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Physics-Driven ML-Based Modelling for Correcting Inverse Estimation

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Paper Link: https://arxiv.org/abs/2309.13985

Science and Engineering Problem

Observation
y

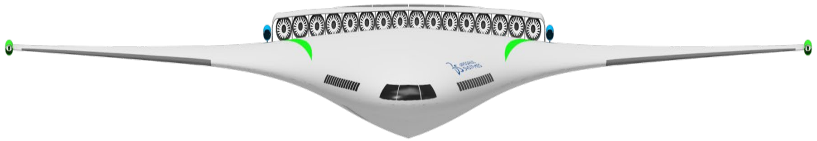
Well-posed; have a good theorem/model to simulate

Forward Problem $F(x)$

State
x

Inverse Problem $G(y)$

ill-posed; does not have mature theorem/model to sovle



ML model

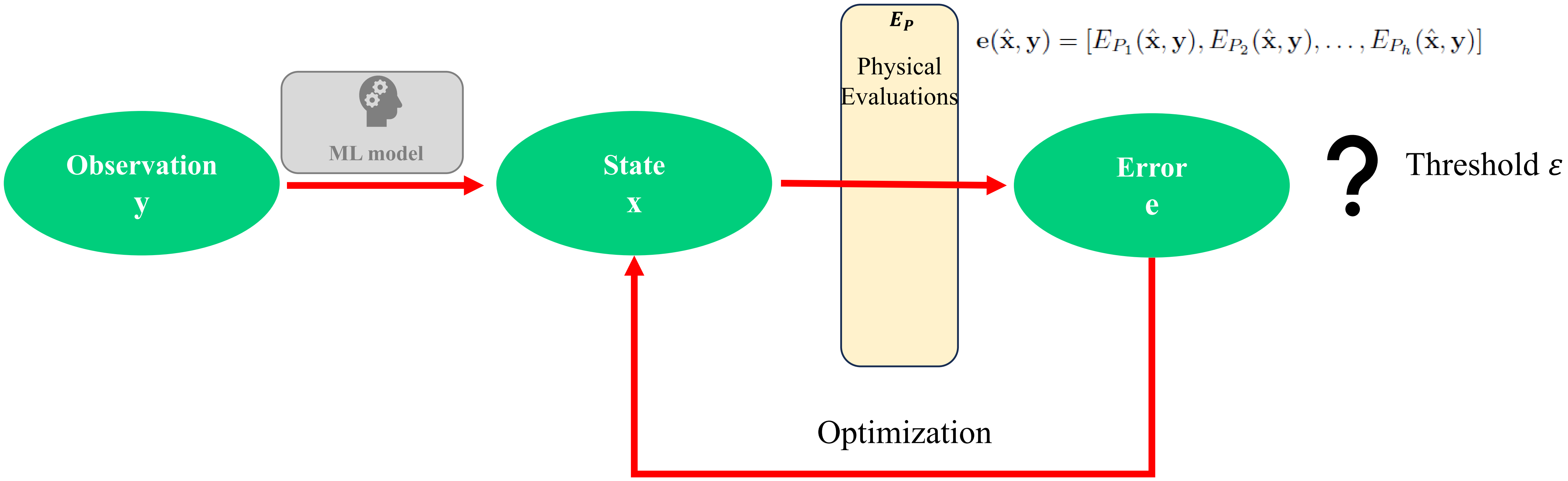
Efficient

Turbofan Engine Design parameters

Reliable?

Image credit: The Economic Times

Balance Efficiency and Reliability



$$\min_{\hat{\mathbf{x}} \in \mathcal{X}} e(\hat{\mathbf{x}}) = \sum_{i=1}^{h} w_i E_{P_i}(\hat{\mathbf{x}})$$

Optimization Problem:

1. find a feasible state $\hat{\mathbf{x}}$
2. by querying the physical evaluations as less times as possible

