

# A BRIEF REVIEW OF HYPERPARAMETER OPTIMIZATION METHODS FOR MACHINE LEARNING

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by Dr. Cherie Ding.

# OUTLINE

1. Introduction
2. Methods
3. Results
4. Discussion
5. Conclusion
6. References

# INTRODUCTION

# MACHINE LEARNING

- Learn from data
- Accuracies > 99% possible
- Real-world applications

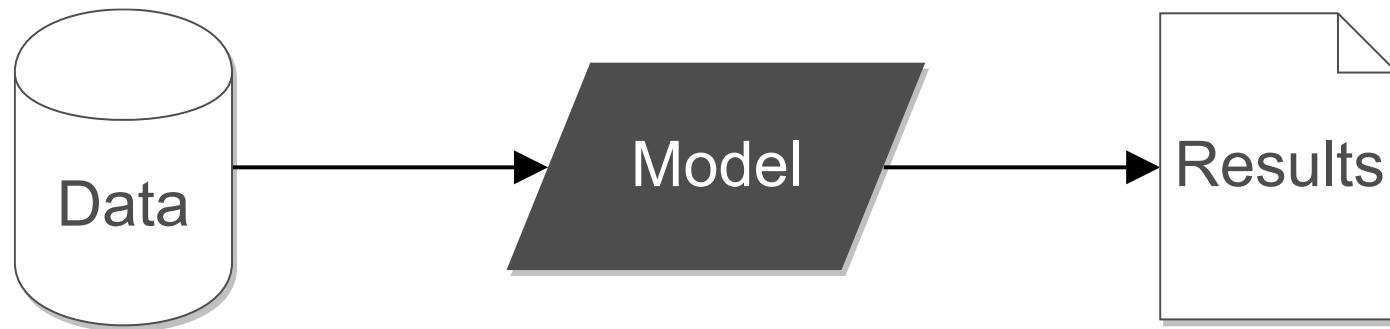


# MEDICAL IMAGE DIAGNOSES

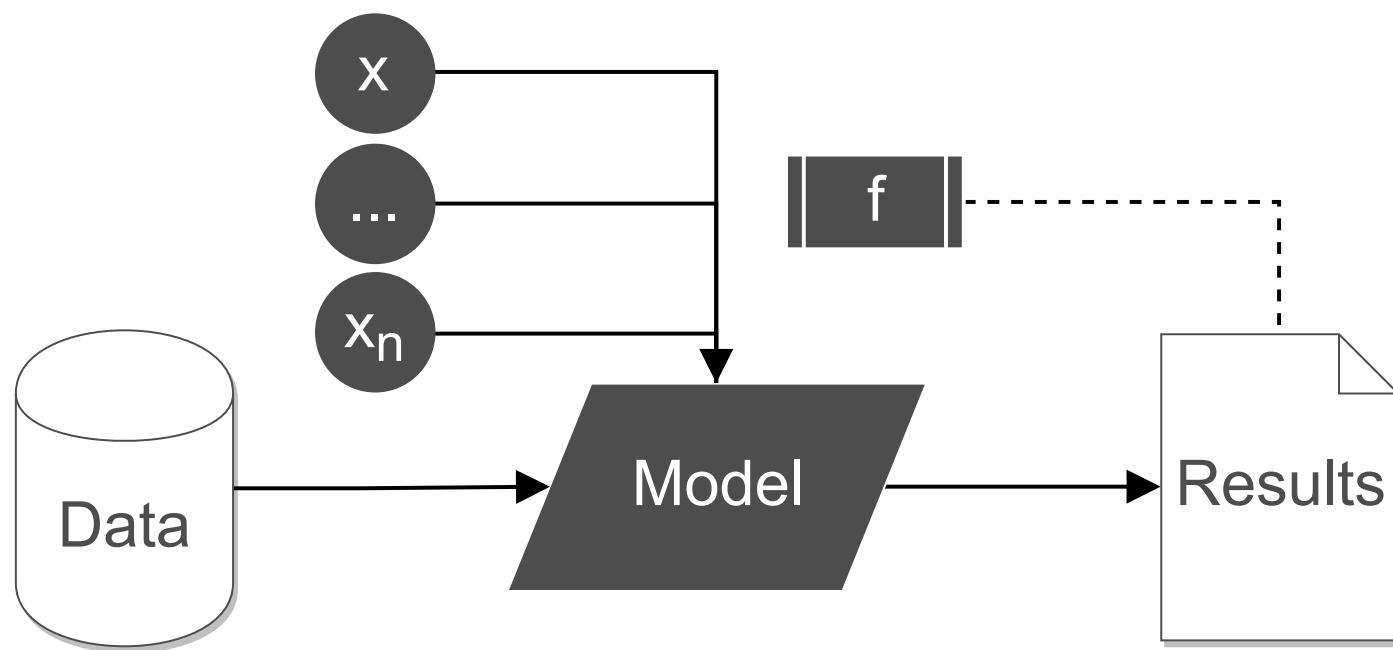
Hurricane Harvey Flooding  
Simonton, Texas  
November 20, 2016 (Left)  
August 30, 2017 (Right)



