A machine learning approach targeting parameter estimation for PFT coexistence modeling using ELM-FATES

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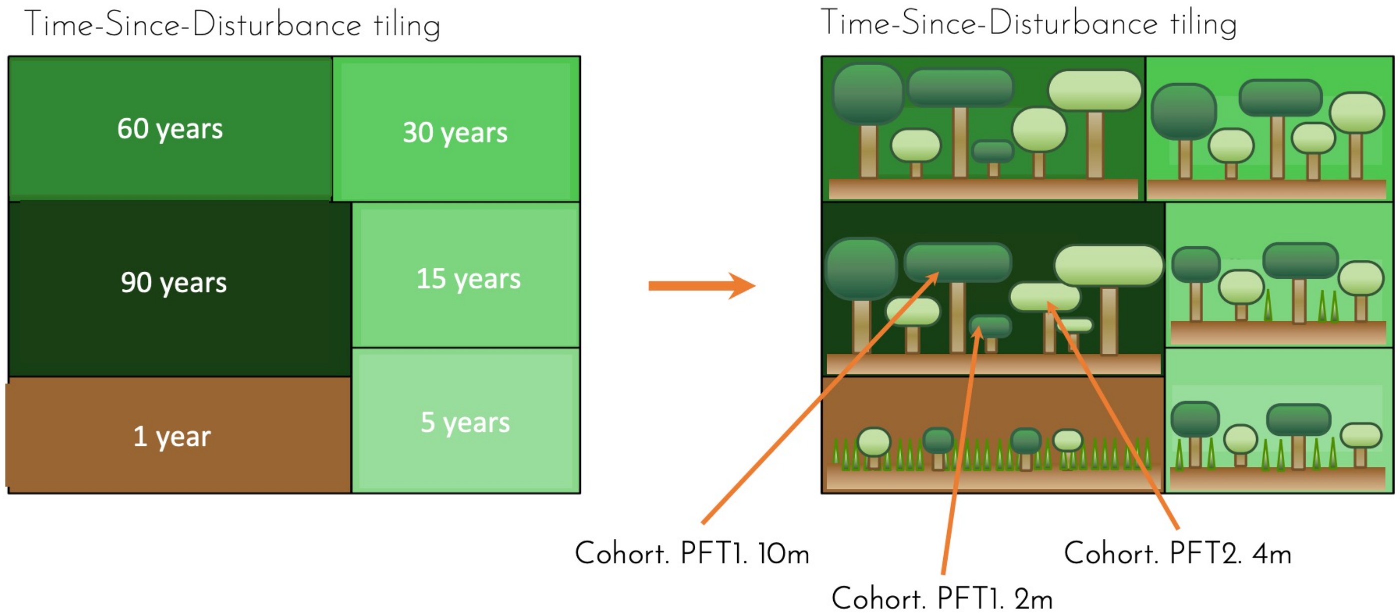
Challenge in modeling PFTs coexistence in FATES

- FATES is a “cohort-based" VDM model
  represent competition/coexistence between different plant functional types (PFTs)
- The challenge is to reasonably simulate the coexistence of PFTs



Each tile contains cohorts of plants, defined by PFT and size

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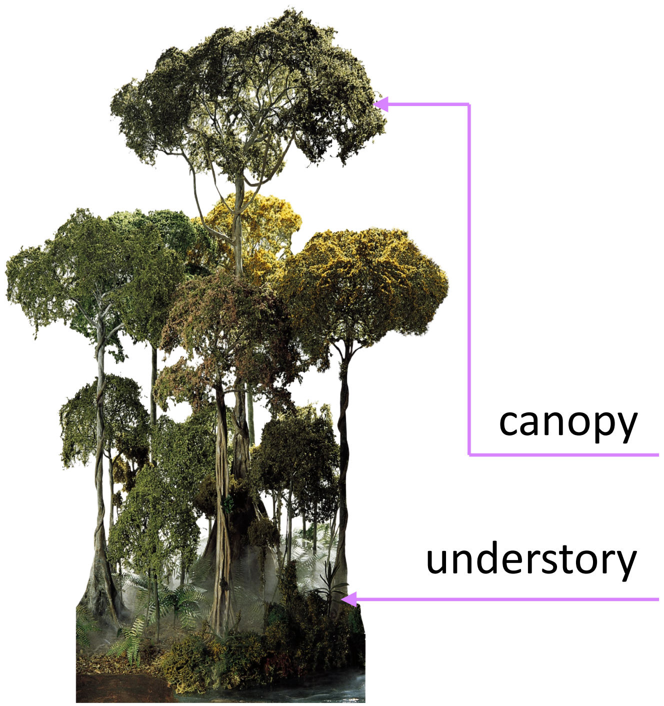
Coexistence theory and modeling

Niche-based coexistence theory

- Environmental Filtering: convergence in strategy to adapt to the surrounding environment
- Niche partitioning: divergence in strategy to ensure differentiation in resource requirements

Humid rainforest



Coexistence theory and modeling

Niche-based coexistence theory

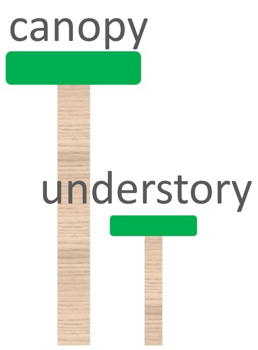
- Environmental Filtering — convergence in strategy
- Niche partitioning — divergence in strategy

FATES

Represent mechanisms/process

Reasonable trait parameter values

- C4 vs. C3 PFT
- Vertical canopy structure



Research goal and testbed

Research goal

Utilize machine learning (ML) to

- alleviate the challenge of modeling PFTs coexistence
- reduce model errors against observations

