From Tuning to Guarantees: Statistically Valid Hyperparameter Selection

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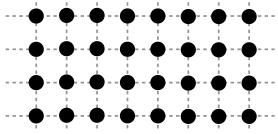


 Hyperparameter selection is a key step in the deployment of pre-trained AI models.

• Examples:

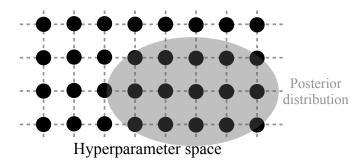
- inference parameters, such as test-time resources, prompt templates, temperature, or decision thresholds
- implementation parameters, such as arithmetic precision

- Traditional approaches are of best effort nature, targeting empirical performance.
 - No formal statistical guarantees
- Examples: Grid search [Bergstra and Bengio, 2012]

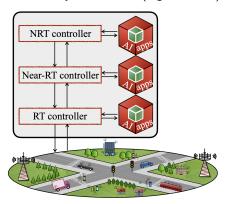


Hyperparameter space

- Traditional approaches are of best effort nature, targeting empirical performance:
 - No formal statistical guarantees
- Examples: Bayesian optimization [Snoek, Larochelle, and Adams, 2012]



- The deployment of AI in sensitive domains such as healthcare [Dzau et al., 2023] and engineering [Simeone, Park, and Zecchin, 2025] requires rigorous statistical guarantees.
- Example: Al-native wireless systems in 6G (e.g., O-RAN)



- Reliability requirements are application specific, e.g., probability of error, latency, fairness, ...
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- Reliability requirements are application specific, e.g., probability of error, latency, fairness, ...
- Hyperparameter λ is said to be **reliable** if the AI model meets the reliability requirement when run with hyperparameter λ .
- Statistical validity in hyperparameter selection:

$$\Pr[\lambda \text{ is not reliable}] \leq \delta,$$

for a user-specified $0 < \delta < 1$ (Pr[·] is over data used for selection).



Discussion & Reflection

How should we think about reliability in practice?

Consider an application you care about (e.g., LLM prompting, RL policies, model selection, or wireless systems), and reflect on:

- What does it mean for a hyperparameter to be reliable? (e.g., stable accuracy, low risk under distribution shift, robustness across seeds)
- Which failures actually matter? (e.g., performance drops, fairness violations, safety constraints)
- What evidence would convince you that a hyperparameter is safe to deploy?
- How would you formalize these notions statistically?

We will revisit these questions as we connect reliability to FDR, risk control, and hypothesis testing.

Learn-Then-Test (LTT)
 [Angelopoulos, Bates, Candès, et al., 2021] formalizes statistically valid hyperparameter selection via multiple hypothesis testing (MHT).

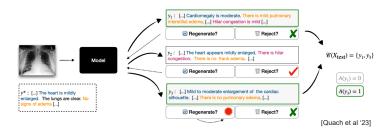






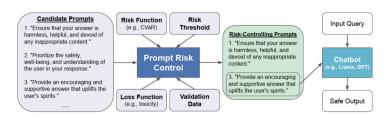
Learn-Then-Test: Some Applications

 Calibrating thresholds for test-time scaling (generation of multiple answers) in LLMs [Quach et al., 2023]



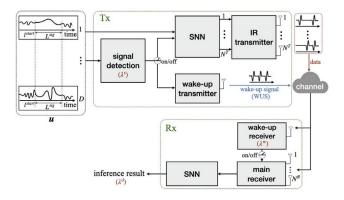
Learn-Then-Test: Some Applications

- Recommendation systems (learning to rank) [Angelopoulos, Krauth, et al., 2023]
- Information retrieval [Xu et al., 2024]
- Prompt template selection for LLMs [Zollo et al., 2023]



Learn-Then-Test: Some Applications

- Telecommunication systems [Simeone, Park, and Zecchin, 2025]
- Neuromorphic computing [Jiechen Chen et al., 2024]

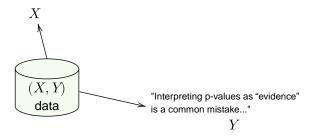


Overview

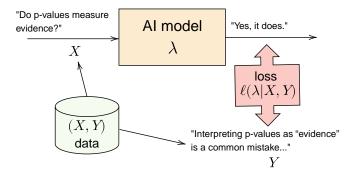
- Learn-Then-Test
- Generalizing Learn-Then-Test:
 - Beyond the Average Risk
 - Adaptive Hyperparameter Selection
 - Incorporating Prior Information
 - Selection with Autoevaluation
- Conclusions

• Data (X, Y) with X = input and Y = output

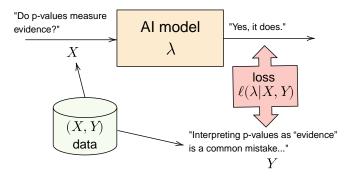
"Do p-values measure evidence?"