# MACHINE LEARNING PROCESS



# MACHINE LEARNING MODEL



# HYPERPARAMETERS

- Adjustable values
- Affect learning performance
- Before learning process

# HYPERPARAMETER OPTIMIZATION

- Adjustable values  $x \dots x_n$
- Affect performance measure  $f$
- Find optimal  $x \dots x_n$

$$\operatorname{argmax}_{x \dots x_n} f(x \dots x_n)$$

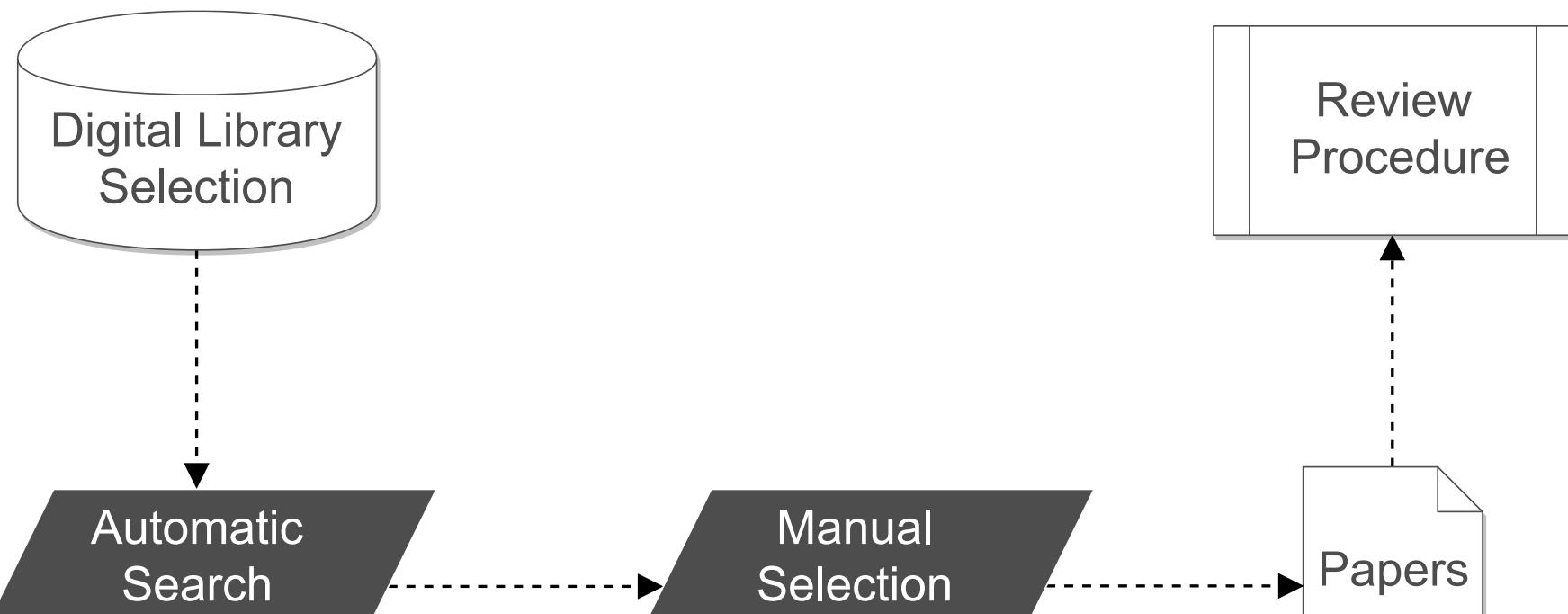
## OBJECTIVES

For hyperparameter optimization:

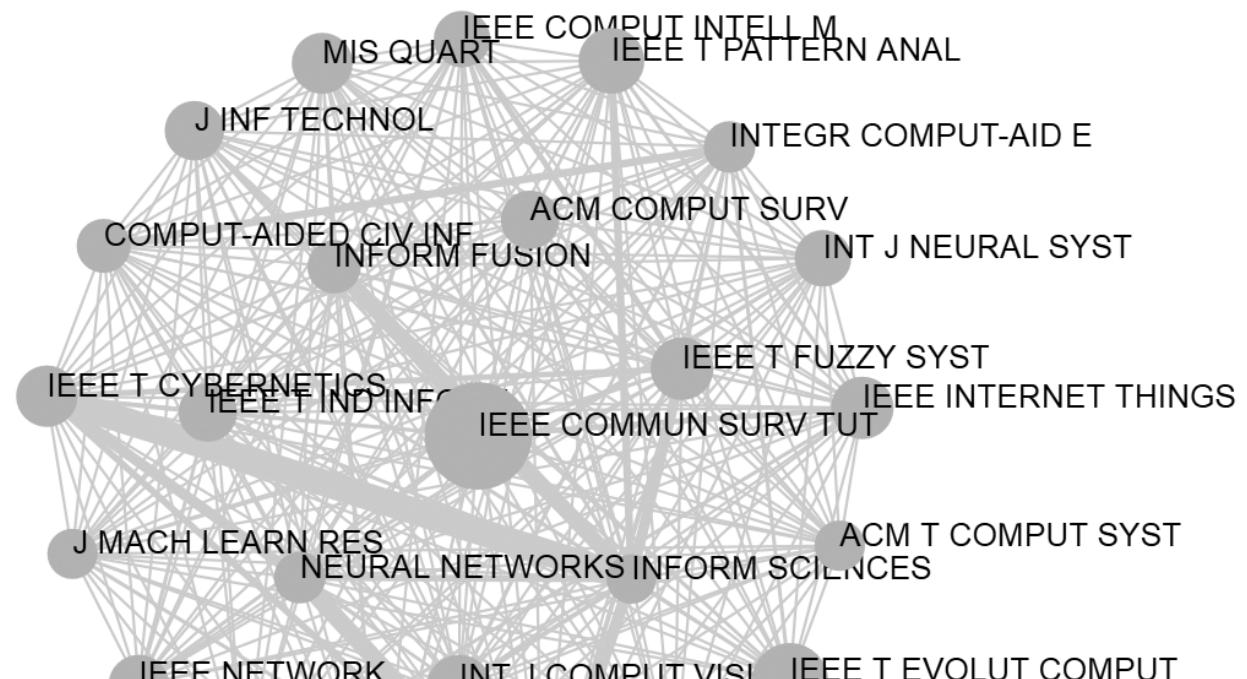
1. Summarize recent methods
2. Discuss limitations
3. Propose improvements and future directions

# METHODS

# METHODS PROCESS



# DIGITAL LIBRARY SELECTION



## AUTOMATIC SEARCH QUERIES

| Query          | Value                        |
|----------------|------------------------------|
| Publication    | IEEE or ACM                  |
| Year           | 2014 to October 5, 2017      |
| Title contains | hyperparameter, optimization |

