An Autotuning-based HPO Framework for Mixed-kernel SVM Classifications in Science and Engineering on Aurora

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Scalable Tools Workshop, Madison, WI, July 26-30, 2026

Mixed-kernel Support Vector Machine (SVM)

- A popular classification method widely used in science and engineering

- Handles both linear and nonlinear classifications
- When data is not linearly separable, kernel functions are used as preprocessing methods to be applied to the training data to transform it to higher-dimensional space in order to make the data linearly separable.

- Some popular nonlinear kernel functions: polynomial, Gaussian, and Sigmoid
  - In general, the Gaussian outperforms the polynomial in both accuracy and convergence time
  - The Gaussian has interpolation ability and is effective at identifying local properties
  - The Sigmoid is better suited for identifying global characteristics but has a relatively weak interpolation ability

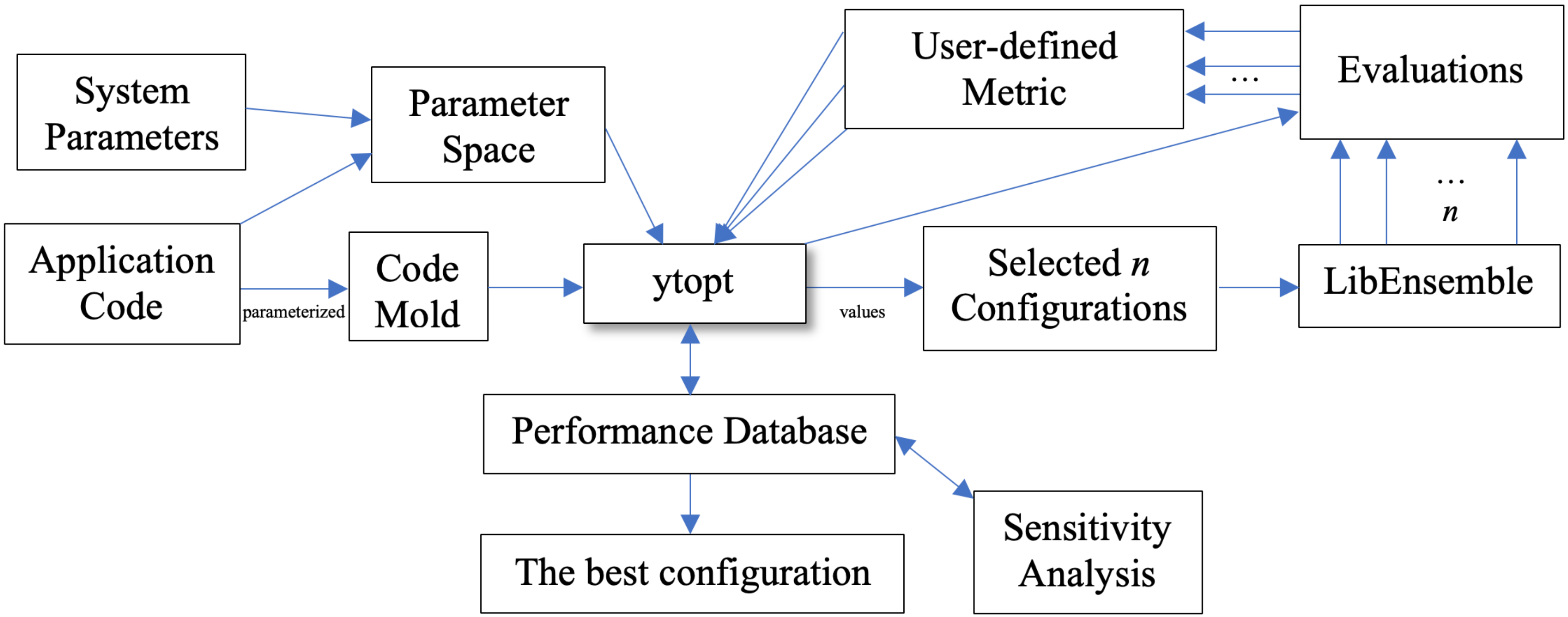
- The mixed kernel between the Gaussian and Sigmoid in SVMs takes the advantages of both kernels.

Background, Motivations, and Our Approach

- In our DOE ASCR-funded Microelectronics projects Threadwork and BIA,
  - Mixed-kernel heterojunction transistor device was developed by Northwestern U.
  - Application driver focuses on HEP detector datasets

- **Approach**: Use mixed kernel SVMs to process HEP detector datasets
  - Utilize *SVC* from scikit-learn to implement a mixed-kernel SVM model
    - *SVC(C=C, kernel=lambda x, y: ExperimentalKernel().mixed_kernel(x, y, mixed_ratio, sigmoid_ratio, coef0, gaussian_ratio))*
  - In HEP, commonly use grid search to conduct initial hyperparameter optimization with the focus on the mixed ratio, sigmoid ratio, and gaussian ratio and obtained the accuracy 83.4% as the baseline
  - Use our autotuning tool ytopt to conduct hyperparameter optimization for five hyperparameters: the mixed ratio, sigmoid ratio, gaussian ratio, the regularization parameter C, and the parameter coef0 in SVC.

ytopt-libe: Asynchronous Autotuning Framework



https://journals.sagepub.com/doi/10.1177/10943420241286476

https://github.com/ytopt-team/ytopt/tree/main/ytopt-libe

Methodology of the Autotuning Framework ytopt

- The search method within ytopt uses Bayesian optimization, where a dynamically updated Random Forest surrogate model that learns the relationship between the configurations and the performance metric, is used to balance exploration and exploitation of the search space.

  - In the exploration phase, the search evaluates parameter configurations that improve the quality of the surrogate model,
  - In the exploitation phase, the search evaluates parameter configurations that are closer to the previously found high-performing parameter configurations.
  - The balance is achieved through the use of the lower confidence bound (LCB) acquisition function that uses
    - the surrogate model' predicted values of the unevaluated parameter configurations
    - and the corresponding uncertainty values (standard deviation).

Two Asynchronous Aspects of the ytopt-libe

- *The asynchronous aspect of the search* allows the search to avoid waiting for all the evaluation results before proceeding to the next iteration.
  - As soon as an evaluation is finished, the data is used to retrain the surrogate model, which is then used to bias the search toward the previous promising configurations.

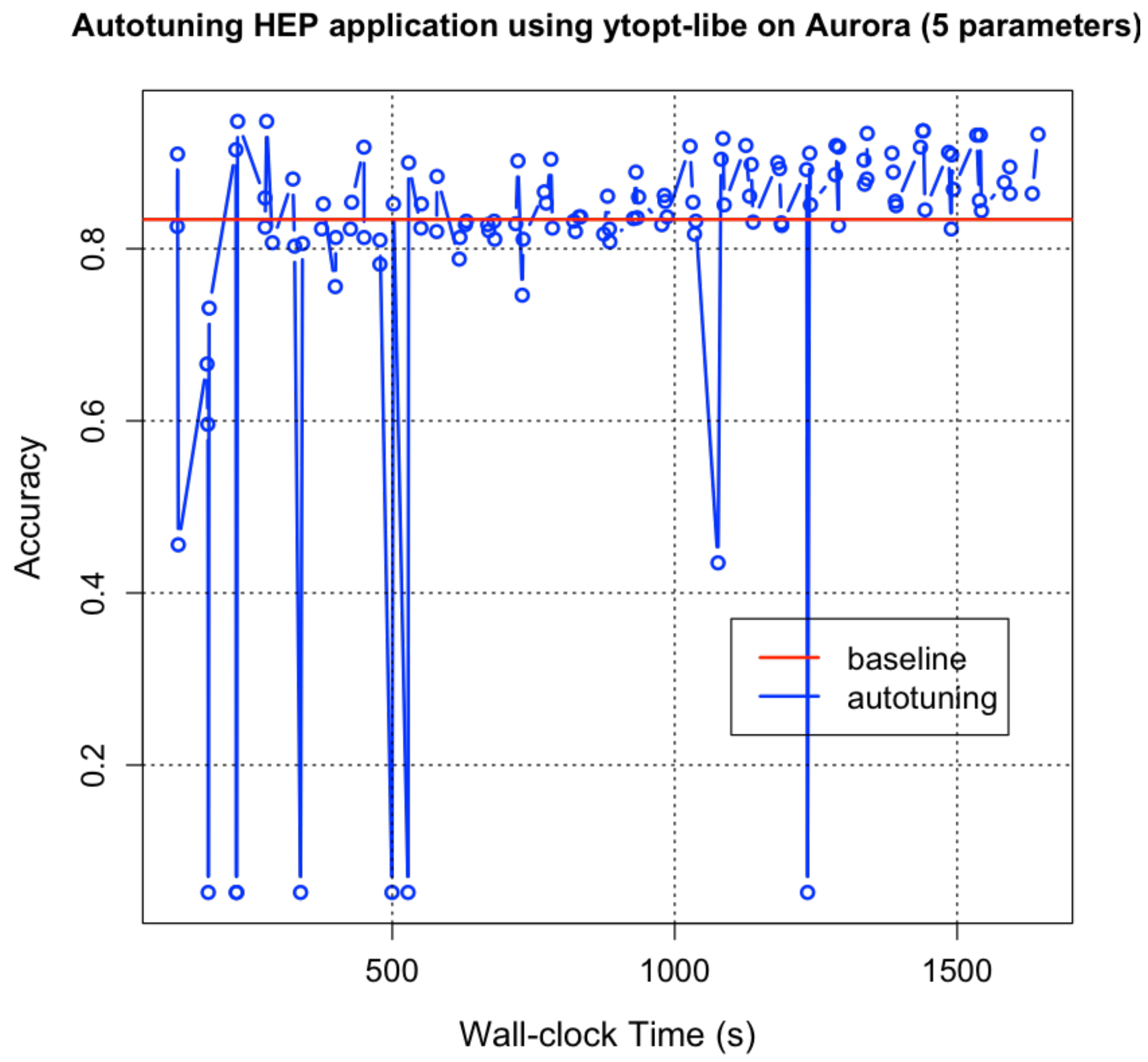
- *The asynchronous aspect of the evaluation* allows ytopt-libe to evaluate multiple selected parameter configurations in parallel by using the asynchronous and dynamic task manager libEnsemble.