• $\ell(\lambda|X,Y) = \textbf{loss}$ at data point (X,Y) under hyperparameter λ (e.g., 0-1 loss)



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• $R(\lambda) = \mathbb{E}_{(X,Y)}[\ell(\lambda|X,Y)] = \text{average risk (e.g., probability of error)}$

Examples of Losses in Different Applications

Reliability depends on how we measure failure. Different applications call for different choices of loss $\ell(\lambda \mid X, Y)$:

- Classification / LLM prompting 0–1 loss, misclassification rate, token-level error, or a scoring loss (e.g., NLL/perplexity).
- **Regression / Forecasting** Squared error $(Y \hat{Y})^2$, absolute error $|Y \hat{Y}|$, pinball loss for quantiles.
- Structured Prediction / Detection mAP drop, IoU-based penalties, object-miss penalties, calibration errors (ECE/MCE).
- Reinforcement Learning / Control Negative return, constraint violation counts, regret, safety-critical failure events.
- LLM-based agents / LLM judging Preference loss, pairwise defeat probability (Bradley-Terry), task-success or factuality loss.
- Wireless / Telecom Scheduling Throughput deficit, latency violation, outage probability, or risk of violating QoS thresholds.

Once the loss is fixed, reliability means keeping its expected value $R(\lambda)$ acceptably low.

• Reliability condition:

$$\lambda$$
 is reliable $\Leftrightarrow R(\lambda) \leq \alpha$,

where α is a user-specified threshold

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Parameter	Significance
α	Reliability requirement: $R(\lambda) \le \alpha$
δ	Maximum allowed failure rate for the hyperparameter selection strategy

Conventional Hyperparameter Selection

• Given some **held-out data** $\mathcal{D} = \{(X, Y)\}$, conventional methods directly optimize standard **empirical risk estimates**

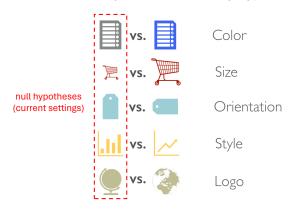
$$\hat{R}(\lambda|\mathcal{D}) = \frac{1}{|\mathcal{D}|} \sum_{(X,Y) \in \mathcal{D}} \ell(\lambda|X,Y)$$

over hyperparameter λ .

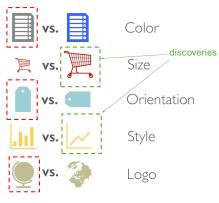
Statistical validity not guaranteed.

- LTT provides reliability guarantees by framing hyperparameter selection as **multiple hypothesis testing** (MHT).
- MHT underlies scientific discovery, A/B testing, ...

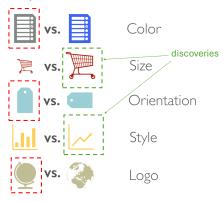
- LTT provides reliability guarantees by framing hyperparameter selection as **multiple hypothesis testing** (MHT).
- MHT underlies scientific discovery, A/B testing, ...
- MHT considers simultaneously a number of binary hypotheses.



- Each hypothesis is tested by collecting data (e.g., click-through rates)...
- ... producing a decision for the null hypothesis or for the alternative hypothesis (discovery).



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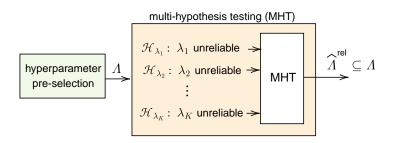
 Goal: Control error rate metrics such as the family-wise error rate (FWER):

 $Pr[any false discovery] \leq \delta$

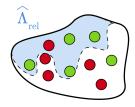
• ① Determine a set Λ of **candidate hyperparameters** using any methodology, such as grid search [Bergstra and Bengio, 2012] or Bayesian optimization [Snoek, Larochelle, and Adams, 2012].