XGBoost

&

SHAP

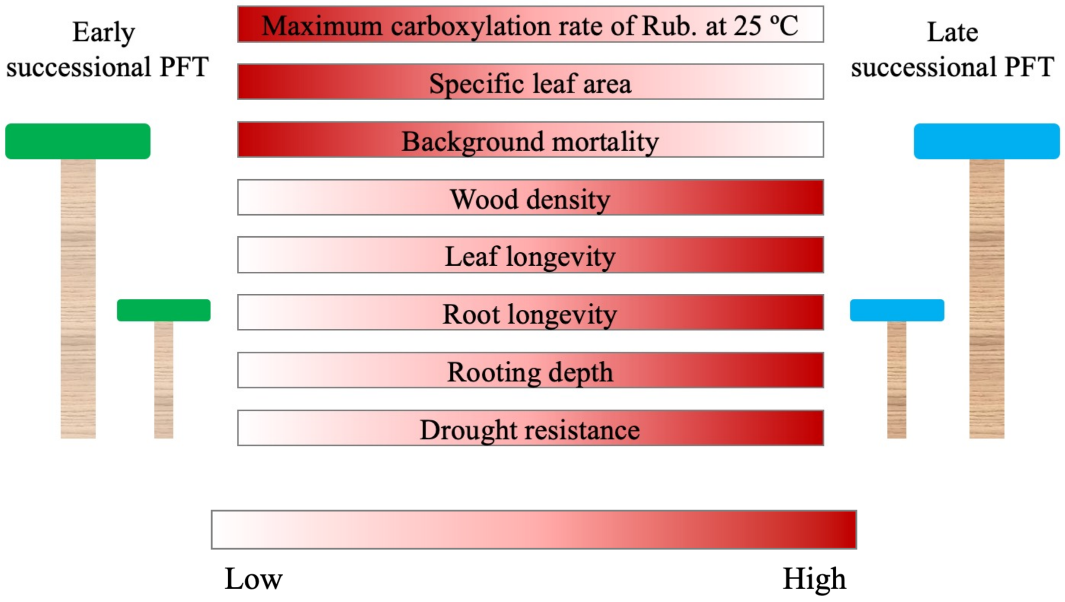
Testbed

- a tropical forest site: Manaus

Model configuration

Two PFTs represented in FATES

- Early vs. late successional broadleaf evergreen tropical tree
- 11 parameters, trait ranges based on tropical tree measurements



Parameter name	Early PFT	Late PFT	Range
Maximum carboxylation rate of Rub. at 25 ºC, canopy top	$V_{cmax,early} > V_{cmax,late}$		40–105
Specific leaf area, canopy top	$SLA_{early} > SLA_{late}$		0.005–0.04
Background mortality rate	$M_{bk,early} > M_{bk,late}$		0.005–0.05
Wood density	$WD_{early} < WD_{late}$		0.2–1.0
Leaf longevity	$L_{leaf,early} < L_{leaf,late}$		0.2–3.0
Maximum size of storage C pool, relative to the maximum size of leaf C pool	same		0.8–1.5

Overall flowchart and research questions

P1. Parameter sampling

Latin hypercube sampling, and tradeoffs

$V_{cmax,early} > V_{cmax,late}, SLA_{early} > SLA_{late}$

$M_{bk,early} > M_{bk,late}, WD_{early} < WD_{late}$

$L_{leaf,early} < L_{leaf,late}$

P2. Initial FATES experiments

Exp-OBS, consideration of observed trait relationships

Exp-CTR

P3. Build ML models and sensitivity analysis

ML models train and test

SHAP importance analysis

P4. Parameter selection and validation

Exp-ML, ELM-FATES simulation using ML selected parameters

Specific research questions

- Q1: Whether observed trait relationships can improve PFTs coexistence?
- Q2: Can simple parameter correlations be constructed to improve PFTs coexistence?
- Q3: Can ML selected parameter values improve PFTs coexistence?

Q1 → Observed trait relationships cannot improve PFTs coexistence modeling

Two experiment ensembles

- Exp-CTR, traits tradeoffs
- Exp-OBS, traits tradeoffs + observed trait relationships

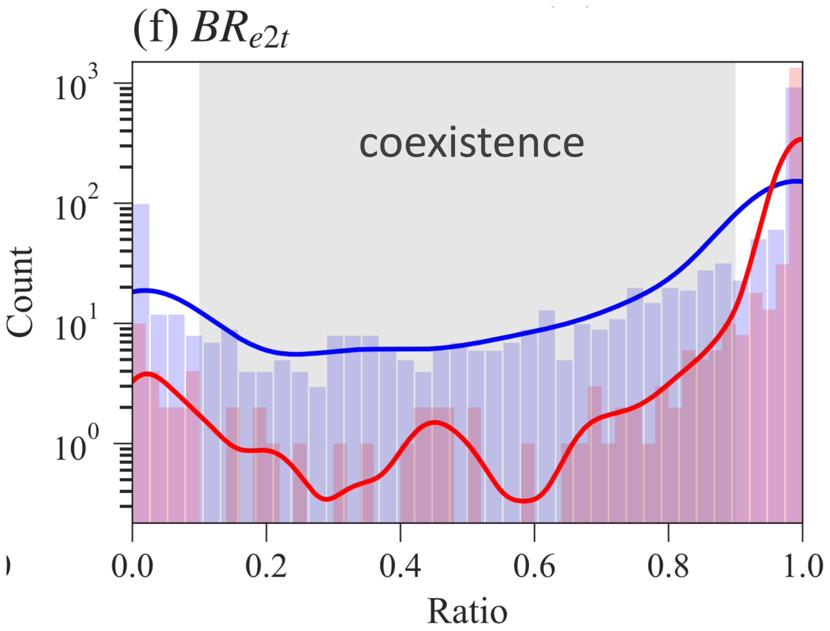
→ degraded the PFT coexistence simulations

Koven et al. (2020) and Longo et al. (2020):

$$M_{bk} = 0.0082 \times e^{(0.0153 \times V_{cmax})} \quad (1)$$

$$L_{leaf} = 0.0001 \times SLA^{(-2.32)} \quad (2)$$

$$WD = -0.583 \times \ln(SLA) - 1.6754 \quad (3)$$



PFT coexistence :
Biomass ratio between early PFT and total biomass

$BR_{e2t} \in (0.9, 1.0]$, "early"
$BR_{e2t} \in [0.1, 0.9]$, "coexistence"
$BR_{e2t} \in [0.0, 0.1)$, "late"