Mixed Kernel SVMs for HEP Detectors

Tunable mixed-kernel SVM enables efficient data filtering for tracking systems and smart pixel HEP detectors

- Use Smart Pixel Datasets generated from Fermi Lab
  - This dataset comprises the charge deposited in each pixel per time slice upon pion interaction with the silicon pixel detectors, along with the truth information of each interacting pion.
- Utilize *SVC* from popular scikit-learn to implement a mixed-kernel SVM model to distinguish between low and high transverse momentum tracks
  - `SVC(C=C, kernel=lambda x, y: ExperimentalKernel().mixed_kernel(x, y, mixed_ratio, sigmoid_ratio, coef0, gaussian_ratio))`
- Use ytopt to conduct hyperparameter optimization for five hyperparameters: the mixed ratio, sigmoid ratio, gaussian ratio, the regularization parameter C, and the parameter coef0 in SVC.

Autotuning the HEP Application with 5 parameters



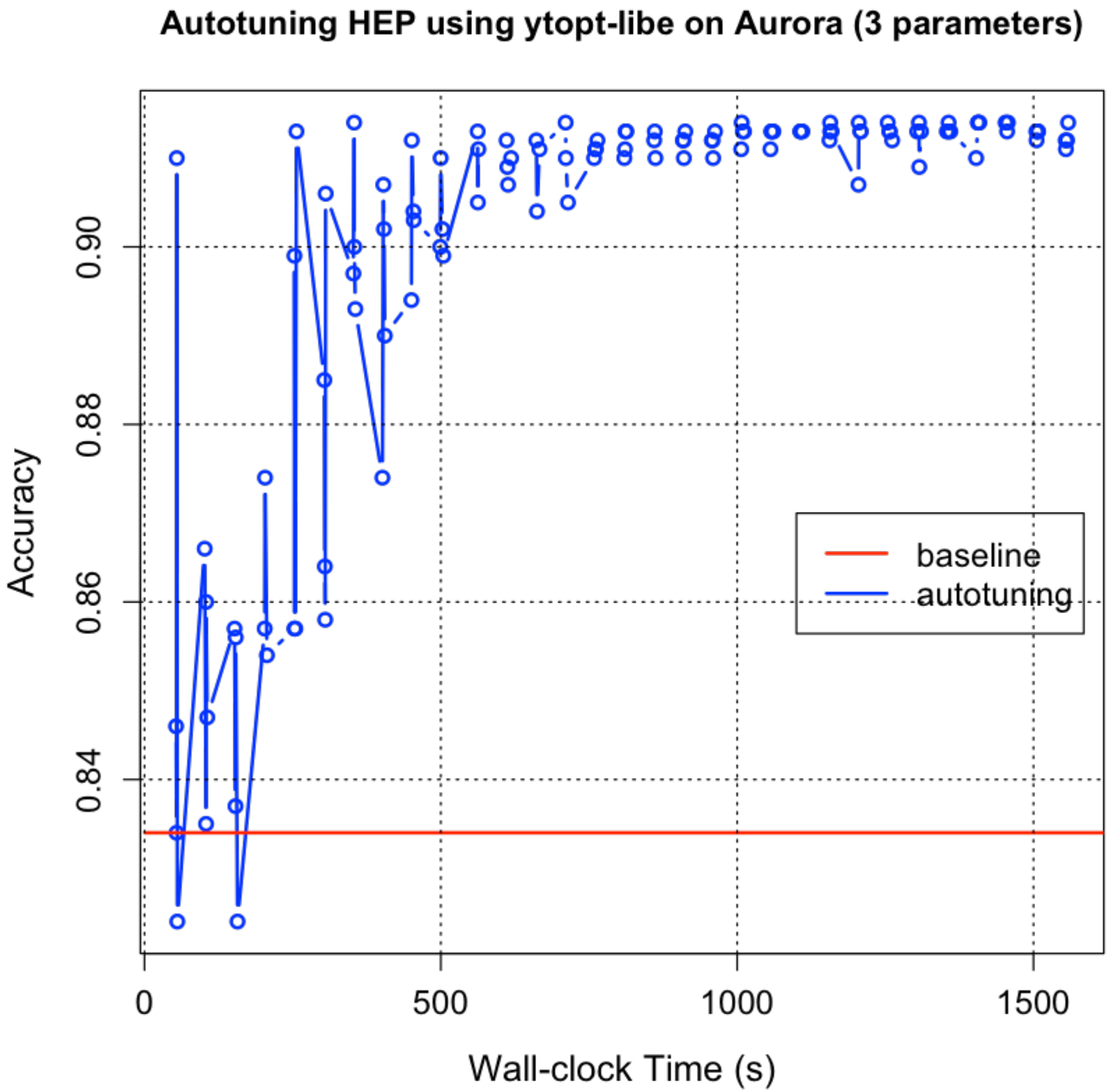
What We Observed

- SVC from scikit-learn:
  - Keep the ranges the same for the mixed ratio, sigmoid ratio, and gaussian ratio
  - the regularization parameter C
    - Common to all SVMs
    - The default value 1.0
    - The strength of regularization for training data is inversely proportional to C
      - If the data has a lot of noisy observations, decrease C (more regularization)
    - Must be positive real number
    - Set the large range [0.1, 100]

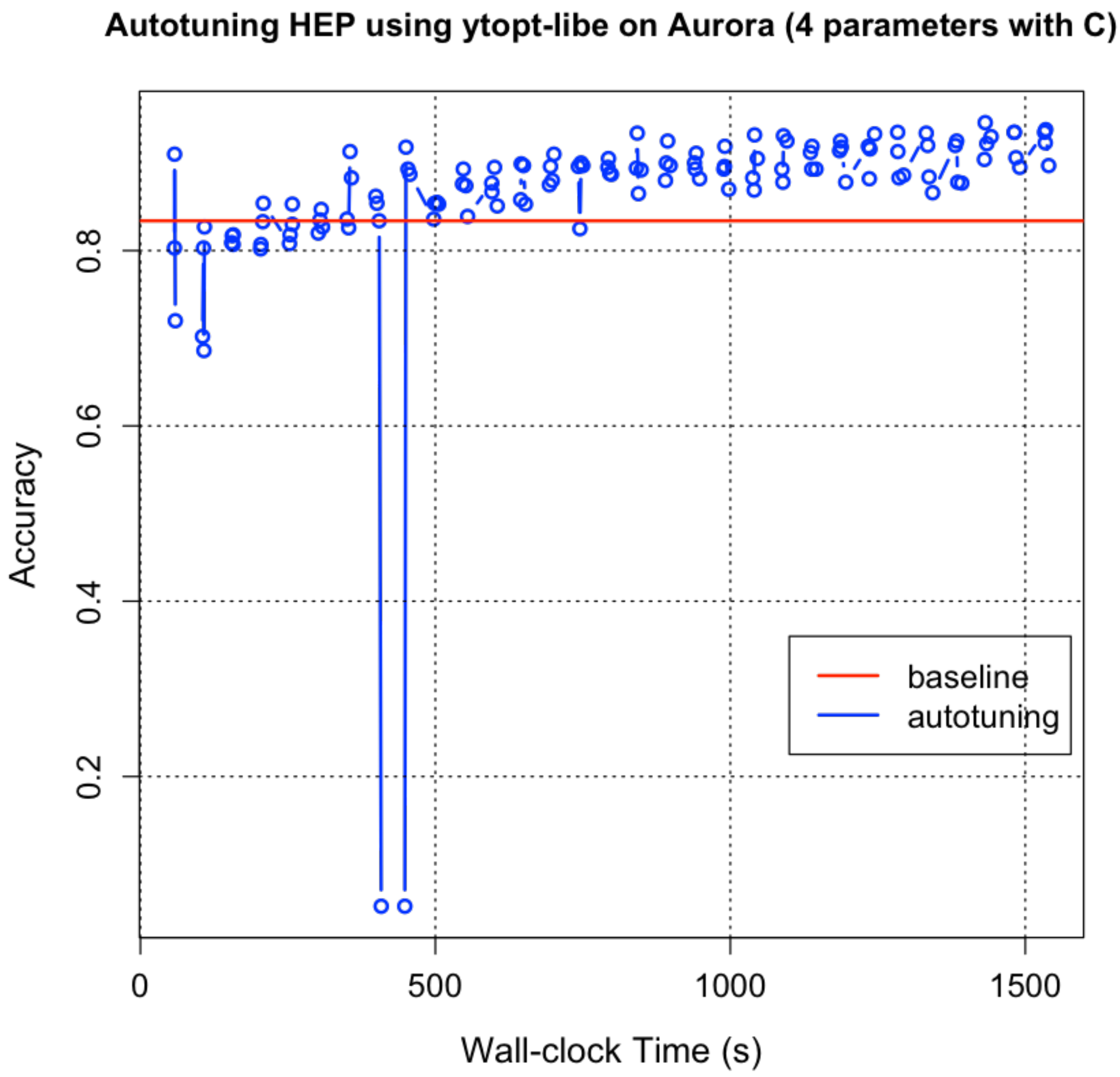
  - the parameter coef0
    - Significant in the sigmoid kernel
    - The default value 0.0
    - Positive or negative real number
    - Set the large range [-15, 15]