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- ② Apply MHT for hyperparameter selection within set Λ:
 - Test a **null hypothesis** for each candidate hyperparameter λ :

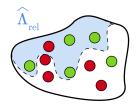
$$\mathcal{H}_{\lambda}$$
: λ is unreliable, i.e., $R(\lambda) > \alpha$



- igcup reliable hyperparams Λ^{rel}
- lacksquare unreliable hyperparams Λ^{unrel}



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 m rel}$
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- By using MHT, the subset $\hat{\Lambda}^{rel}$ of selected hyperparameters satisfies **error** rate control guarantees.
- Notably, the family-wise error rate (FWER) guarantee coincides with the statistical validity condition

 $\Pr[R(\lambda) > \alpha \text{ for a selected } \lambda] \leq \delta.$

 Given some held-out data D = {(X, Y)}, evaluate standard empirical risk estimates

$$\hat{R}(\lambda|\mathcal{D}) = \frac{1}{|\mathcal{D}|} \sum_{(X,Y)\in\mathcal{D}} \ell(\lambda|X,Y)$$

for every $\lambda \in \Lambda$.

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• A larger value of the **estimated reliability** margin $(\alpha - \hat{R}(\lambda|\mathcal{D}))^+$ provides more evidence that λ is reliable.

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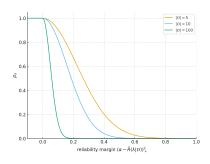
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- Thus, a statistic of the form

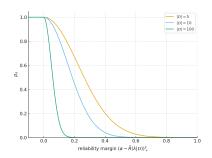
$$p_{\lambda} = e^{-2|\mathcal{D}|(\alpha - \hat{R}(\lambda|\mathcal{D}))_{+}^{2}}.$$

will tend to be small when λ is reliable.

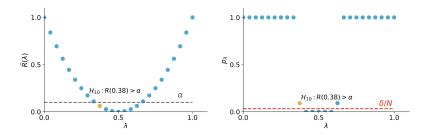


- If the loss is bounded within [0,1], the statistic p_{λ} is a **p-value** for the null hypothesis \mathcal{H}_{λ} .
- A small p-value p_{λ} indicates evidence that the hyperparameter λ is reliable:

$$\Pr[p_{\lambda} \leq \delta \mid \lambda \text{ is unreliable}] \leq \delta,$$
 for $0 < \delta < 1.$



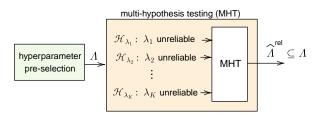
Why Empirical Risk Alone Is Not Reliable



- ullet Empirical risk $\hat{R}(\lambda)$ can underestimate the true risk due to finite-sample noise.
- This may cause an **unreliable** hyperparameter to falsely appear safe.
- LTT converts these empirical risk gaps into valid p-values, ensuring unreliable hyperparameters cannot "slip through" by chance.

Figure reproduced from Angelopoulos, Bates, Candès, et al., 2021.

• We have a set of p-values p_{λ} , one for each hyperparameter $\lambda \in \Lambda$.



- Examples of FWER-controlling MHT procedures:
 - Bonferroni correction

$$\lambda \in \hat{\Lambda}^{\mathsf{rel}}$$
 if $p_{\lambda} \leq rac{\delta}{|\Lambda|}$

Fixed sequence testing

Error Rates in Multiple Hypothesis Testing

- When testing many hypotheses simultaneously (e.g., many hyperparameters), different types of errors can occur.
- Two common error metrics:
 - FWER (Family-Wise Error Rate): Probability of making at least one false discovery.
 - FDR (False Discovery Rate): Expected proportion of false discoveries among all discoveries.
- These metrics control different risks, and are used for different applications.

Family-Wise Error Rate (FWER)

• In hyperparameter selection, a "false discovery" means:

Selecting a hyperparameter λ that is actually unreliable.

• **FWER** measures the probability of making *any* such mistake:

$$\mathsf{FWER} = \mathsf{Pr} \left(\exists \lambda \in \hat{\Lambda}^{\mathrm{rel}} : R(\lambda) > \alpha \right).$$

• Goal of LTT: Ensure

$$\mathsf{FWER} \leq \delta,$$

which exactly matches the notion of statistical validity in hyperparameter selection.