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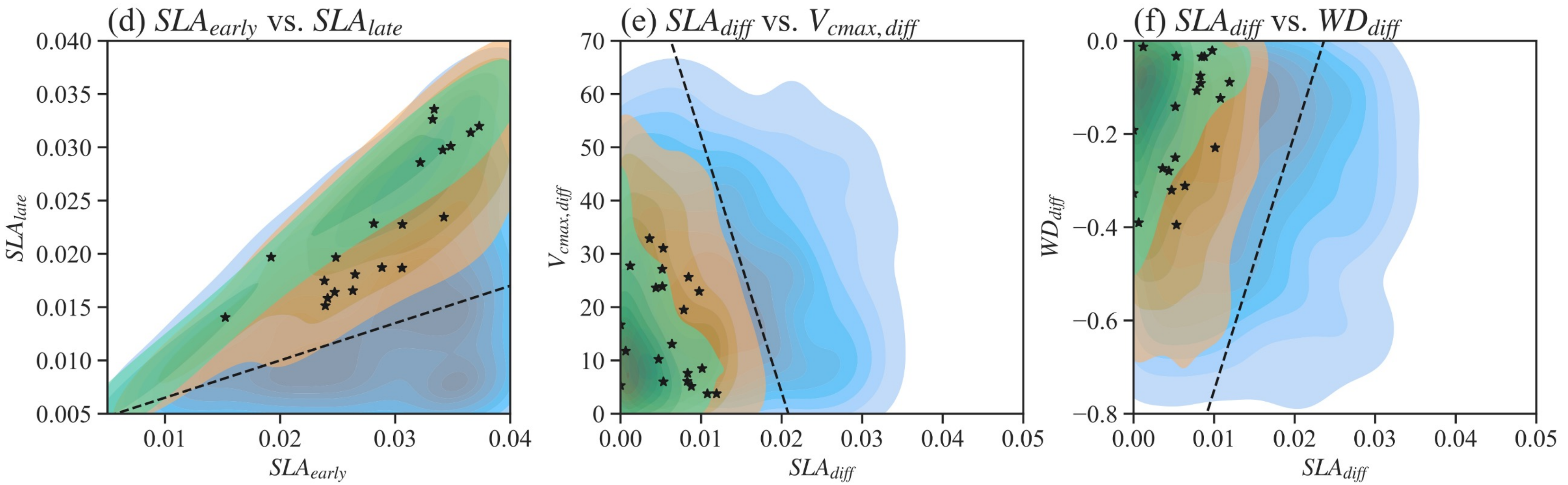
Q2 → Simple constructed correlations are also insufficient

Based on Exp-CTR, build empirical simple parameter correlations



- Early
- Coexistent
- Late

★ optimal case:
1) coexistence,
2) relative bias of water/energy/carbon < 15%

- $SLA_{late} > 0.35 \times SLA_{early} + 0.003$
- $V_{cmax,diff} < -4800 \times SLA_{diff} + 100$
- $WD_{diff} > 55 \times SLA_{diff} - 1.3$

→

Within these constrained parameter spaces,

- Coexisting cases increases from 20.6% to 32.6%
- 67.4% is still either early or late
- Optical cases account only about **2.3%**