- Some abnormal cases with the very low accuracy 5.2%
- Why? This motivates us to investigate what really happened here

Autotuning the HEP Application with 3 parameters with C=1.0 and coef0=0.0



Autotuning the HEP Application with 4 parameters with C=[0.1, 100] and coef0=0.0



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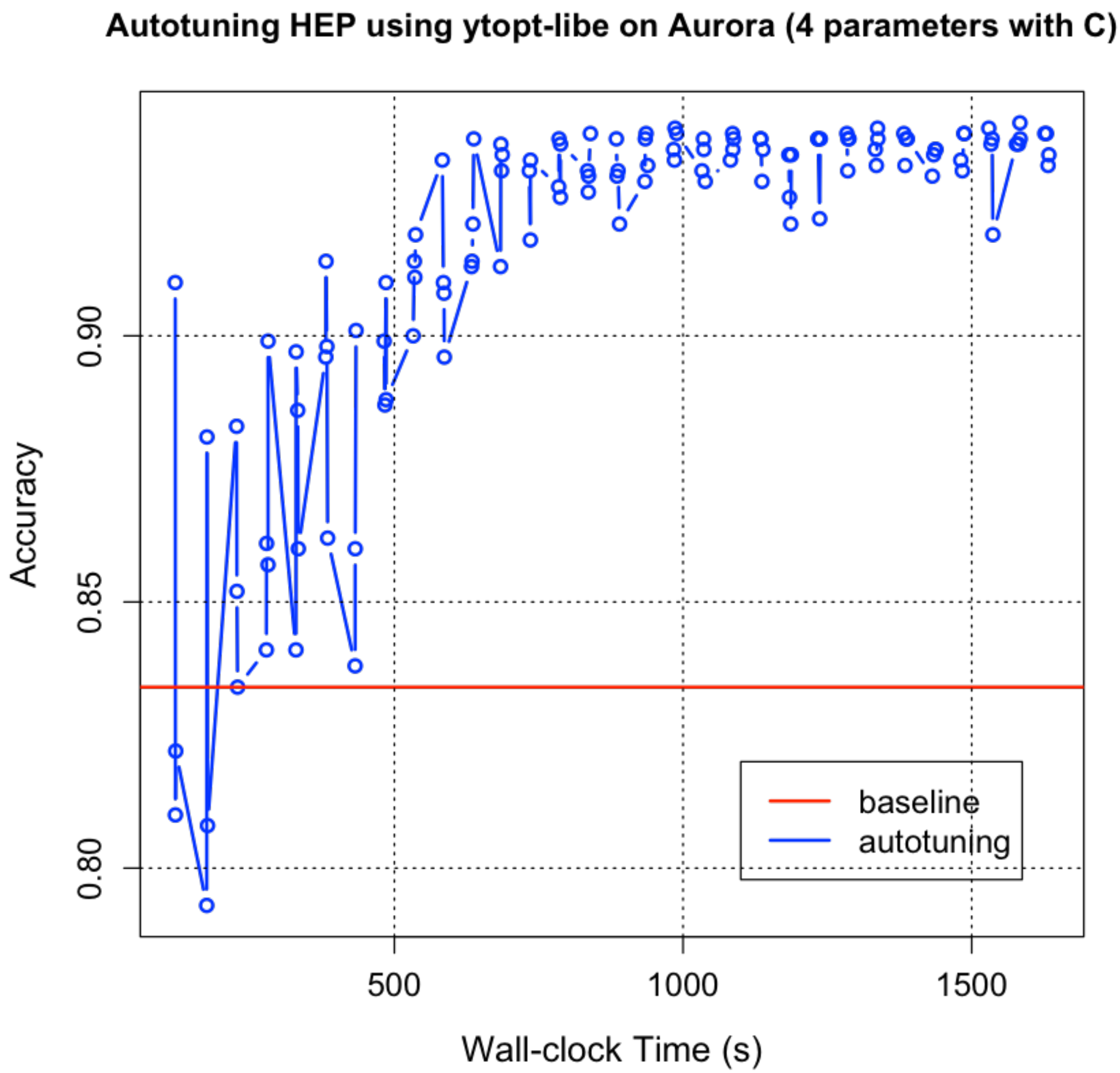
Autotuning the HEP Application with 4 parameters with C=[0.37, 10] and coef0=0.0