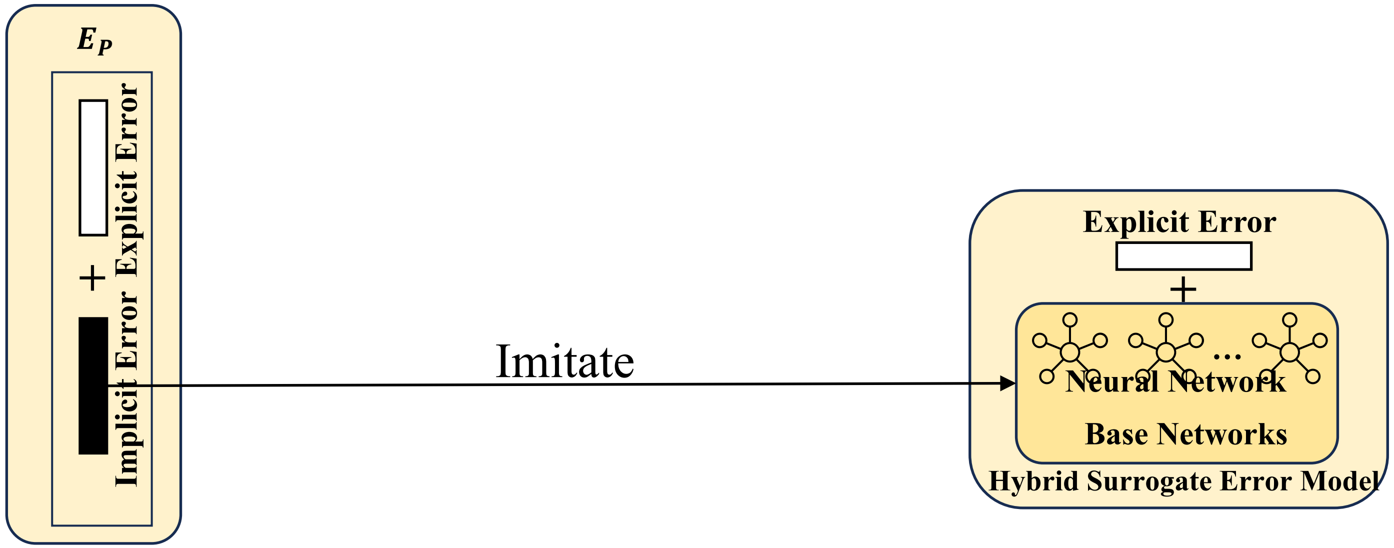
Design: Hybrid Surrogate Error Model

Cheap but accurate model of $\boldsymbol{E_P}$

De-black box:
Explicit Error: error element that is efficient to calculate and differentiable
Implicit Error: error element that is (1) time-consuming to calculate or (2) indifferentiable

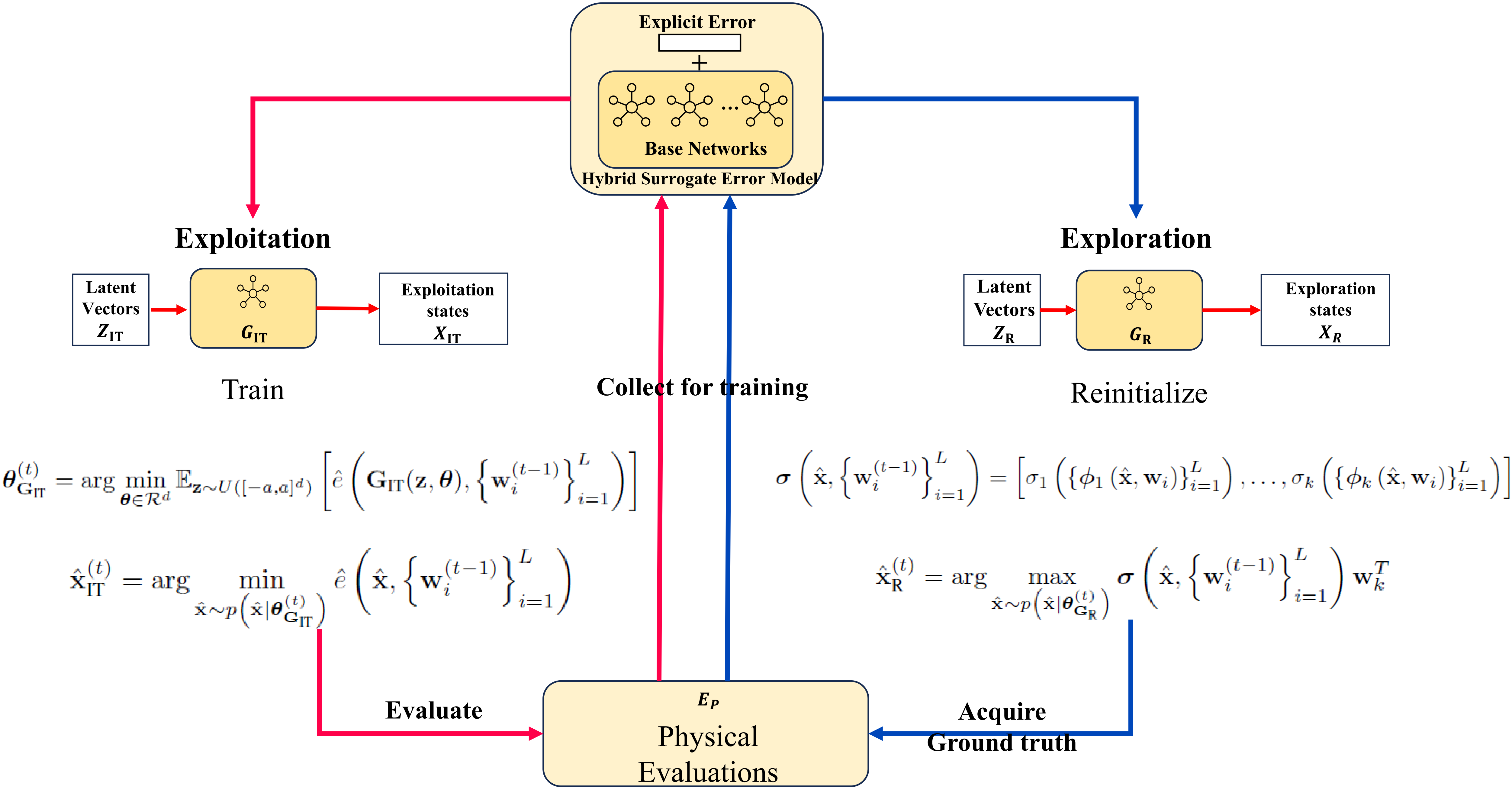
Ensemble Learning:
Reduce estimation uncertainty
increase estimation robustness