• Very conservative: tries to avoid even a single unreliable choice.

False Discovery Rate (FDR)

- In set-valued prediction problems (e.g., multi-label classification), we may output several items at once.
- FDR measures the *expected proportion* of incorrect predictions:

$$\mathsf{FDR}(T) = \mathbb{E}\left[\frac{\#\{\mathsf{false \ predictions}\}\}}{\mathsf{max}\{1,\#\{\mathsf{predictions}\}\}}\right].$$

- Unlike FWER, FDR does not penalize a single mistake heavily.
- FDR is appropriate when:
 - We produce many items at once (e.g., a set of labels),
 - and we care about the average purity of the set.
- Examples of notable FDR-controlling procedures:
 - Benjamini-Hochberg (BH) procedure [Benjamini and Hochberg, 1995]
 - Benjamini-Yekutieli (BY) [Benjamini and Yekutieli, 2001]

Example 1: Multi-Label Classification with FDR Control

- Task: multi-label classification on MS COCO.
 - Each image X has a set of labels $Y \subseteq \{1, ..., K\}$.
 - Base model $\hat{f}(x) \in [0,1]^K$ outputs class-wise probabilities.
- We predict a set of labels

$$T_{\lambda}(x) = \{z \in \{1, \dots, K\} : \hat{f}_{z}(x) \ge \lambda\}$$

and we want to control the **false discovery rate** (FDR) of wrong labels in $T_{\lambda}(X)$.

• LTT chooses λ so that FDR is controlled at level (α, δ) .

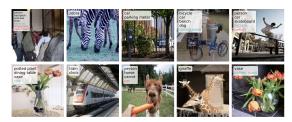
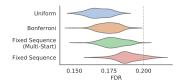


Figure reproduced from Angelopoulos, Bates, Candès, et al., 2021.

Example 1: Multi-Label Classification with FDR Control

- Dataset: MS COCO, n = 4000 calibration points, 1000 validation points.
- Candidate thresholds: $\Lambda = \{0, 0.001, \dots, 1\}$.
- LTT compares different MHT procedures:
 - Uniform (no multiple testing correction)
 - Bonferroni
 - Fixed-sequence testing
 - Fixed-sequence testing with multiple starting points
- Goal: control FDR at level $\alpha = 0.2$ with failure probability $\delta = 0.1$.



Method	50%	75%	90%	99%	99.9%
Uniform	3	4	6	11	13
Bonferroni	3	4	7	11	14
Fixed Sequence (Multi-Start)	3	4	7	11	14
Fixed Sequence	3	5	7	12	14

Figure reproduced from Angelopoulos, Bates, Candès, et al., 2021.

Try LTT Yourself!

Interactive LTT Notebook & Code

The following GitHub repo contains a simple, self-contained implementation of Learn-Then-Test (LTT) that you can run immediately on Colab or locally.



https://github.com/amirfar76/neurips25-valid-hparam-tutorial

Generalizing Learn-Then-Test: Beyond the Average Risk

Beyond the Average Risk

- LTT controls the average risk $R(\lambda) = \mathbb{E}_{(X,Y)}[\ell(\lambda|X,Y)]$.
- In some applications, it may be preferable to control:
 - a quantile of the loss $\ell(\lambda|X,Y)$: quantile risk
 - functionals of the data distribution: information-theoretic measures

Controlling the Quantile Risk: Example

• Wireless scheduling problem:

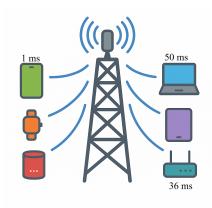


 Reliability requirement using the average risk: Ensure that the average user delay is less than 10 ms

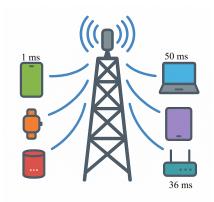
$$R(\lambda) \le \alpha = 10 \text{ ms}$$

with a probability no smaller than 90% ($\delta=0.1$)

Controlling the Quantile Risk: Example



Controlling the Quantile Risk: Example



- Reliability requirement using the quantile risk:
 - \bullet At least 90% of the users must have a delay smaller than 10 ms

$$R_q(\lambda) \leq \alpha = 10 \text{ ms}$$

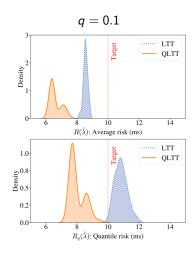
with q = 0.1

Quantile Learn-Then-Test

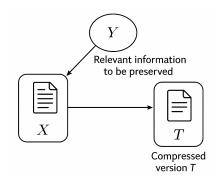
- Quantile LTT (QLTT) [Farzaneh, Park, and Simeone, 2024] extends LTT to control the quantile risk.
- Invert a confidence interval on the desired quantile to obtain a p-value.