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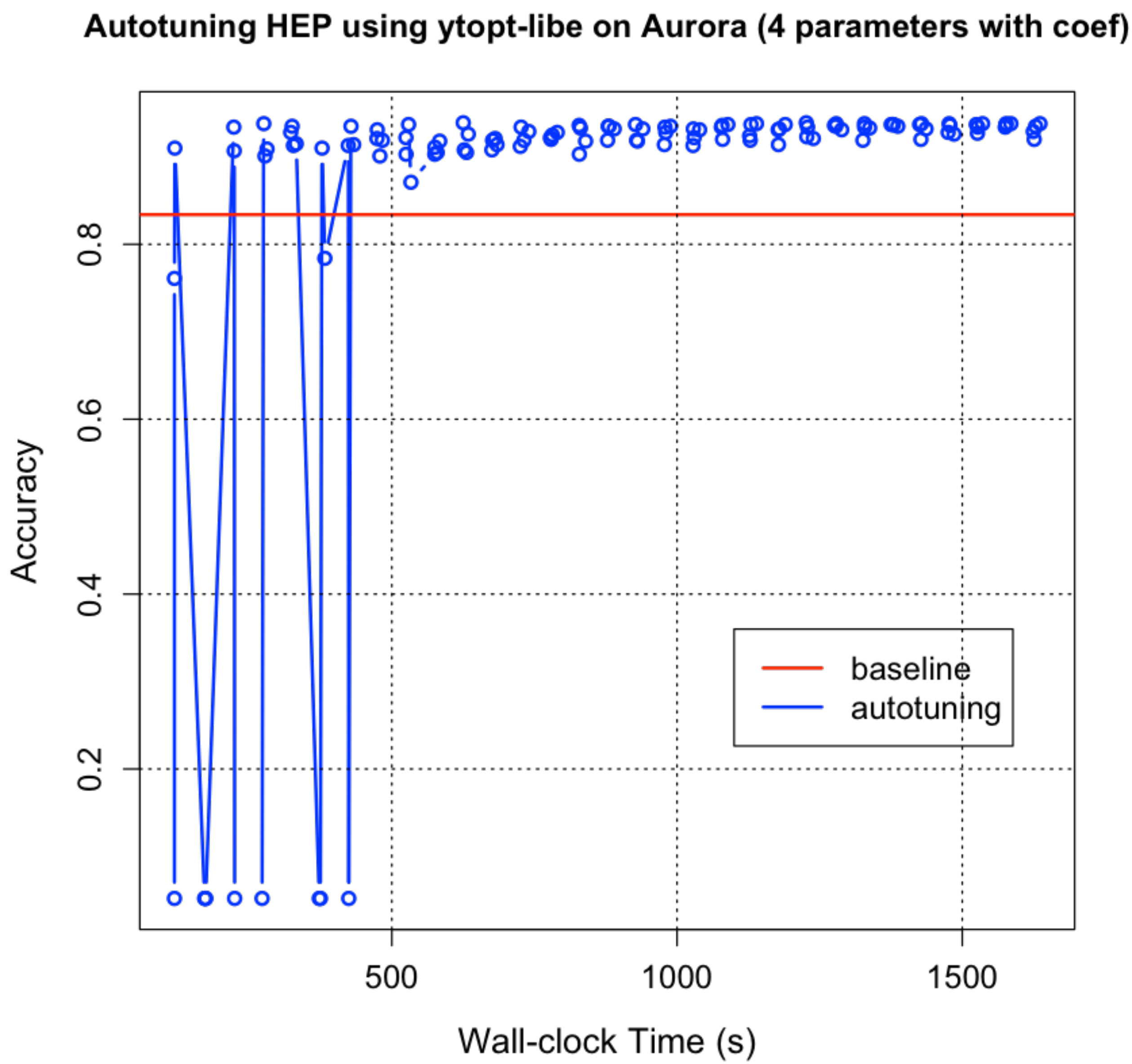
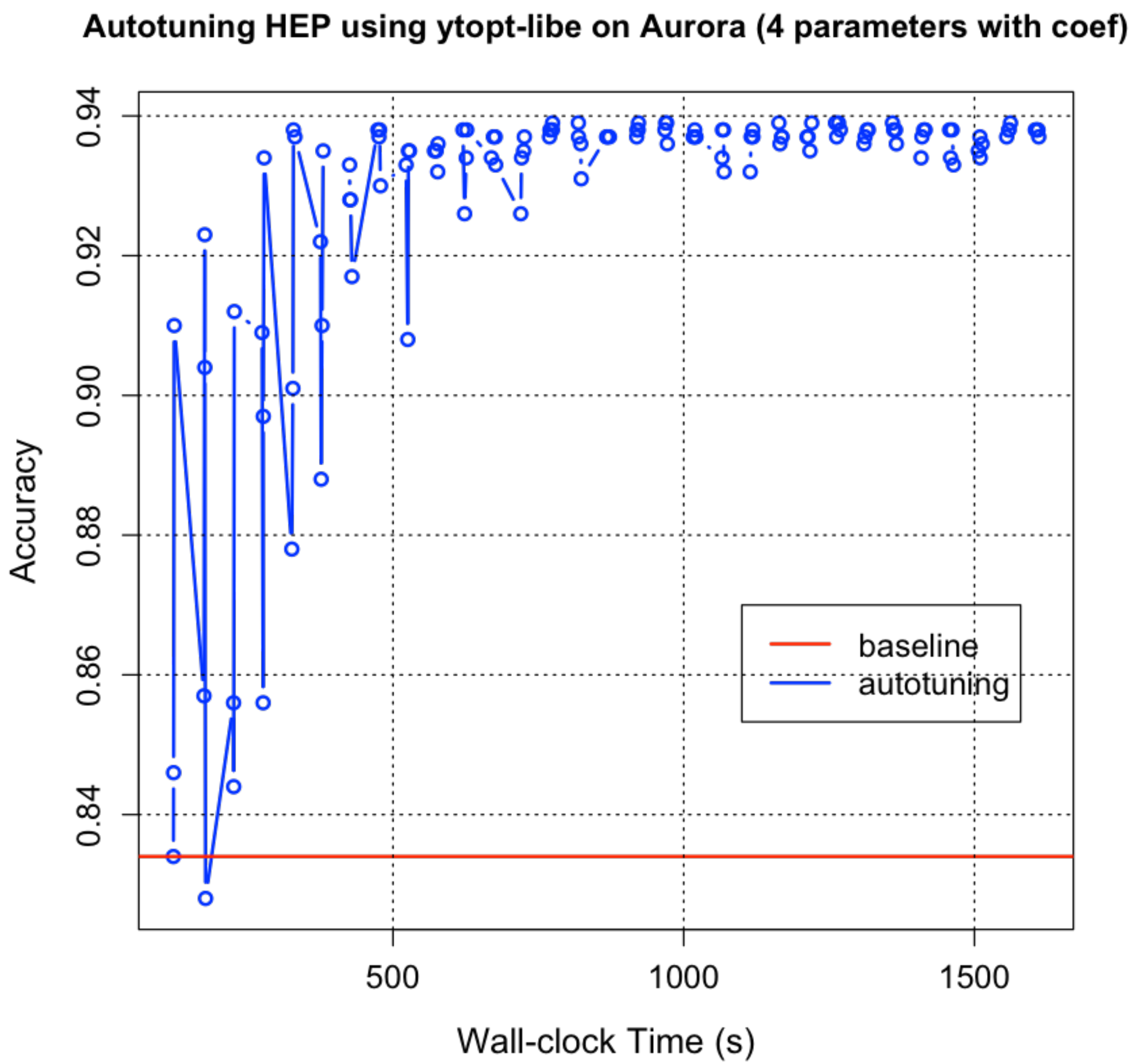
Autotuning the HEP Application with 4 parameters with C=1.0 and coef0=[-15, 15]



Autotuning the HEP Application with 4 parameters with C=1.0 and coef0=[-1, 1]



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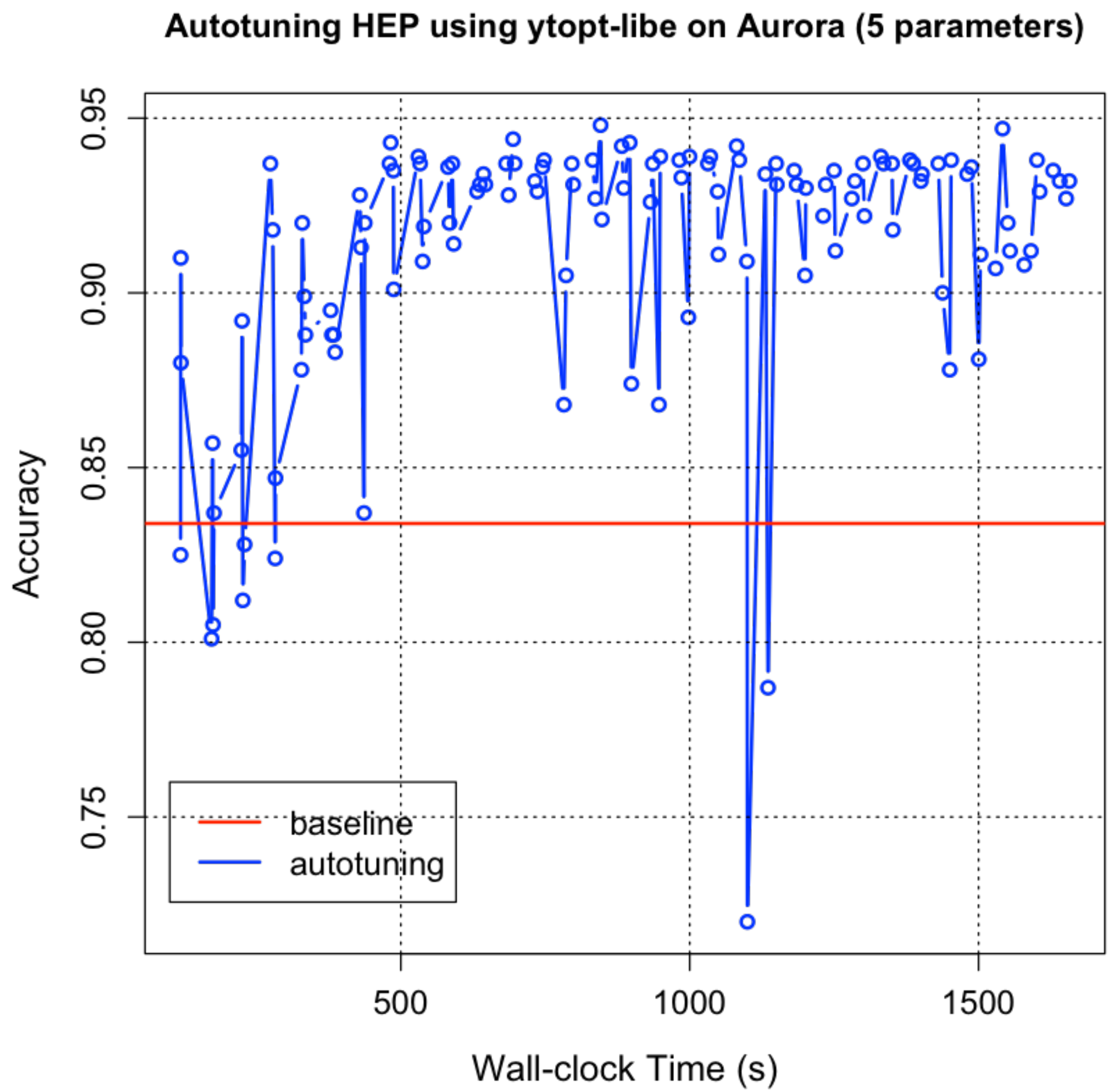
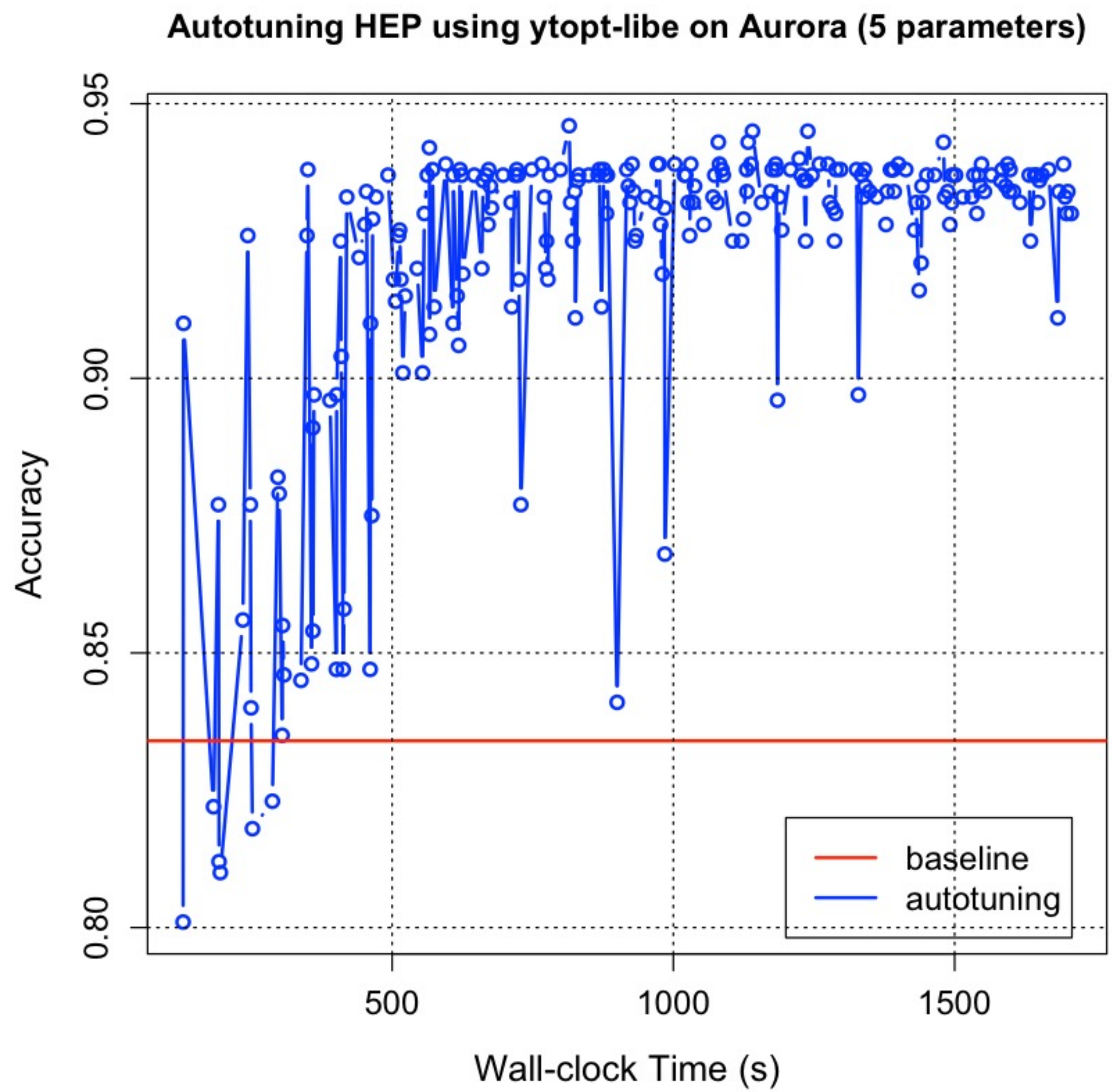
Autotuning the HEP Application with 5 parameters with C=[0.37, 10] and coef0=[-1, 1] on 4 Aurora nodes