Build ML surrogate models

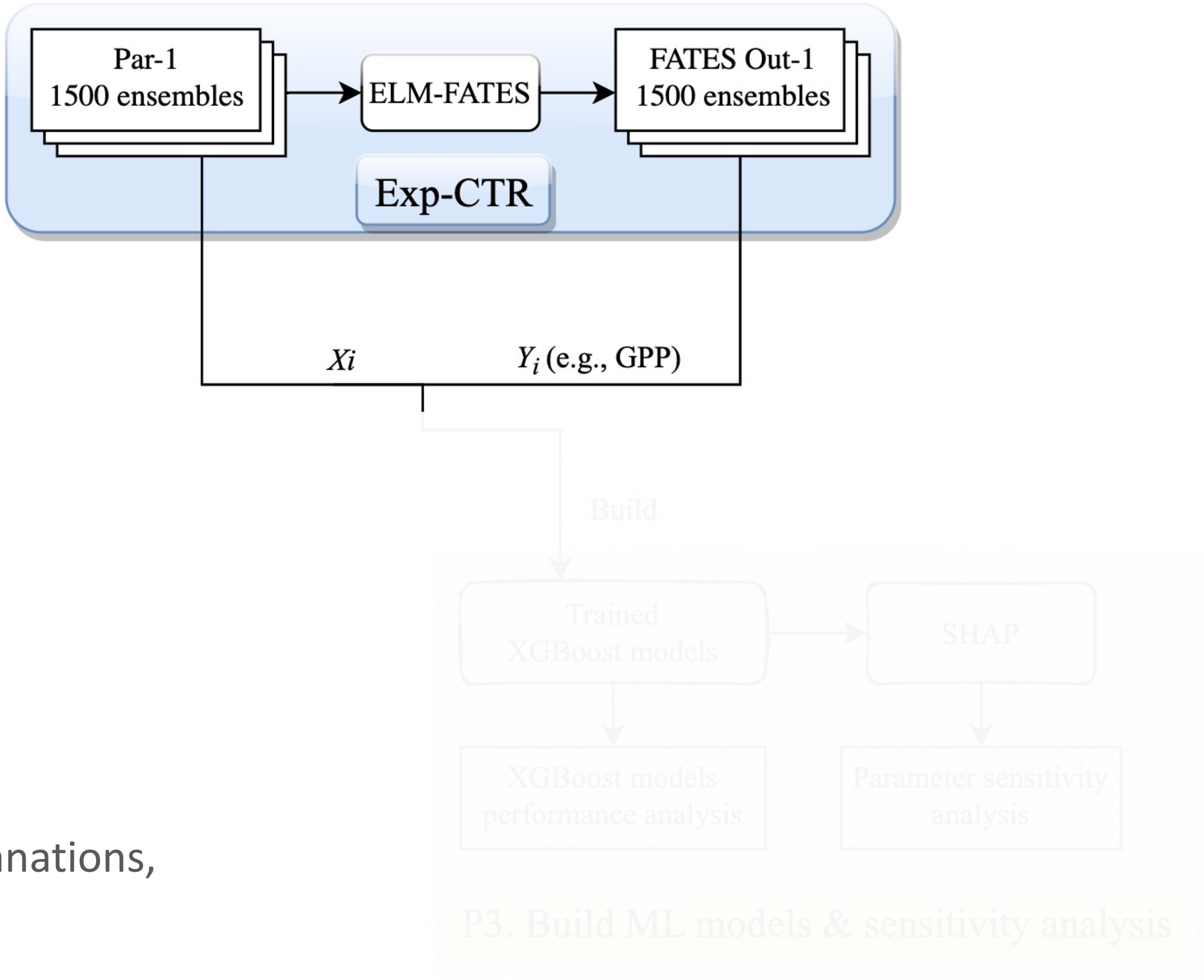
In Exp-CTR, 1500 samples of

- *Xn*, parameters and their difference

  e.g., $V_{cmax,early}$, SLA_{diff},

- *Yi*, ELM-FATES outputs

  e.g., ET, SH, GPP, AGB, BW



Build emulators

$$Y_i = \boldsymbol{f}_i\,(X_1, X_2, X_3, \ldots)$$

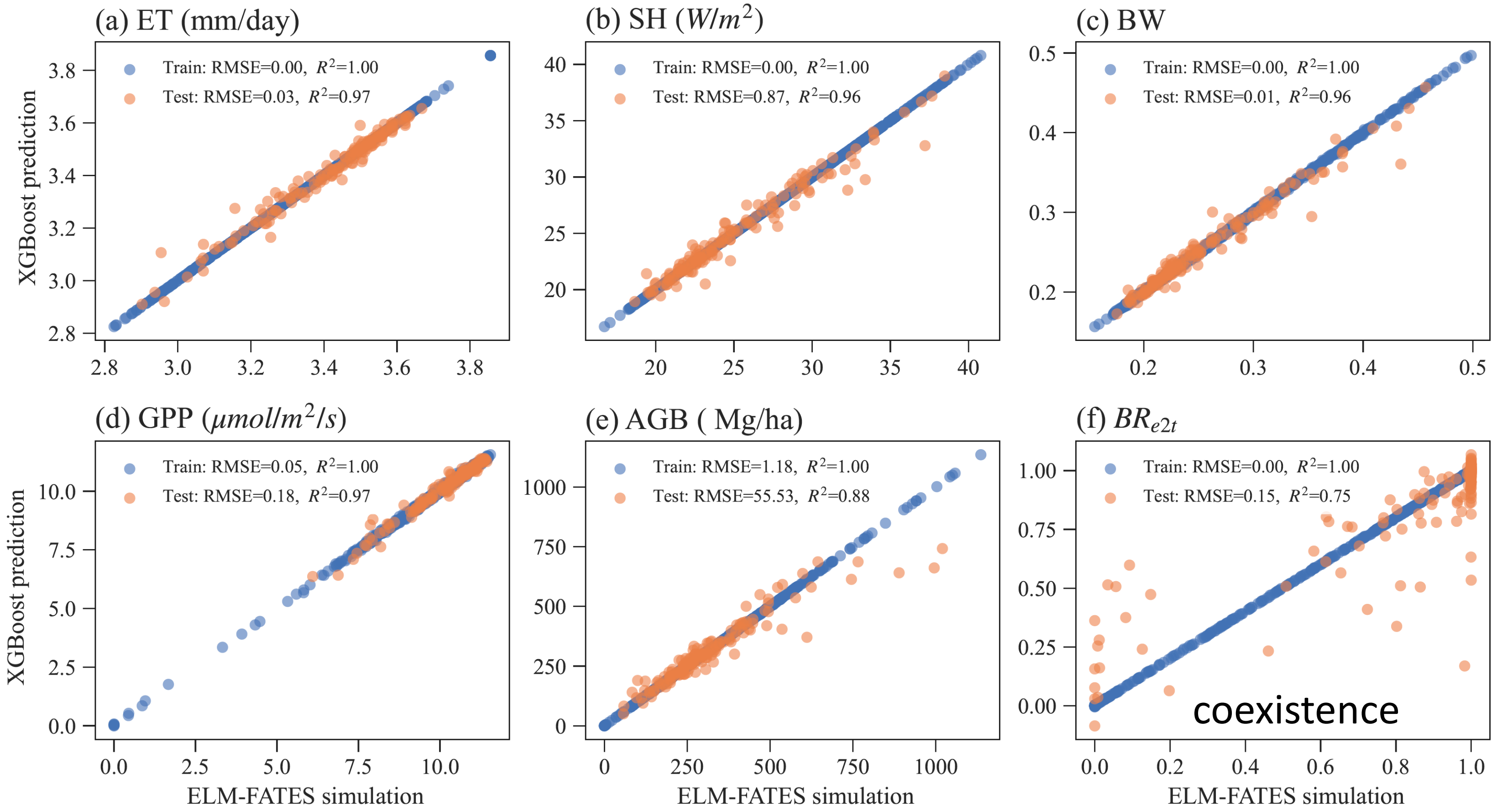
Machine learning algorithm
e.g., XGBoost (Chen et al., 2016)

SHAP (SHapley Additive exPlanations, Lundberg et al., 2017)

Parameters selection

ML surrogate models have good performance

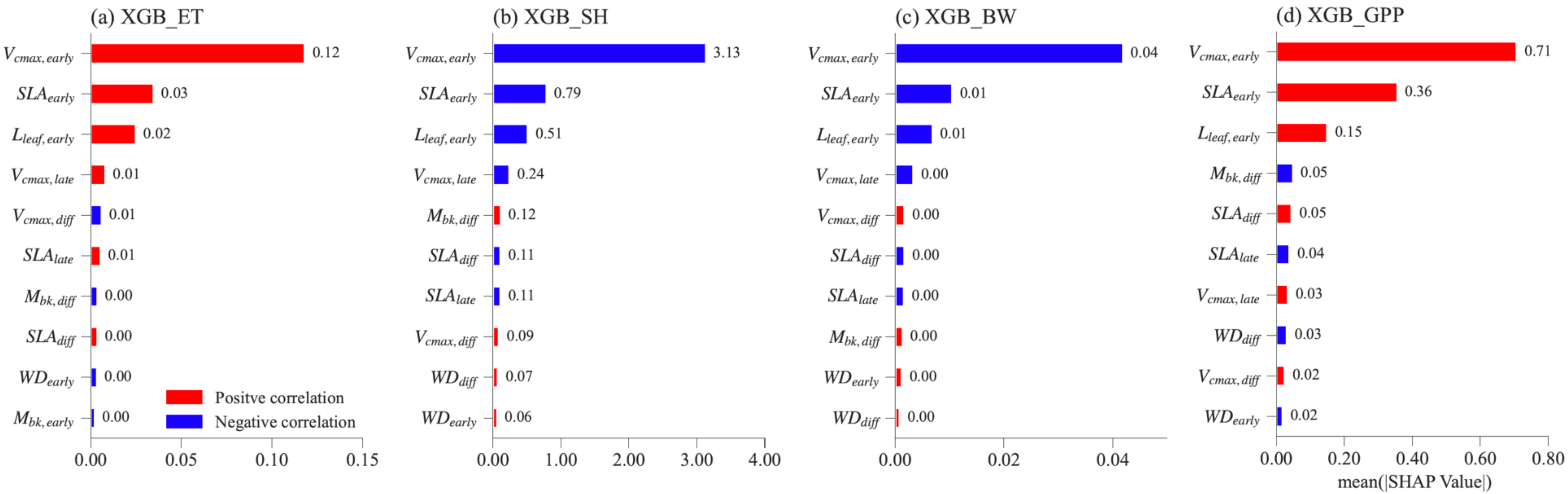
- 6 XGBoost surrogate models: ET, SH, BW, GPP, AGB, and BR_{e2t}
- Overall good performance in training and testing samples
  - AGB and BR_{e2t} are relatively difficult to emulate