Quantile Learn-Then-Test

- Quantile LTT (QLTT) [Farzaneh, Park, and Simeone, 2024] extends LTT to control the quantile risk.
- Invert a confidence interval on the desired quantile to obtain a p-value.



- X = input
- Y = target variable
- $(X, Y) \sim P_{XY}$, with P_{XY} unknown
- Goal: Extract a compressed representation T ~ P_{T|X} of X that is sufficiently relevant for predicting Y.



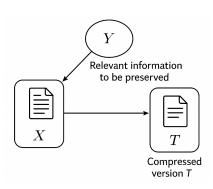
• Mutual information:

$$I(A; B) = \mathbb{E}_{P_{AB}} \left[\log_2 \left(\frac{P_{AB}}{P_A \cdot P_B} \right) \right]$$

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 Information Bottleneck (IB) problem [Tishby, Pereira, and Bialek, 2001; Zaidi, Estella-Aguerri, and Shamai, 2020]:



• Given data $\mathcal{D} = \{(X, Y)\} \underset{\text{i.i.d.}}{\sim} P_{XY}$, one can produce the estimates $\hat{I}(X; T)$ and $\hat{I}(T; Y)$.

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- Introduce a Lagrange multiplier $\lambda > 0$ to tackle the unconstrained problem [Alemi et al., 2017]

$$\underset{P_{T|X}}{\mathsf{minimize}} \quad \underbrace{\hat{J}(X;T)}_{\mathsf{size}} - \lambda \underbrace{\hat{J}(T;Y)}_{\mathsf{relevance}}.$$

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• Reliability requirement: Select the hyperparameter λ to guarantee the relevance constraint

$$I(T; Y) \ge \alpha$$

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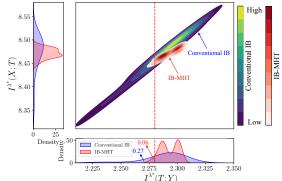
• Since the joint distribution P_{XY} is not known, one can only ensure the **probabilistic relevance constraint**:

$$\Pr\left[I(T;Y)<\alpha\right]\leq\delta$$

where δ is a user defined probability

• **IB-MHT** [Farzaneh and Simeone, 2024] inverts a confidence interval on the mutual information to obtain p-values for each candidate Lagrange multiplier, allowing the use of LTT.

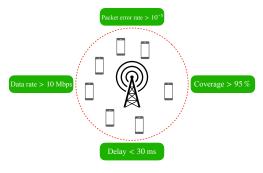
- **IB-MHT** [Farzaneh and Simeone, 2024] inverts a confidence interval on the mutual information to obtain p-values for each candidate Lagrange multiplier, allowing the use of LTT.
- Image processing example: Joint distributions of the mutual informations I(T;Y) and I(X;T) obtained by using a conventional IB solver [Alemi et al., 2017] and IB-MHT ($\delta=0.1$)



Generalizing Learn-Then-Test: Multi-Objective Optimization

Multi-Objective Optimization

- LTT only controls a single risk function $R(\lambda)$.
- In some applications, there are multiple risk functions to be controlled.

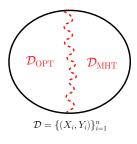


$$\min_{\lambda \in \Lambda} \{R_{L_c+1}(\lambda), R_{L_c+2}(\lambda), \dots, R_L(\lambda)\}$$

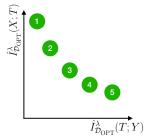
subject to $R_I(\lambda) < \alpha_I$ for all $1 \le I \le L_c$,

Pareto Testing

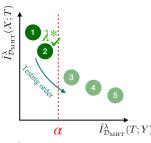
• To address this, Pareto testing (PT) [Laufer-Goldshtein et al., 2023] takes the following steps.