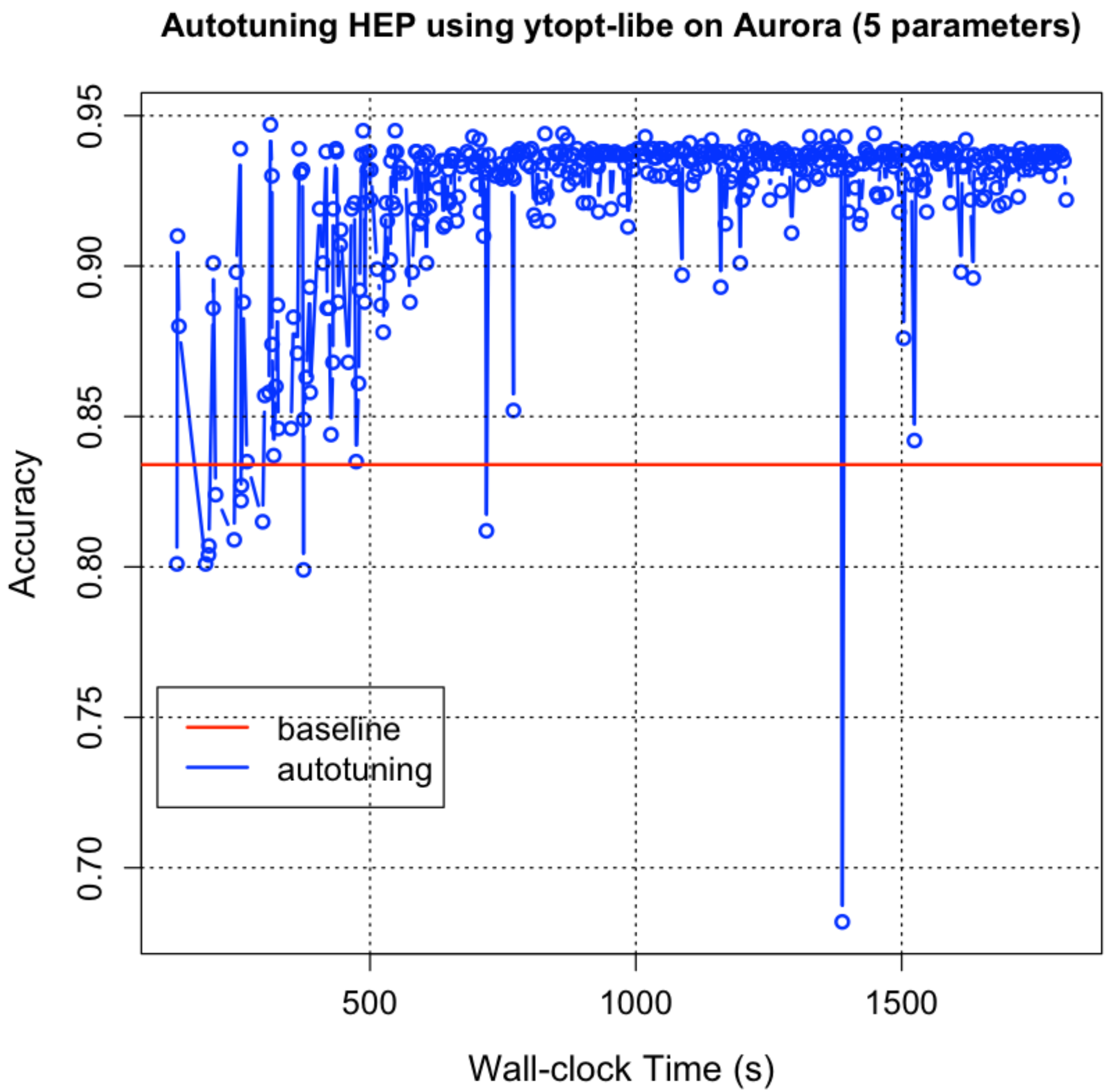
Accuracy:
94.8%

Autotuning the HEP Application with 5 parameters with C=[0.37, 10] and coef0=[-1, 1] on 8 nodes