Which parameters are important

- Only 3 features dominate the prediction of ET, SH, BW, and GPP

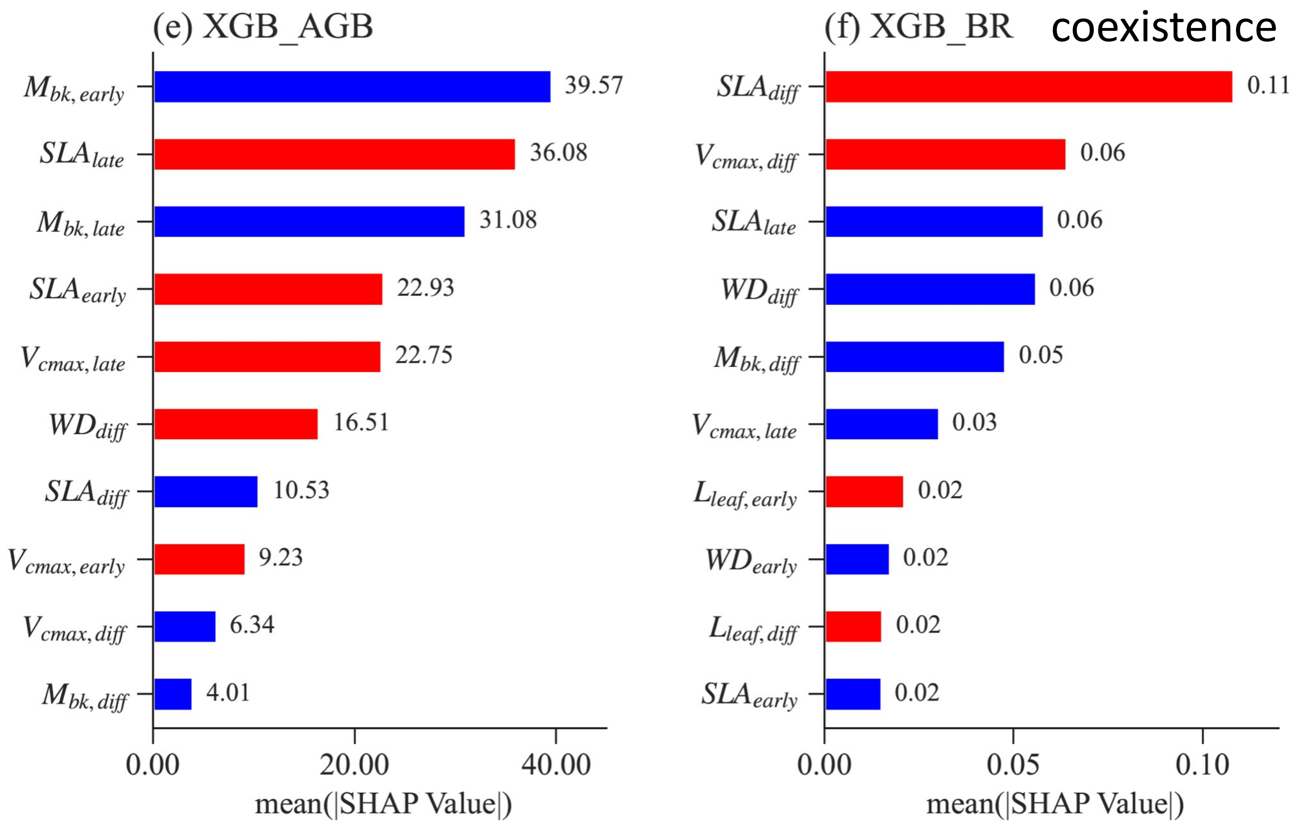
$$V_{cmax,early}$$
$$SLA_{early}$$
$$L_{leaf,early}$$



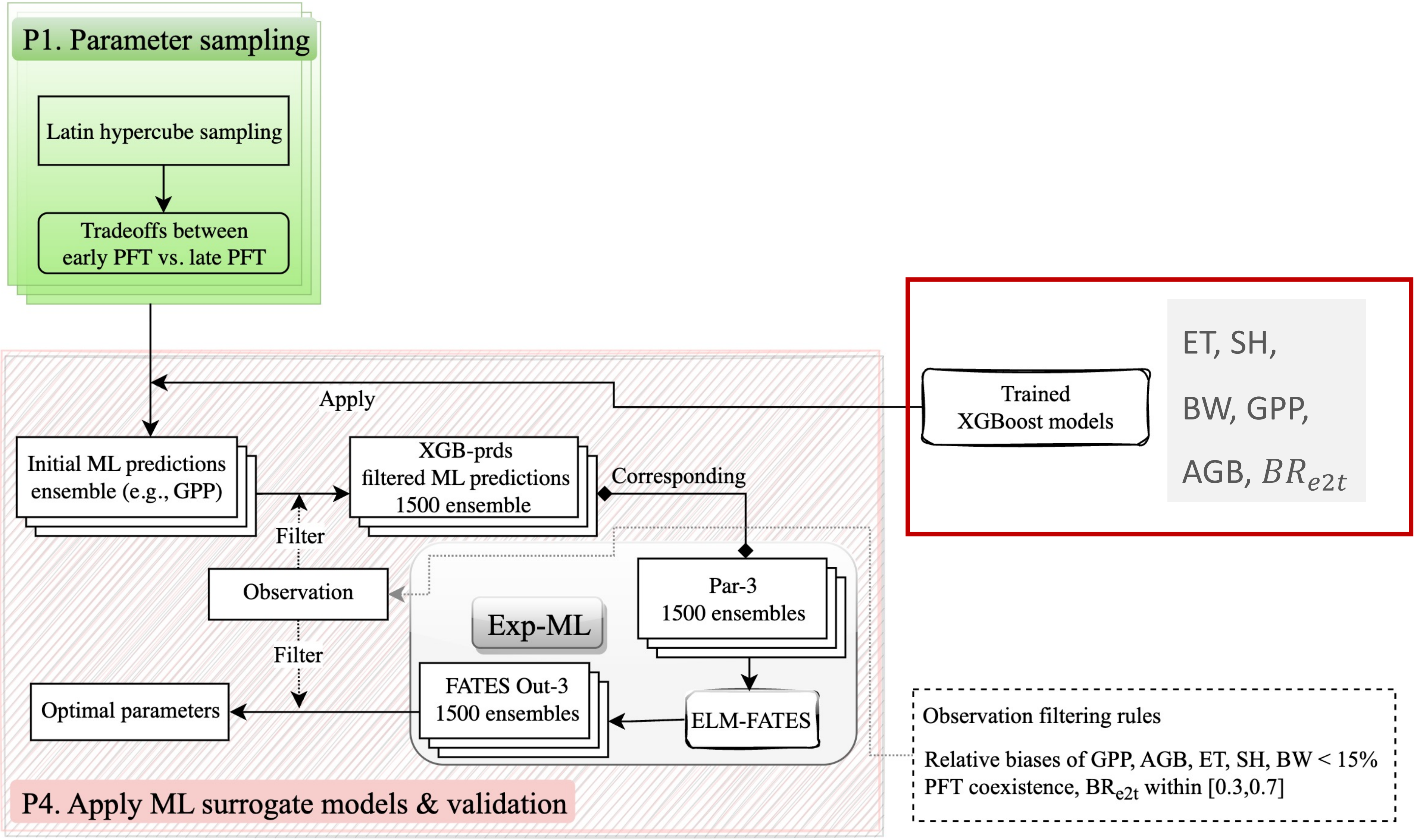
Which parameters are important

- More than 6 features are most important for predicting AGB and BR_{e2t}
- Trait parameter differences between early and late PFT are very important