(1) Split data set \mathcal{D}



② Estimate Pareto frontier using $\mathcal{D}_{\mathrm{OPT}}$



 $\begin{array}{c} \text{ (3) Sequential FWER-} \\ \text{ controlling MHT using} \\ \mathcal{D}_{\text{MHT}} \end{array}$

Try PT Yourself!

Interactive PT Notebook & Code

The following GitHub repo contains a simple, self-contained implementation of Pareto Testing (PT) that you can run immediately on Colab or locally.

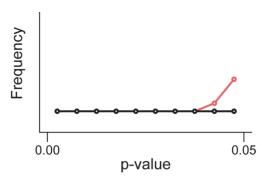


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Generalizing Learn-Then-Test: Adaptive Hyperparameter Selection

- LTT is a **batch** method operating on a **fixed data set**.
- In practice, collecting data and evaluating the loss of a model can be expensive: it may require interactions with the real world, simulations, optimizations, ...
- It is thus useful to carry out testing **sequentially**, **discarding** less performing hyperparameters and **terminating** as soon as possible.

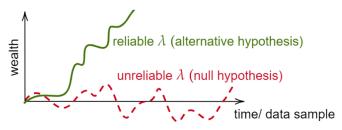
- LTT does not support adaptive hyperparameter selection:
- p-values do not allow for optional continuation: p-hacking [Head et al., 2015].



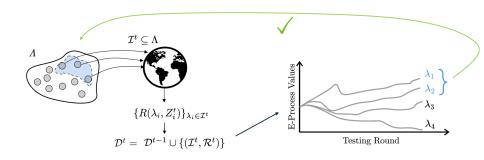
• E-values are a (nonparametric, composite) generalization of likelihood ratios [Shafer and Vovk, 2019, Ramdas and Wang, 2024], which are more robust than p-values.

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- Specifically, the sequential extension of e-values, known as e-processes, supports optional continuation (by Ville's theorem).

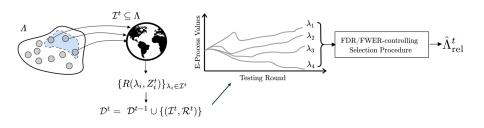
- **E-values** are a (nonparametric, composite) generalization of likelihood ratios [Shafer and Vovk, 2019, Ramdas and Wang, 2024], which are more robust than p-values.
- Specifically, the sequential extension of e-values, known as **e-processes**, supports **optional continuation** (by Ville's theorem).
- An e-process has the **game-theoretic** interpretation of accumulated wealth for a strategy **betting** on the reliability of a hyperparameter.



- Adaptive LTT (aLTT) [Zecchin, Park, and Simeone, 2024]
 - ullet Test a subset $\mathcal{I}^t \subseteq \Lambda$ of hyperparameters at each testing round t
 - ullet Update **e-process** for each hyperparameter $\lambda \in \mathcal{I}^t$
 - Stop, producing a set $\Lambda^{\rm rel}$, or continue

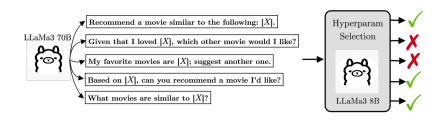


 Thanks to the anytime validity properties of e-processes, aLTT supports optional continuation and adaptive termination, while guaranteeing FWER control.

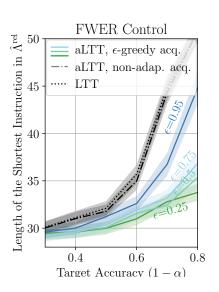


Example

- Prompt template selection from a set Λ of LLM-generated candidate prompts.
- Reliability requirement: Average error rate of the answer
- Post-selection optimization: Minimize average prompt length



Example



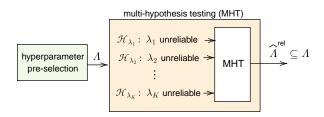
Generalizing Learn-Then-Test: Incorporating Prior Information

Incorporating Prior Information

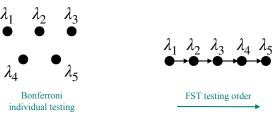
- In some applications, one may have prior information about the relative reliability level of different hyperparameters.
- Examples:
 - a higher resource utilization may imply higher accuracy
 - use LLM-as-a-judge