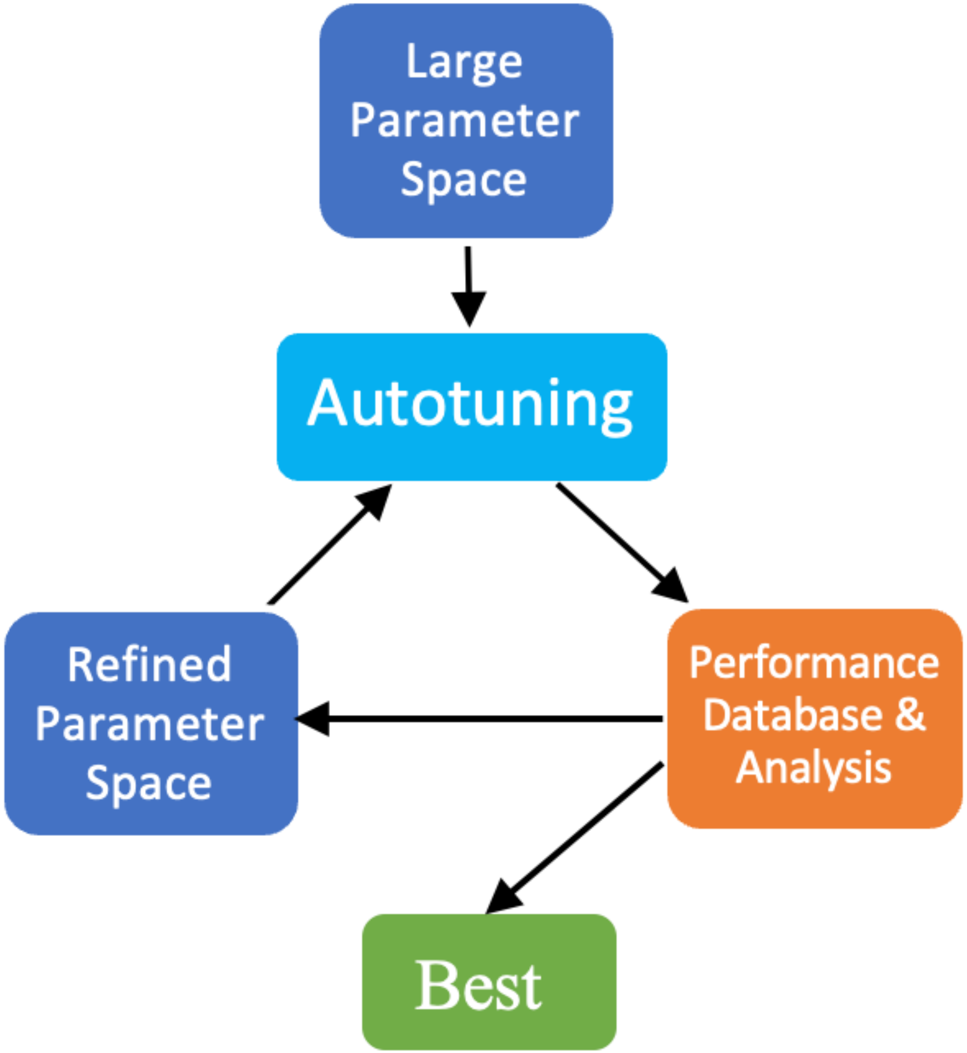
Accuracy: 94.8%

Autotuning the HEP Application with 5 parameters with C=[0.37, 10] and coef0=[-1, 1] on 16 nodes



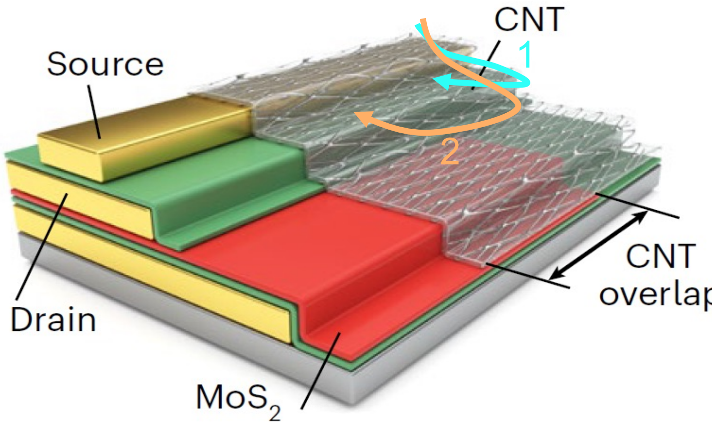
Accuracy: 94.8%

Autotuning-based HPO Framework



Mixed Kernel Heterojunction (MKH) Transistor

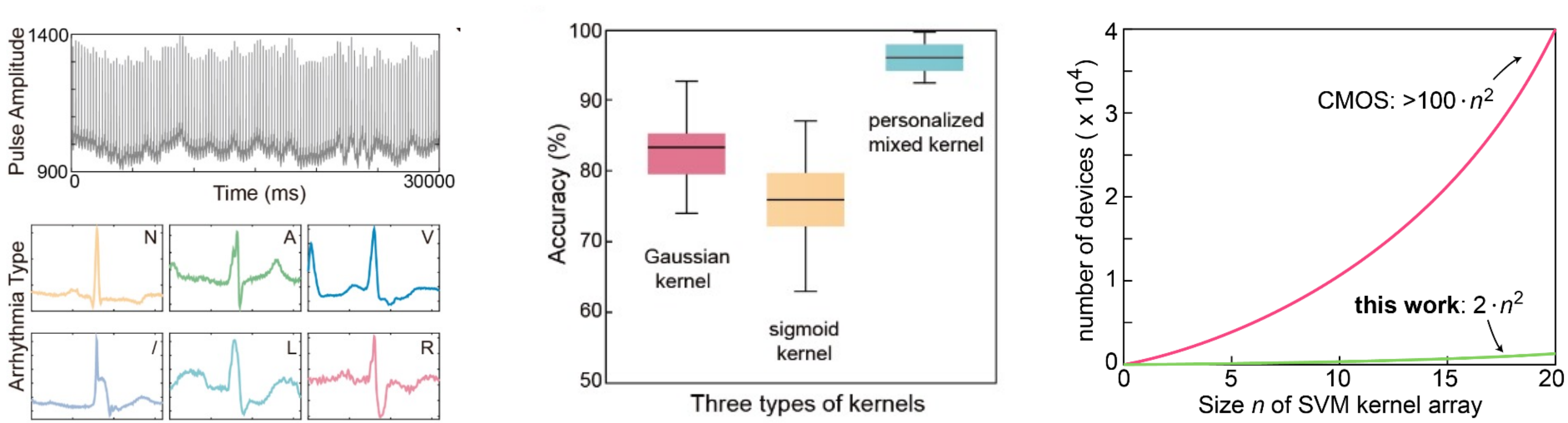
- CNT-MoS_2 vdW p-n heterojunctions with *lateral offsets*
- Dual-gated structure achieves tunable Gaussian and sigmoid kernel functions for efficient SVM classification



*Yan, Qian, Sangwan, Hersam et al., Nature Electronics **6**, 862 (2023)*

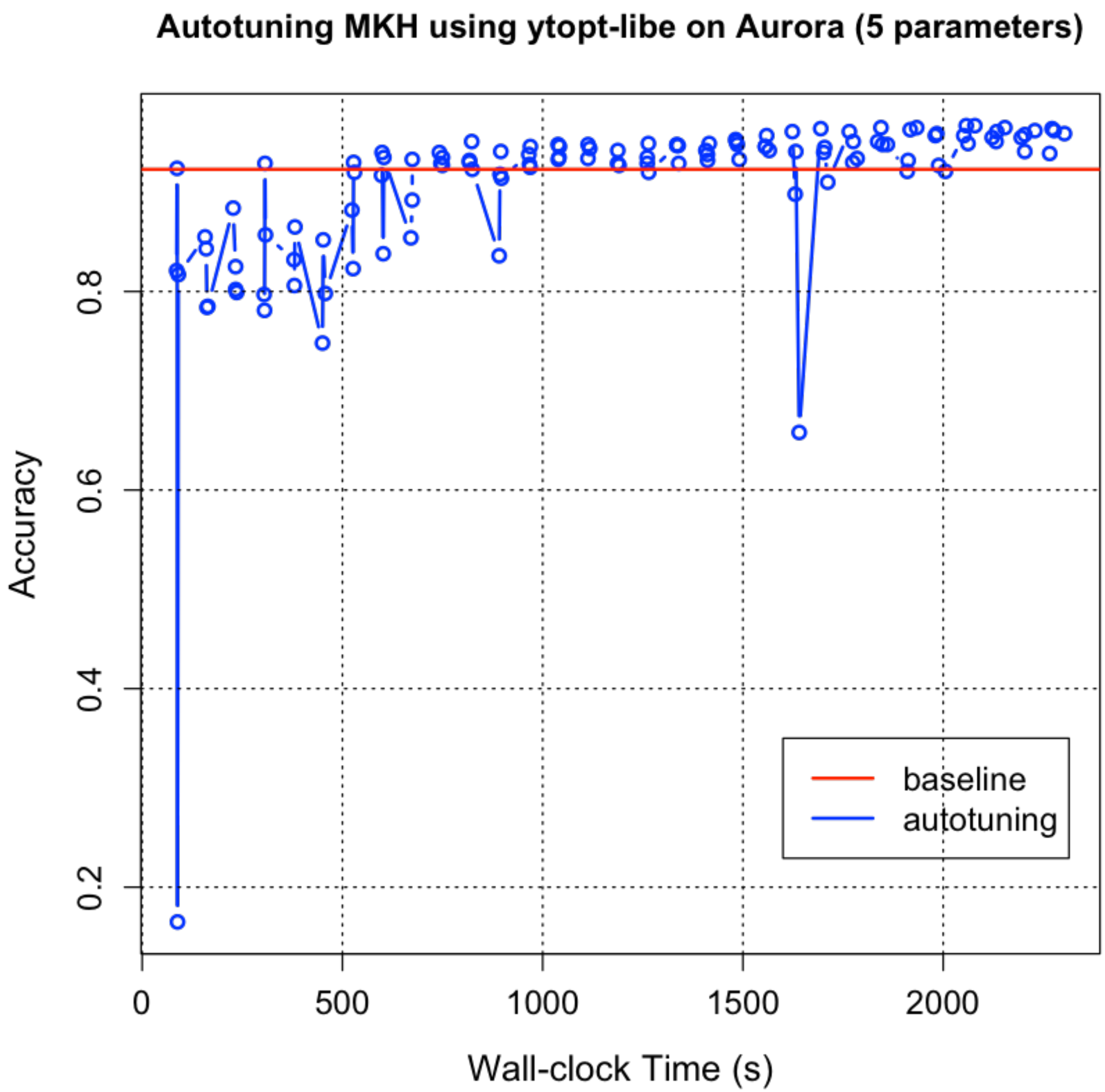
Heterojunction Transistor—Applications

- Two devices → full tunability of all hyperparameters
- SVM with mixed kernels → efficient arrhythmia detection in electrocardiogram (ECG) signal