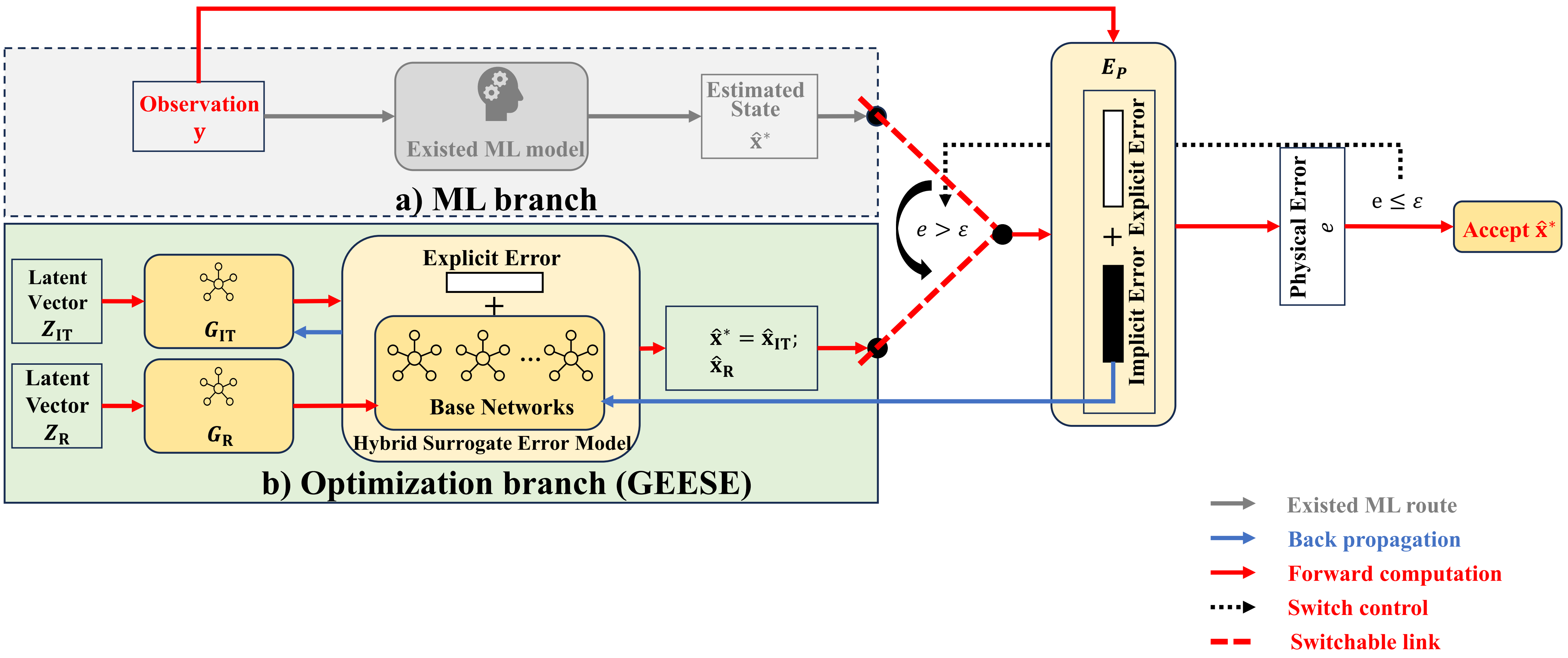
$$\hat{\mathrm{e}}_{\mathrm{im}}\left(\hat{\mathbf{x}},\{\mathbf{w}_i\}_{i=1}^{L}\right)=\frac{1}{L}\sum_{i=1}^{L}\phi\left(\hat{\mathbf{x}},\mathbf{w}_i\right)$$