Incorporating Prior Information

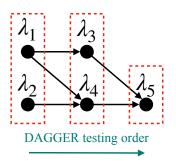


 Prior information can inform the MHT step, e.g., via fixed-sequence testing (FST):



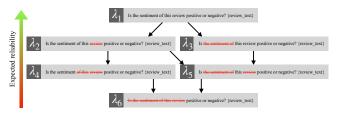
Reliability Graph-based Pareto Testing

- However, prior information possibly extracted from separate data may be much richer than a simple linear ordering.
- Reliability graph-based Pareto testing (RG-PT) [Farzaneh and Simeone, 2025] operates MHT over a directed acyclic graph (via DAGGER [Ramdas, Jianbo Chen, et al., 2019]).



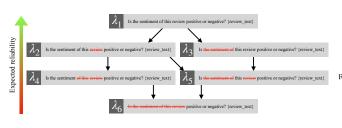
Example

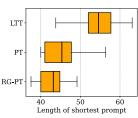
• Prompt template optimization



Example

Prompt template optimization





(Pareto testing [Laufer-Goldshtein

et al., 2023])

Generalizing Learn-Then-Test: Hyperparameter Selection with Autoevaluation

Reliable Hyperparameter Selection via Autoevaluation

- LTT requires held-out data (X, Y) to estimate the risk (and compute p-values or e-values).
- However, labels Y may be scarce.

Reliable Hyperparameter Selection via Autoevaluation

- LTT requires held-out data (X, Y) to estimate the risk (and compute p-values or e-values).
- However, labels Y may be scarce.
- **R-AutoEval** [Boyeau et al., 2024, Eyre and Madras, 2024, Schneider et al., 2024] allows for reliable hyperparameter selection via LTT by assuming:
 - limited labeled data
 - abundant unlabeled data



Reliable Hyperparameter Selection via Autoevaluation

 R-AutoEval incorporates synthetic labels through prediction-powered inference (PPI) [Angelopoulos, Bates, Fannjiang, et al., 2023]



PPI risk estimate = estimate with unlabeled data

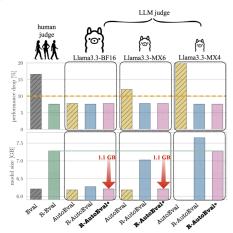
- bias correction using labeled data

R-AutoEval+

• R-AutoEval+ [Park, Zecchin, and Simeone, 2025] dynamically tunes its reliance on synthetic data, reverting to conventional methods based only on labeled data when the autoevaluator is insufficiently accurate.

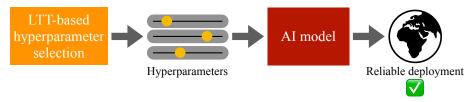
R-AutoEval+

- R-AutoEval+ [Park, Zecchin, and Simeone, 2025] dynamically tunes its
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- Post-training quantization of LLMs



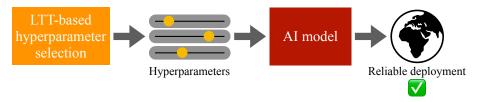
Conclusions

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- Hyperparameter selection is a key step in the deployment of pre-trained AI models.
- Multiple hypothesis testing provides a principled statistical framework to ensure statistical guarantees (Learn-Then-Test).
- This talk has reviewed several practical extensions:
 - quantile risk and information-theoretic measures
 - adaptive selection
 - prior information for structured testing
 - autoevaluation

Conclusion



- Hyperparameter selection is a key step in the deployment of pre-trained AI models.
- Multiple hypothesis testing provides a principled statistical framework to ensure statistical guarantees (Learn-Then-Test).
- This talk has reviewed several practical extensions:
 - quantile risk and information-theoretic measures
 - adaptive selection
 - prior information for structured testing
 - autoevaluation
- Future work:
 - extension to training-time hyperparameter setting (e.g., freeze-thaw)
 - large-scale deployment in engineering settings (e.g., O-RAN)

Live Q&A with Anastasios Angelopoulos

University of California, Berkeley
Author of the original Learn–Then–Test (LTT) framework

people.eecs.berkeley.edu/~angelopoulos

We will now switch to the live Zoom session.

Please feel free to ask questions about LTT, conformal prediction, multiple hypothesis testing, or broader reliability topics.

Acknowledgments

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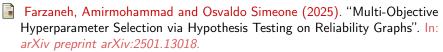


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