  e.g, SLA_{diff}, $Vcmax_{diff}$

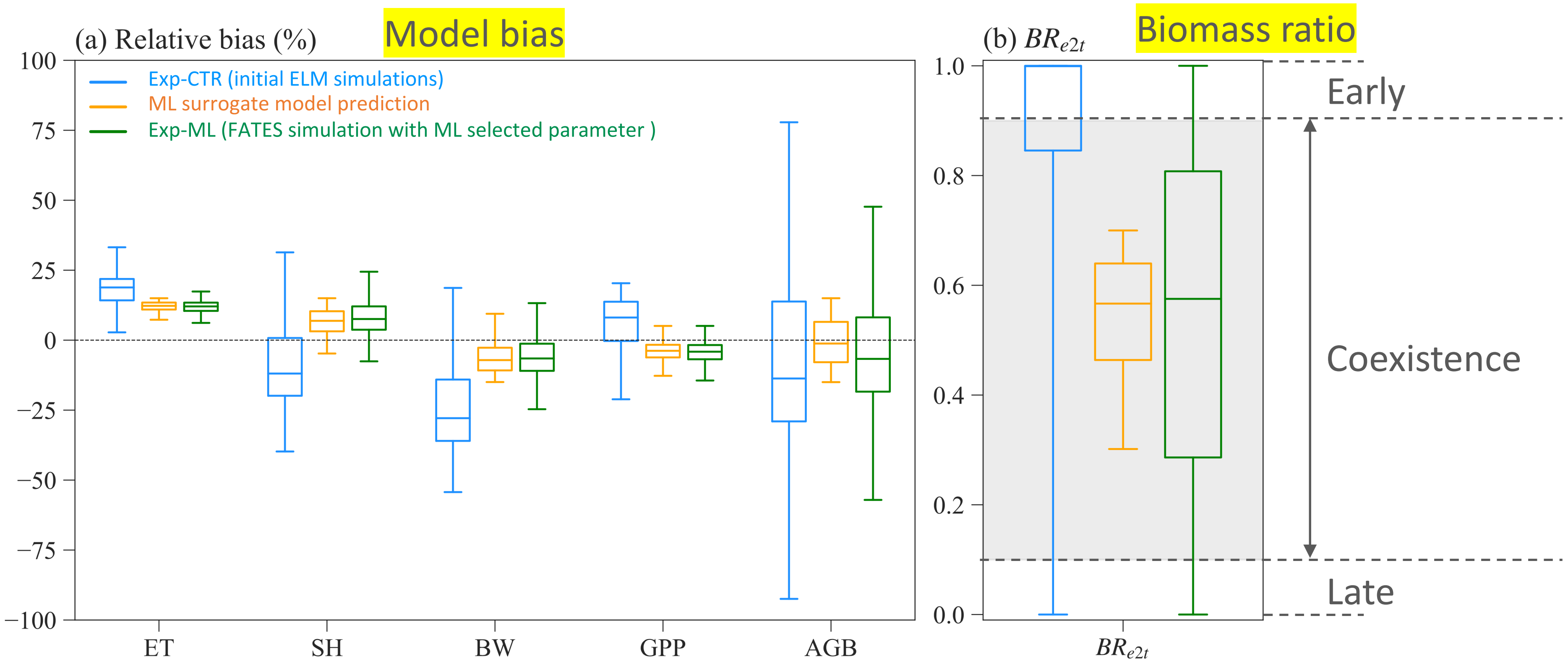


Parameter selection using ML surrogate models



ML selected parameter values largely improve FATES simulation

- ML selected parameters → better capture observations
- ML selected parameters → more well-coexistent runs



ML selected parameter values largely improve FATES simulation

Compared with **Exp-CTR** and **Exp-ML** have

- 3.6 times more coexistence cases, 20% →73%
- 23.6 times more optimal cases, 1.4%→33%, with higher model accuracy

Category	BR_{e2t} ∈[0.1, 0.9]	|AGB_bias| < 15%	|GPP_bias| < 15%	|ET_bias| < 15%	|SH_bias| < 15%	|BW_bias| < 15%	Exp-CTR		Exp-ML		Ratio
							count	percent	count	percent	
Late							130	8.7%	174	11.6%	1.3
Coexistence							309	20.6%	1097	73.1%	3.6
Early							1059	70.6%	229	15.3%	0.2
All dead							2	0.1%	0	0.0%	
Total							1500		1500		
Add observation constraints	+						309	20.6%	1097	73.1%	3.6
	+	+					98	6.5%	620	41.3%	6.3
	+	+	+				85	5.7%	618	41.2%	7.3
	+	+	+	+			23	1.5%	572	38.1%	24.9
	+	+	+	+	+		23	1.5%	502	33.5%	21.8
	+	+	+	+	+	+	21	1.4%	495	33.0%	23.6

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Parameter tradeoffs align with niche-based coexistence theory