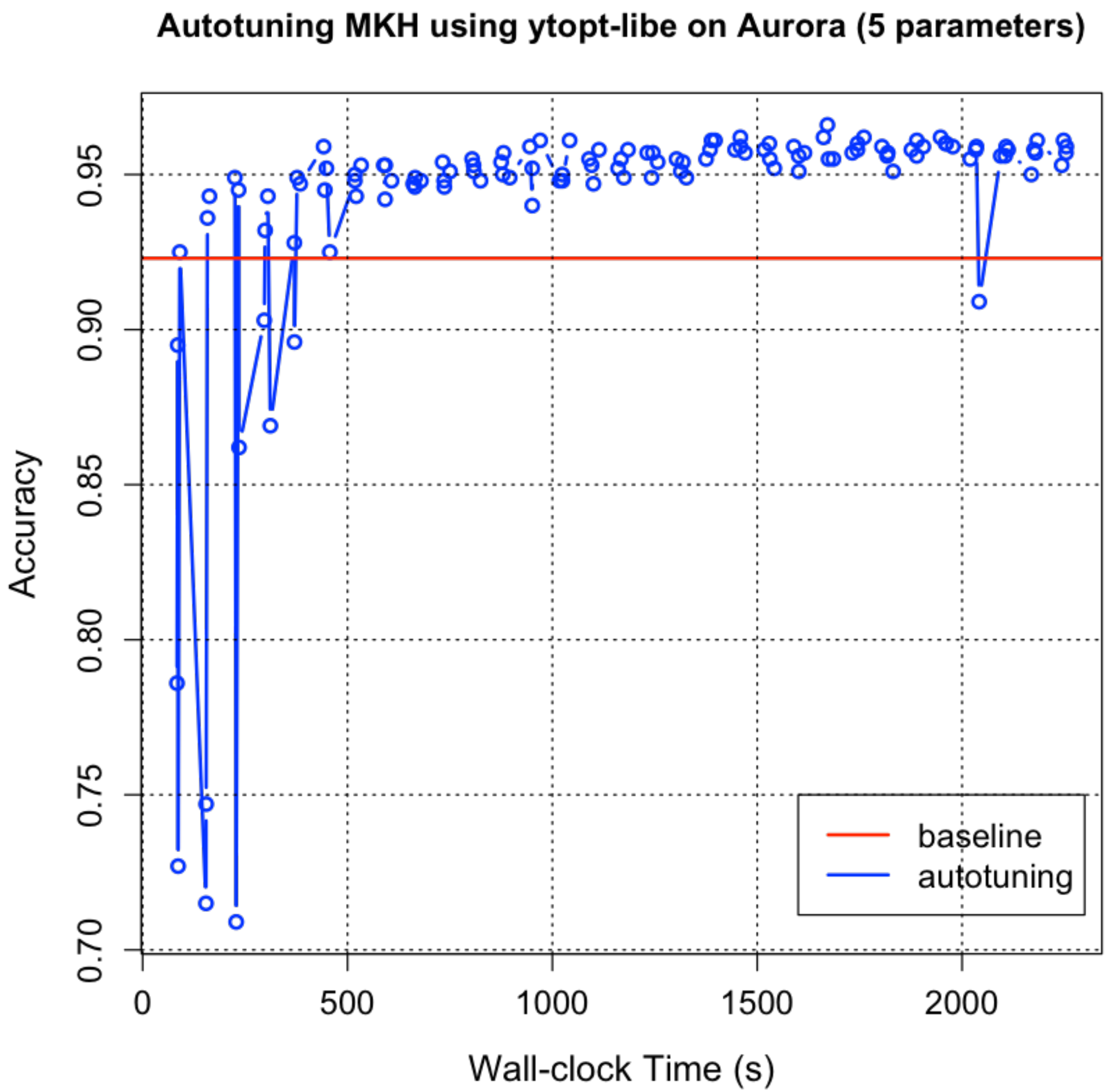


*Yan, Qian, Sangwan, Hersam et al., Nature Electronics **6**, 862 (2023) with **less than 95% average accuracy***

Autotuning the MKH Application with 5 parameters with C=[0.1, 100] and coef0=[-15, 15] on 4 nodes

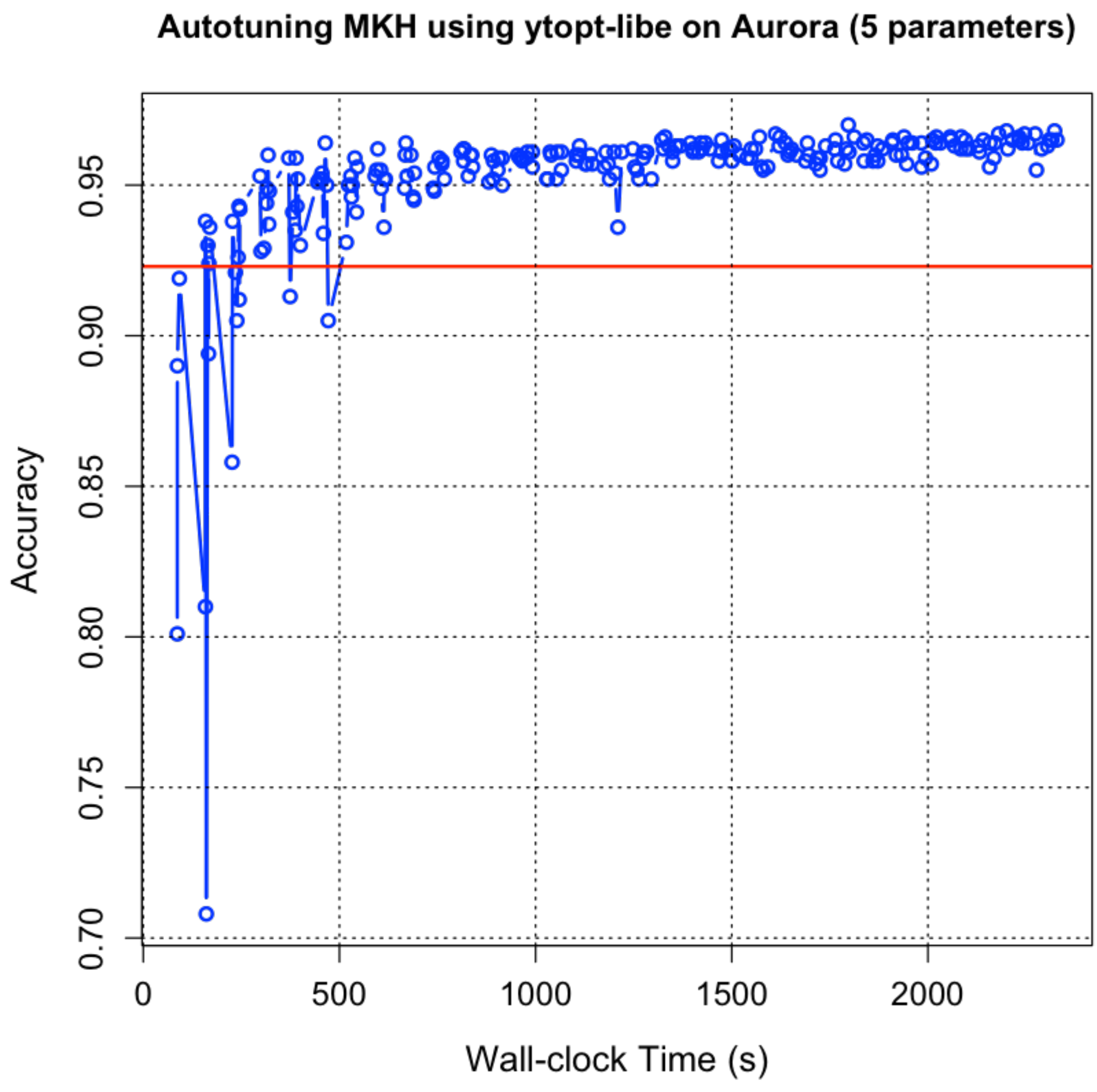


Autotuning the MKH Application with 5 parameters with C=[0.37, 10] and coef0=[-1, 1] on 4 nodes