## MANUAL SELECTION CRITERIA

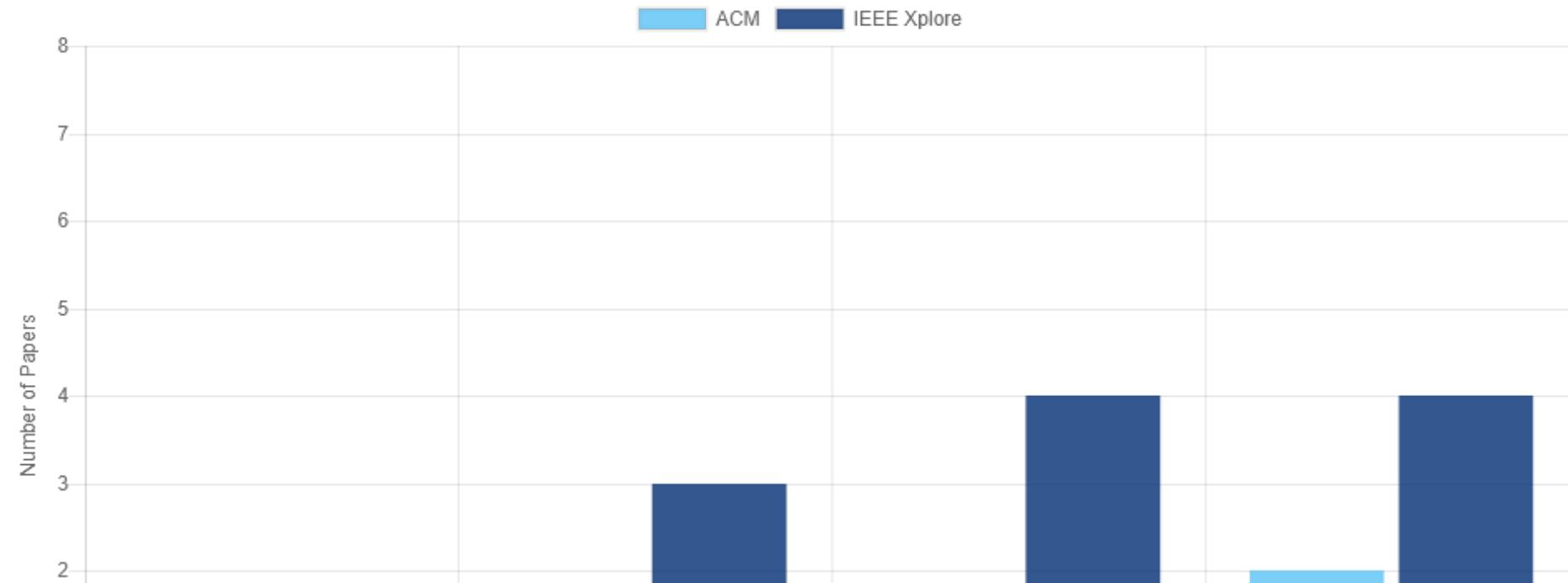
| Criteria  | Description                                  |
|-----------|--|
| Detailed  | specific methods and results, $\geq 8$ pages |
| Relevant  | mention hyperparameter optimization          |
| Practical | experiments, benchmarks, applications        |