Environmental Filtering

convergence in strategy

Niche partitioning

divergence in strategy

Niche-based coexistence theory

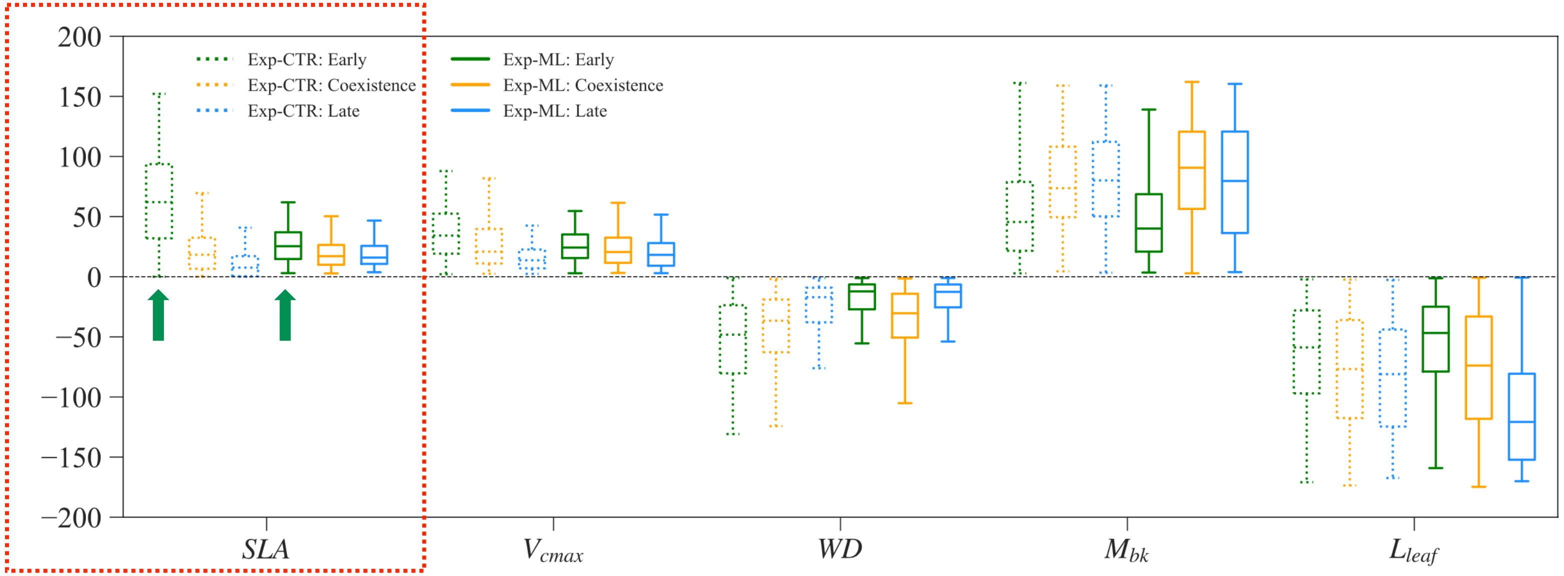
Relative difference should not be considerable

- Large difference in SLA more likely favors the early PFT

Some degree of differences should exist

- Small difference in SLA more likely favors the late PFT
- For Exp-CTR, coexistence have intermediate differences in SLA, V_{cmax}, WD, M_{bk} and L_{leaf}
- For Exp-ML, coexistence have intermediate differences in SLA, V_{cmax}, and L_{leaf}

M_bk and WD show large difference but they show tradeoff to make coexistence



Parameter relative difference (%) between early PFT and late PFT

Parameter tradeoffs align with niche-based coexistence theory

Environmental Filtering

convergence in strategy

Niche partitioning

divergence in strategy

Niche-based coexistence theory

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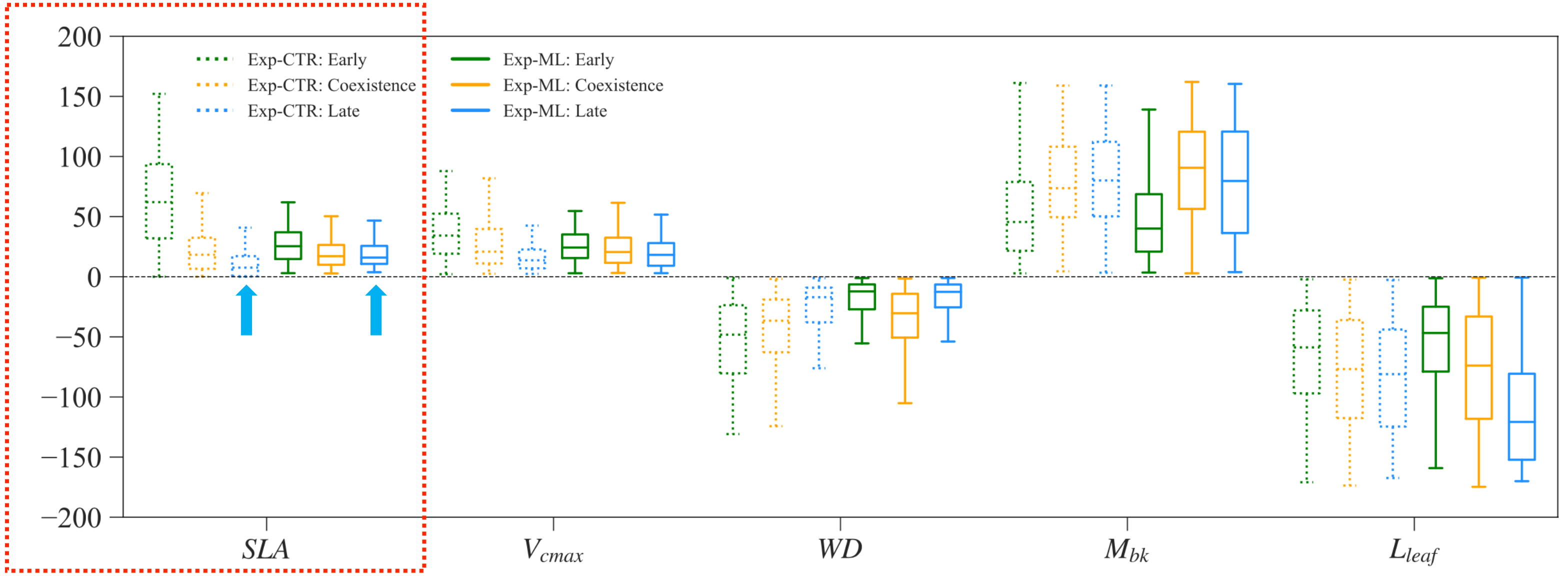

Parameter relative difference (%) between early PFT and late PFT

Parameter tradeoffs align with niche-based coexistence theory

Environmental Filtering

convergence in strategy

Niche partitioning

divergence in strategy

Niche-based coexistence theory

Difference should not be considerable

- Large difference in SLA more likely favors the early PFT

Some degree of differences should exist or balance

- Small difference in SLA more likely favors the late PFT
- For Exp-CTR, coexistence have intermediate differences in SLA, V_{cmax}, WD, M_{bk} and L_{leaf}
- For Exp-ML, coexistence have intermediate differences in SLA, V_{cmax}, and L_{leaf}