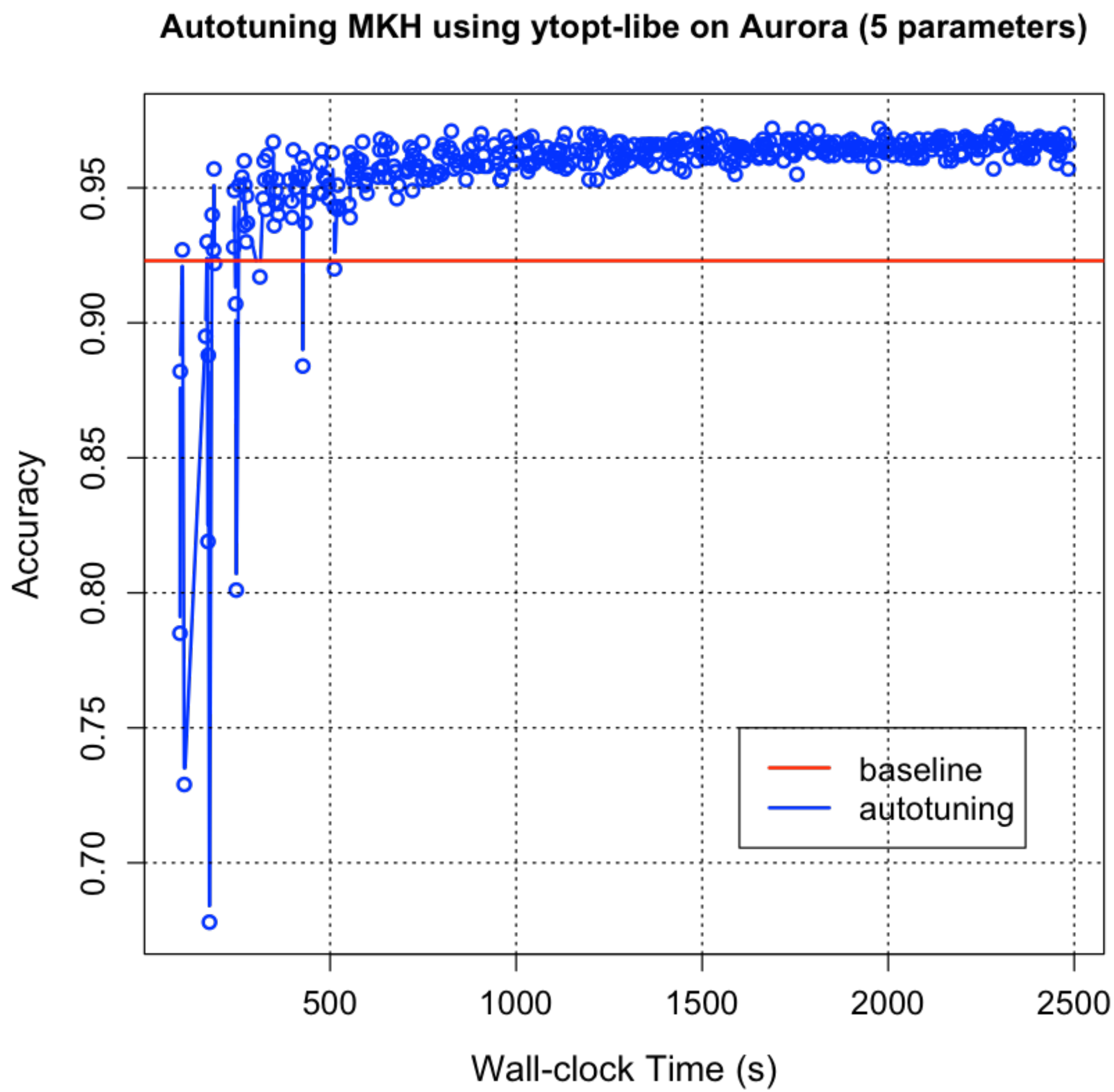
Accuracy: 96.6%

Autotuning the MKH Application with 5 parameters with C=[0.37, 10] and coef0=[-1, 1] on 8 nodes



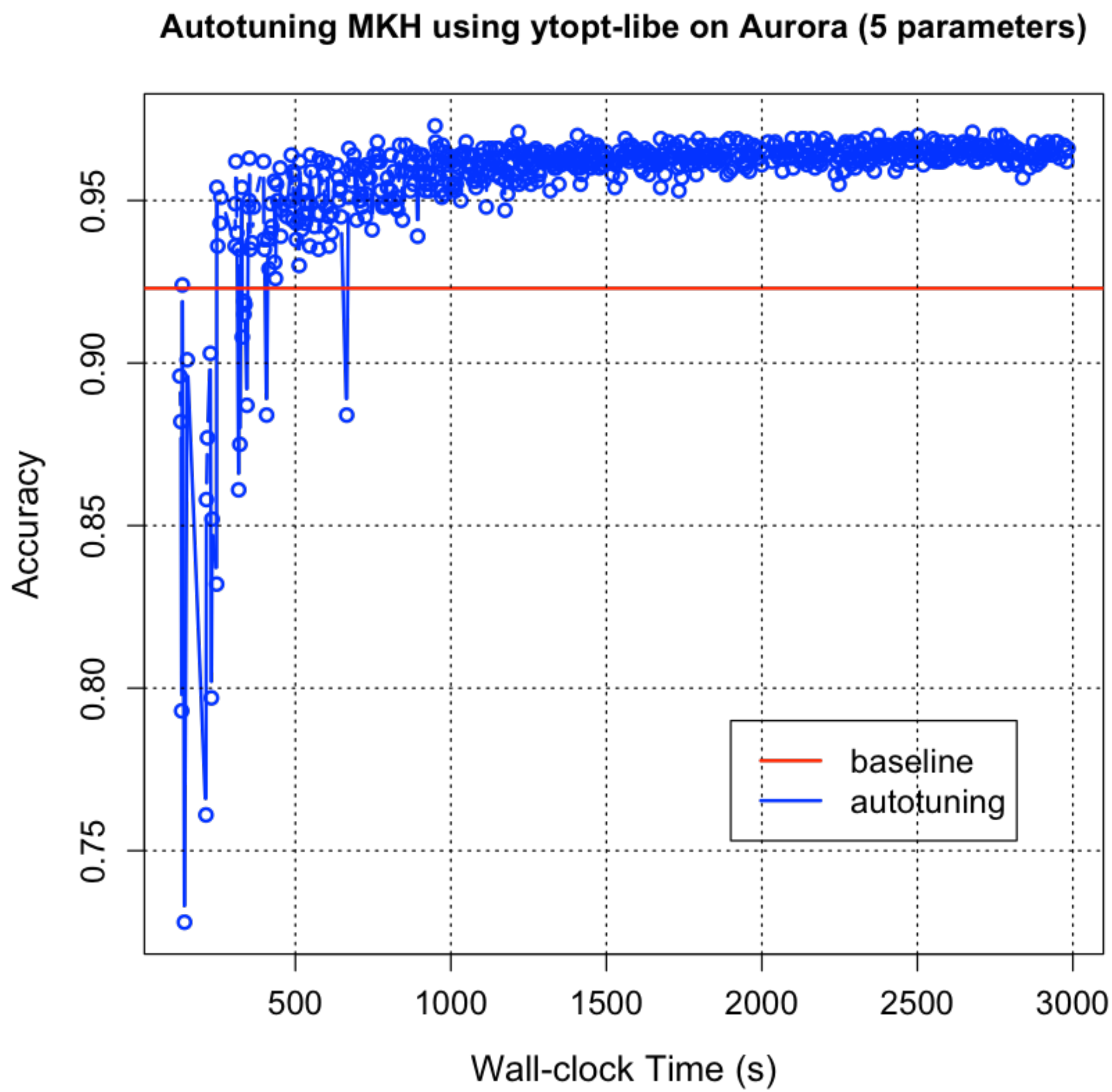
Accuracy: 97%

Autotuning the MKH Application with 5 parameters with C=[0.37, 10] and coef0=[-1, 1] on 16 nodes



Accuracy: 97.3%

Autotuning the MKH Application with 5 parameters with C=[0.37, 10] and coef0=[-1, 1] on 32 nodes



Accuracy: 97.3%

Summary

- We proposed the autotuning-based HPO framework for the mixed-kernel SVM applications in science and engineering on Aurora

- Our experimental results on Aurora show that
  - the optimal selection of hyperparameters in SVMs greatly varies for different applications and datasets
  - Uninformed choices of hyperparameters C and coef0 in the mixed-kernel SVMs resulted in severely low accuracy (5.2%)
  - The proposed framework achieved the highest accuracy for both mixed-kernel SVM applications.

- The implementation codes for both applications are available on our GitHub repo (https://github.com/ytopt-team/ytopt/tree/main/ytopt-libe/svms)

- Futher work: LLM-based HPO (Can AI replace our tools?)

Acknowledgements

This work was supported in part by

– DoE ASCR Microelectronics projects Threadwork and BIA

– DoE ASCR SciDAC RAPIDS3