel sizes, capturing broader patterns and global context.
- higher level: smaller kernel sizes, capturing local patterns and fine grained details.



#### Decoder Architecture

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- First level: the output length is 4, which is meant to predict the mean values of 4 segments, each of which contains 288/4 = 72 points in the forecasted series.
- Second level: the 4 outputs are expanded to16, each represents the mean value of 288/16 = 18 points.
- Expansion: ⟨a, b, c, d⟩ becomes ⟨a, a, a, a, b, b, b, b, c, c, c, c, d, d, d, d⟩, in the **high-dimensional hidden space**.
- By predicting the mean value of different length sub-segments, **extreme values** are represented and spread across

multiple levels in the hierarchy, leading to higher mean values in the segments containing them.



$$
KL(p || q) = \sum p(x) \log \left(\frac{p(x)}{q(x)}\right),
$$

 $\mathcal{L}_i = \text{KL}(\text{softmax}(p_m_i), \text{softmax}(g_m_i)),$ 

$$
\mathcal{L} = RMSE(\hat{y}, y) + \lambda \times \left(\sum_{i=1}^{k} \mathcal{L}_i\right),
$$

#### Motivations:

- $\triangleright$  Kullback-Leibler divergence loss acts as a regularization term that encourages the model to match the target distribution while balancing the sequence generation loss.
- $\triangleright$   $p_{\perp}m_i$  represents the predicted segment mean values in the ith layer, while  $g_m_i$  is the vector of computed ground truth mean values for the segments in the i*th* layer.



**Input**: Dataset with training and inference sequences **Output:** Oversampled training set

**Procedure Oversampling:** 

```
while training set size is not satisfied do
    Randomly sample a sequence including training and
     inference sections:
    if maximum value in inference section \geq T then
        Mark sequence as important;
        Move maximum value to the middle of the inference
         section of the sequence;
        foreach index I in the sequence with step size S do
            Sample starting at I;
            Add sampled sequence to oversampled training
             set:
       end
    end
    else
        Add sequence to oversampled training set;
    end
end
```


 $\triangleright$  Multiple iterations of sampling from the beginning with a specified step size S.



### Baselines:

- FEDFormer
- InFormer
- NLinear
- Dlinear
- NEC+
- EnDecoder, the common encoder-decoder model built with LSTM layers.





#### **Main results**



- Univariate Long-Term (h = 288) Series Forecasting Results.
- Over 1600 test points in the test set were inferenced on all datasets.
- The **best results** are in bold and the second best results are underlined.
- "All" represents the average RMSE of all test samples compared with the ground truth. "High" means larger than the mean value; "Low" includes test samples lower than the mean value.

*In comparison to the three second-best models (NEC+, Nbeats and EnDecoder), SEED achieved, on average, relative RMSE reduction of 31.44%, 34.68%, and 29.67% across the datasets.*



#### **Example comparisons with the second best baselines**

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#### **Effect of the Importance-Enhanced Oversampling Policy**



- To evaluate the impact of this policy, we increased the threshold T while simultaneously decreasing the step size S.
- Increasing the threshold T and decreasing the step size S had a positive impact on the results.
- There is an optimal threshold T value beyond which the policy's effectiveness plateaus.



#### **Effect of the KL Regularization Terms & Segment Expanding**

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We just use T=4, S=8 as an example:

- T4S8: 5-layer without regularization loss terms.
- T4S8-3L: 3-layer SEED with regularization loss terms.
- T4S8-Regu: 5-layer SEED with regularization loss terms, which gives the best result.



## On-Device Prediction for Chronic Kidney Disease

## Alex Whelan, Soham Phadke, David C. Anastasiu

IEEE GHTC 2022





# **Chronic Kidney Disease (CKD)**

- Progressive decline of kidney function
- Approximately 15% of US population affected by CKD







# **Point of Care Testing (PoCT)**

- Kidney Health Monitoring (KHM) System
	- Accessible
	- Fast & Reliable
	- Affordable
- Lateral Flow Assey Test Strip Design



- **Humanitarian assistance**
- Alternative to LAB testing





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## **Related Works**

- SmartBioPhone [1]
- ChemTrainer [2]
- DeepLactate [3]

#### **SmartBioPhone** :

https://pubs.rsc.org/en/Image/Get?imageInfo.ImageType=GA&imageInfo.ImageIdentifier. ManuscriptID=B902354M&imageInfo.ImageIdentifier.Year=2009

## SmartBioPhone™



**DeepLactate** : https://ars.els-cdn.com/content/image/1-s2.0- S0925400522011315-gr3.jpg



#### **ChemTrainer** : https://ars.els-cdn.com/content/image/1-s2.0- S0925400517316519-fx1.jpg





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## **Application Setup**

## ● **[Sign up]**

- Modes of Operation
	- User
	- Researcher







## Application Workflow



## **Localization**

- Hough Circle Transform Method
- Decode Metadata





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## **Feature Extraction**

- HSV Feature Vector Construction (bottom)
- **Randomized Crop (right)**
- **•** Dimensionality Reduction







## **Classification**

- Predictions using estimated glomerular filtration rate **(eGFR)** and **metadata**
- New readings can be used to update models in the cloud database



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## **Evaluation**

- 10-Fold Cross-Validation
- F1 evaluation metric
- Gridsearch (right)





### Model Effectiveness



#### **RGB** Features

#### **HSV** Features







## **Citations**

[1] J. M. Ruano-Lopez, M. Agirregabiria, G. Olabarria, D. Verdoy, D. D. Bang, M. Bu, A. Wolff, A. Voigt, J. A. Dziuban, R. Walczak, and J. Berganzo, "The smartbiophone™, a point of care vision under development through two european projects: Optolabcard and labonfoil," Lab Chip, vol. 9, pp. 1495–1499, 2009.

[2] M. E. Solmaz, A. Y. Mutlu, G. Alankus, V. Kılıc a A. Bayram, and N. Horzum, "Quantifying colorimetric tests using a smartphone app based on machine learning classifiers," *Sensors and Actuators B: Chemical*, vol. 255, pp. 1967–1973, 2018. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S0925400517316519>

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[4] O. Sidorov, "Conditional gans for multi-illuminant color constancy: Revolution or yet another approach?" in *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR) Workshops*, June 2019.



## Selective Partitioned Regression for Accurate Kidney Health **Monitoring**

## Alex Whelan, Ragwa Elsayed, Alessandro Bellofiore,

## David C. Anastasiu

Under Submission



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Color Space Comparison

Phase Angle (degrees)



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### Feature Type Comparison



#### Comparison Against Baselines



#### **Baseline Methods:**

DNN: VGG-inspired CNN-based deep neural network KNN: k-Nearest Neighbor classifier/regressor RF: Random Forest classifier/regressor HBT: Histogram Gradient Boosting Decision Tree classifier/regressor XGB: Extreme Gradient Boosting Tree classifier/regressor DT: Decision Tree classifier/regressor (*not shown in figure*) SVM: Support Vector Machines classifier/regressor (*not shown in figure*)



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# **Questions?**



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