## REVIEW PROCEDURE

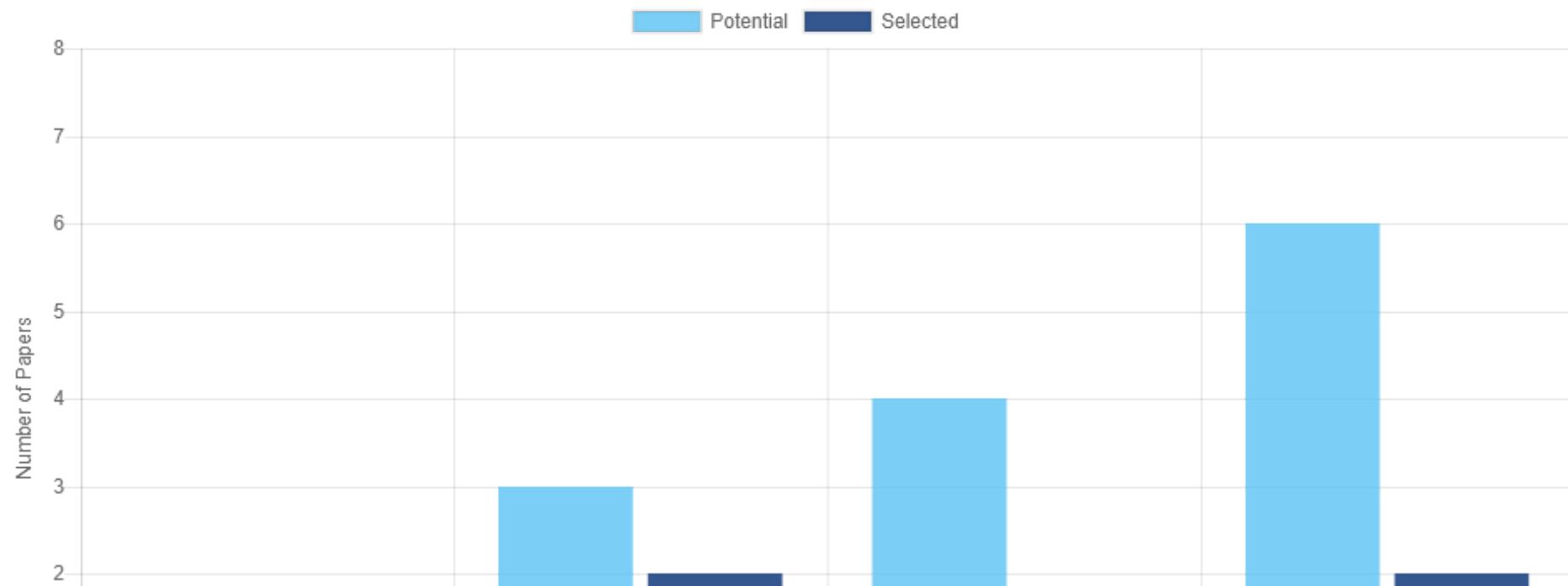
1. Identify methods
2. Summarize methods
3. Summarize experiments and results
4. Discuss limitations, improvements, directions

# RESULTS

# POTENTIAL PAPERS



# SELECTED PAPERS



## HYPERPARAMETER OPTIMIZATION METHODS

1. Simple: **Exhaustive search**
2. Advanced: Model or procedural based search

## SIMPLE METHODS

| Method        | Description                |
|---------------|----------------------------|
| Manual Search | Trial and error            |
| Grid Search   | Predefined range of values |
| Random Search | Randomized range of values |

Ref: [6]

## MANUAL SEARCH

| Hyperparameter | Values |
|----------------|--------|
|----------------|--------|

|       |   |
|-------|---|
| $x_1$ | 5 |
|-------|---|

|       |    |
|-------|----|
| $x_2$ | 10 |
|-------|----|

|       |    |
|-------|----|
| $x_3$ | 15 |
|-------|----|

## GRID SEARCH

| Hyperparameter | Values |
|----------------|--------|
|----------------|--------|

|       |           |
|-------|-----------|
| $x_1$ | 5, 10, 15 |
|-------|-----------|

|       |         |
|-------|---------|
| $x_2$ | 3, 6, 9 |
|-------|---------|

|       |         |
|-------|---------|
| $x_3$ | 2, 4, 6 |
|-------|---------|

## RANDOM SEARCH

### Hyperparameter    Values

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|       |              |
|-------|--------------|
| $x_1$ | 6, 10, 8, 12 |
|-------|--------------|

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|       |          |
|-------|----------|
| $x_2$ | 9, 17, 1 |
|-------|----------|

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|       |       |
|-------|-------|
| $x_3$ | 21, 5 |
|-------|-------|

## ADVANCED METHODS

| Method           | Description                             |
|------------------|---|
| Assumption       | Expert assumptions for particular cases |
| Evolutionary     | Procedurally generated hyperparameters  |
| Sequential Model | Sequentially guided hyperparameters     |

## ASSUMPTION BASED OPTIMIZATION

- Specific algorithms, data, and cases
- Select  $x \dots x_n$  based on assumptions
- e.g. Distribution assumptions

Ref: [1]