$$\hat{e}\left(\hat{\mathbf{x}},\{\mathbf{w}_i\}_{i=1}^{L}\right)=\underbrace{\sum_{j=1}^{k} w_j\left(\frac{1}{L}\sum_{i=1}^{L}\phi_j\left(\hat{\mathbf{x}},\mathbf{w}_i\right)\right)}_{\text{approximated implicit error}}+\underbrace{\sum_{j=k+1}^{h} w_j E_{P_j}(\hat{\mathbf{x}})}_{\text{true explicit error}}$$

Design: Twin Selection




Observation
y
Existed ML model
Estimated State
$\hat{x}^*$
a) ML branch
Latent Vector
Z_{IT}
G_{IT}
Latent Vector
Z_R
G_R
Explicit Error
+
Base Networks
Hybrid Surrogate Error Model
$\hat{x}^* = \hat{x}_{IT}; \hat{x}_R$
b) Optimization branch (GEESE)
$e > \varepsilon$
E_P
Explicit Error
+
Implicit Error
Physical Error
e
$e \leq \varepsilon$
Accept $\hat{x}^*$
Existed ML route
Back propagation
Forward computation
Switch control
Switchable link

Experimental setting

- Three engineering problem: Turbofan Design, 2. Electro-mechanical Actuator Design, 3, Pulse-width Modulation of 13-level Inverters
- Configuration: 100 independent test cases per problem, the allowed query times to physical evaluation E_P is 1000.

Metrics:

Failure times: total failure times in 100 cases

Query times: the average query times needed for correcting state.

Algorithm	Problem 1 State Dimension:11		Problem 2 State Dimension:20		Problem 3 State Dimension:30	
	Failure times	Query times	Failure times	Query times	Failure times	Query times
BOGP	0	3.29 ±1.51	97	973.76 ±144.28	4	112.66 ±229.98
GA	0	64.00 ±0.00	0	130.56 ±63.31	13	231.76 ±339.71
PSO	0	64.00 ±0.00	0	64.00 ±0.00	12	244.16±343.71
CMAES	0	55.67 ±3.28	0	119.44 ±41.80	12	227.42 ±312.17
ISRES	0	65.00±0.00	0	177.64 ±80.51	16	250.05 ±350.16
NSGA2	0	64.00 ±0.00	0	139.52 ±68.56	13	232.40 335.94
UNSGA3	0	64.00 ±0.00	0	140.80 ±79.94	12	227.52 ±330.07
SVPEN	100	1000.00±0.00	100	1000.00±0.00	100	1000.00±0.00
GEESE (Ours)	0	**3.18 ±1.98**	0	**51.65 ±33.01**	**0**	**43.56 ±65.28**

Conclusion and Future Work

- propose a novel approach, GEESE, to correct wrong state estimation through optimization, aiming at delivering both low error and high efficiency.

- a hybrid surrogate error model to provide fast error estimations to reduce simulation cost and to enable gradient based backpropagation of error feedback.

- two generative models to approximate the probability distributions of the candidate states for simulating the exploitation and exploration behaviors.

- GEESE is tested on three real-world SAE inverse problems. Results show that it fails the least number of times in terms of finding a feasible state correction, and requires physical evaluations less frequently in general.

Future work: how to correct high-dimension state estimation?

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Thank you!