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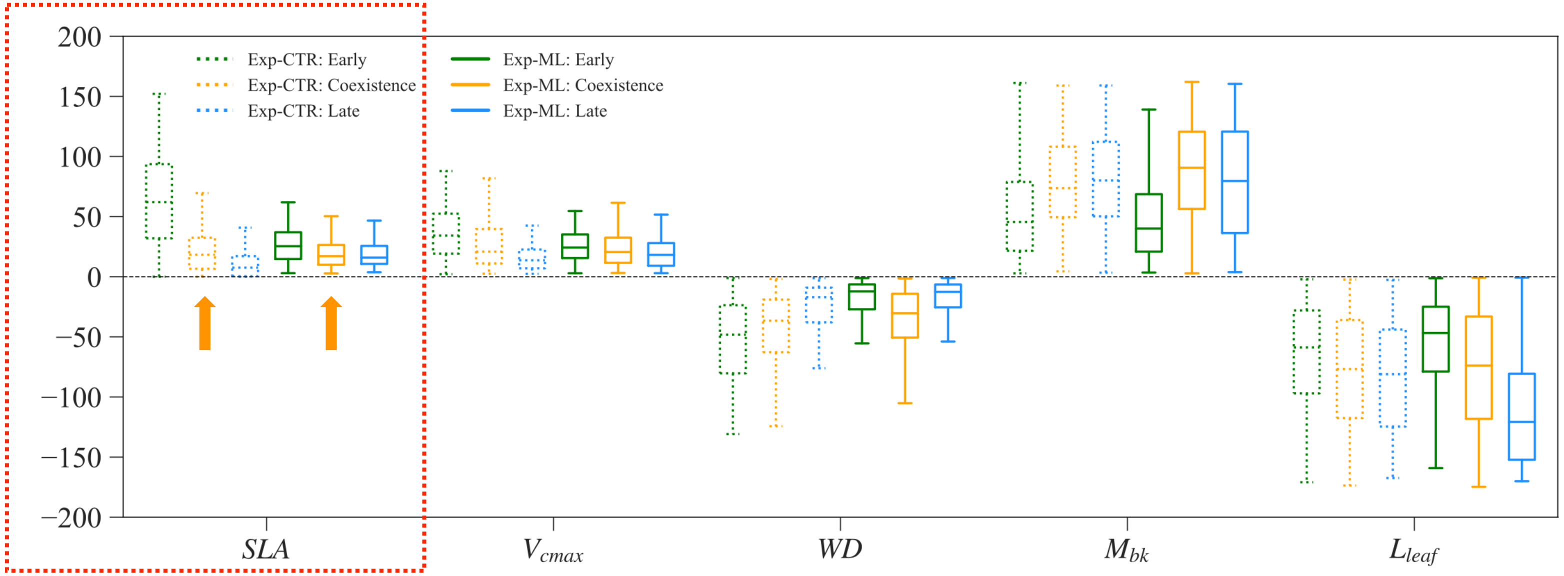
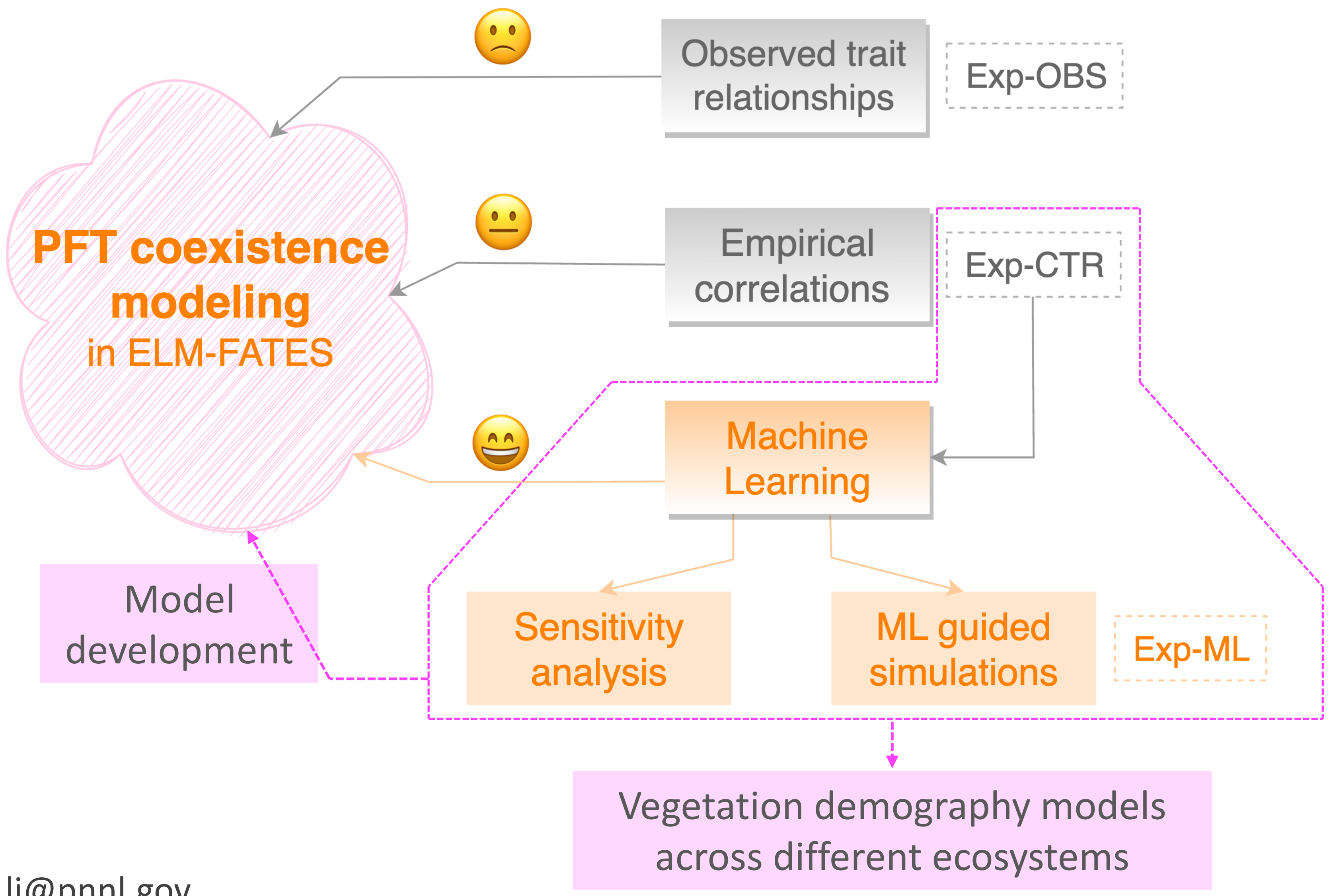


Parameter relative difference (%) between early PFT and late PFT

Take Home Message



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