## EVOLUTIONARY BASED OPTIMIZATION

- Mimic biological evolution
- Evolve and naturally select  $x \dots x_n$
- e.g. Genetic algorithms, particle swarm

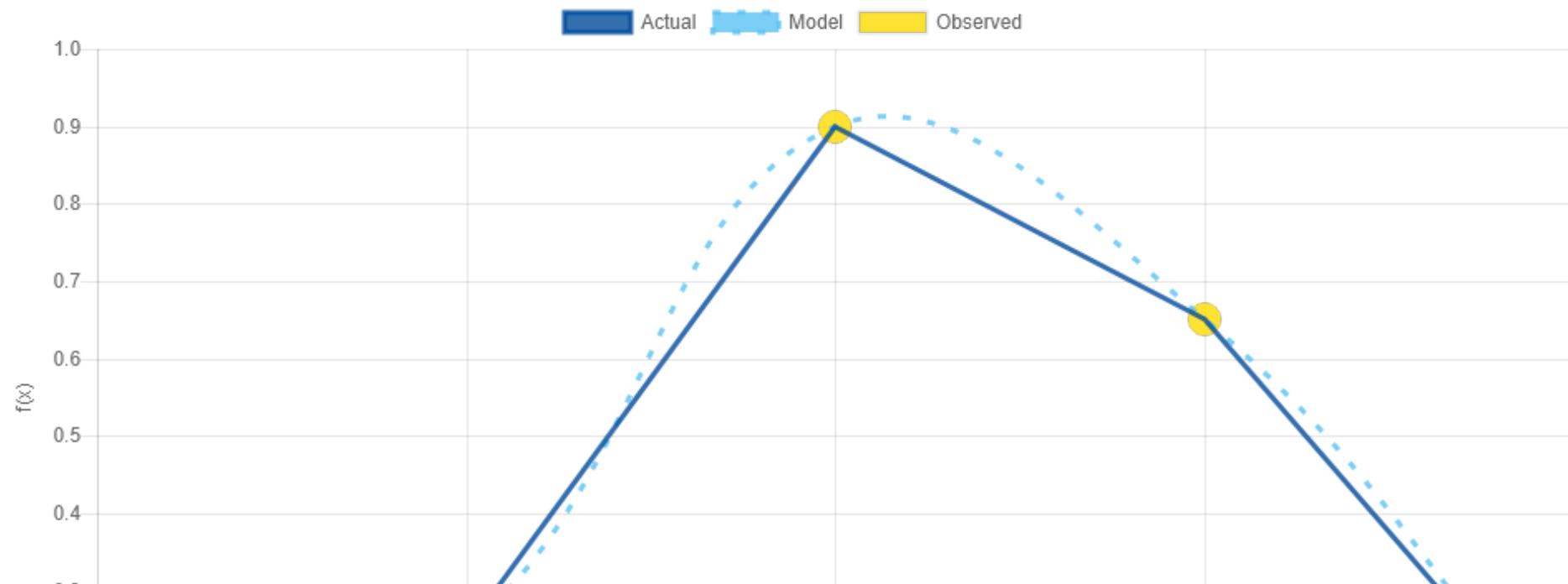
Ref: [7]

## SEQUENTIAL MODEL BASED OPTIMIZATION (SMBO)

- Model performance function  $f$  using  $x \dots x_n$
- Predict next best set of hyperparameters
- e.g. Bayesian optimization

Ref: [8-10]

# SMBO EXAMPLE



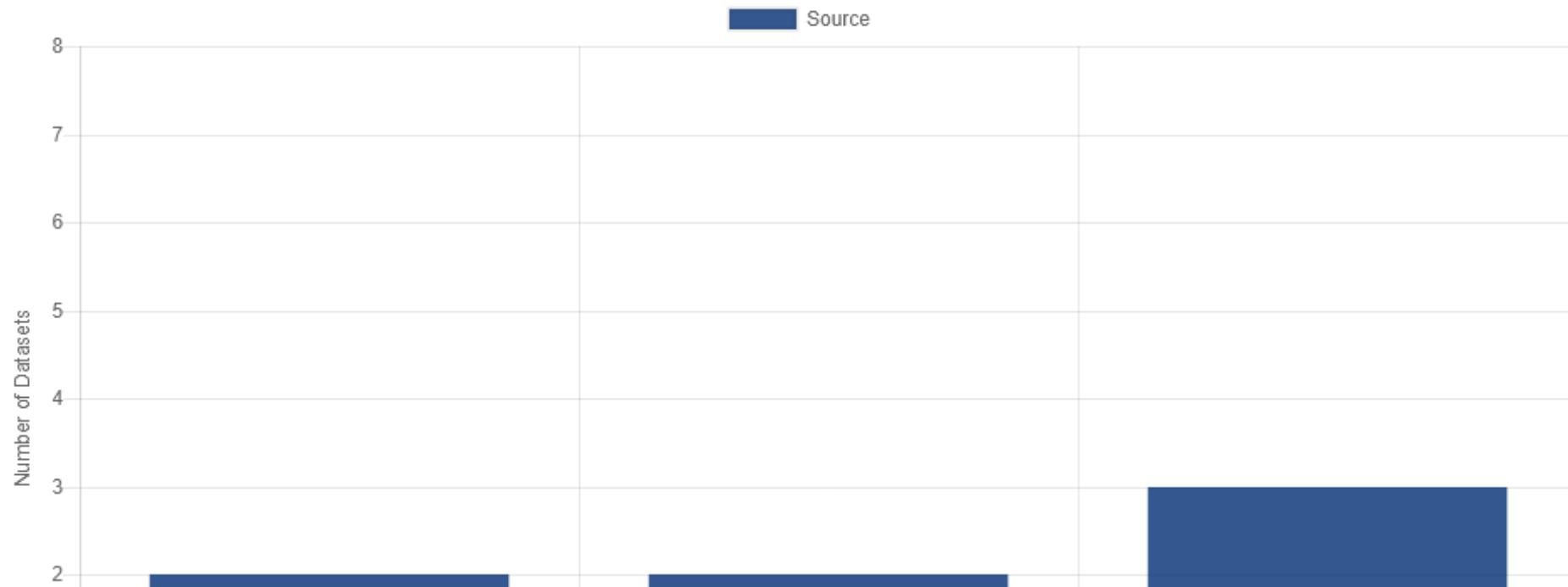
## SMBO IMPROVEMENTS

- Transfer learned hyperparameters [1]
- Discover better starting hyperparameters [2]
- Measure transfer hyperparameters influence [3]
- Consider hyperparameter inter-dependency [4]

## SMBO EXPERIMENTS

- Improved performance (e.g. ~10-20%)
- Better hyperparameters than simple methods
- Same time and iteration constraints

# SMBO DATA



# DISCUSSION

## LIMITATIONS

- Manual constraints selection
- Scalability
- Dataset variability

## MANUAL CONSTRAINTS

- Hyperparameters  $x \dots x_n$
- Performance measure  $f$
- Set of constraints  $C$
- Iteration or steps  $t$

$$\operatorname{argmax}_{x \dots x_n \in C} f(x \dots x_n) \text{ given } t$$

## IMPROVEMENTS AND FUTURE DIRECTIONS

- Automated Machine Learning
- Combining methods
- Sampling

# CONCLUSION

- Reviewed 5 papers
- **SMBO** as an effective framework
- Constraints and scalability
- *Automated Machine Learning*

# REFERENCES

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- [7] D. Whitley, S. Rana, J. Dzubera, and K. E. Mathias, “Evaluating evolutionary algorithms,” *Artificial intelligence*, vol. 85, no. 1, pp. 245– 276, 1996.
- [8] J. Snoek, H. Larochelle, and R. P. Adams, “Practical bayesian optimization of machine learning algorithms,” in *Advances in neural information processing systems*. 2012, pp. 2951–

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- [10] D. R. Jones, M. Schonlau, and W. J. Welch, “Efficient global optimization of expensive black-box functions.” Journal of Global optimization, vol

# THANK YOU

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[github.com/rrwen/slides-rmcs-litreview](https://github.com/rrwen/slides-rmcs-litreview)