Probabilistic Spatio-Temporal Modeling of Land Surface Temperature: A Comparison of IDW, Random Forest, and Sparse Gaussian Processes

Course project Presentation

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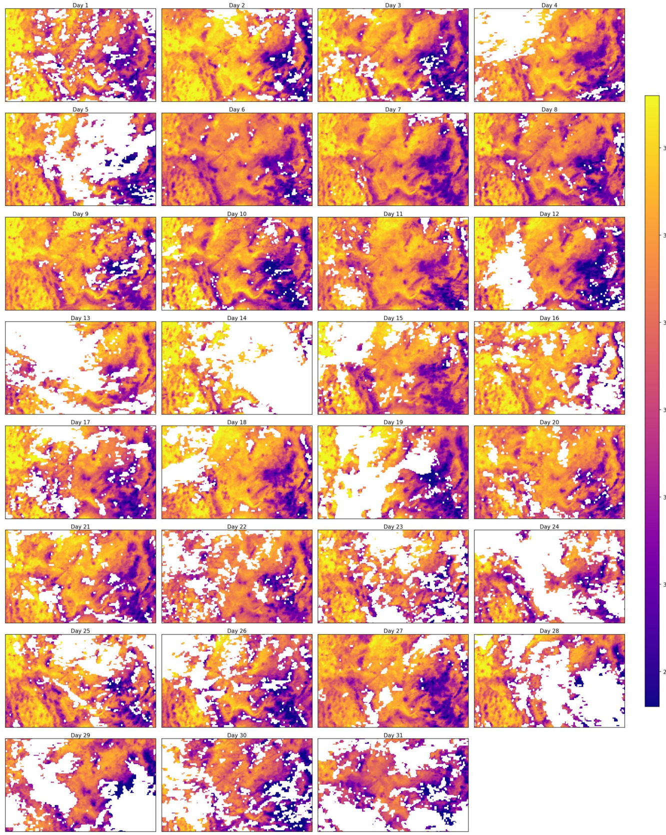
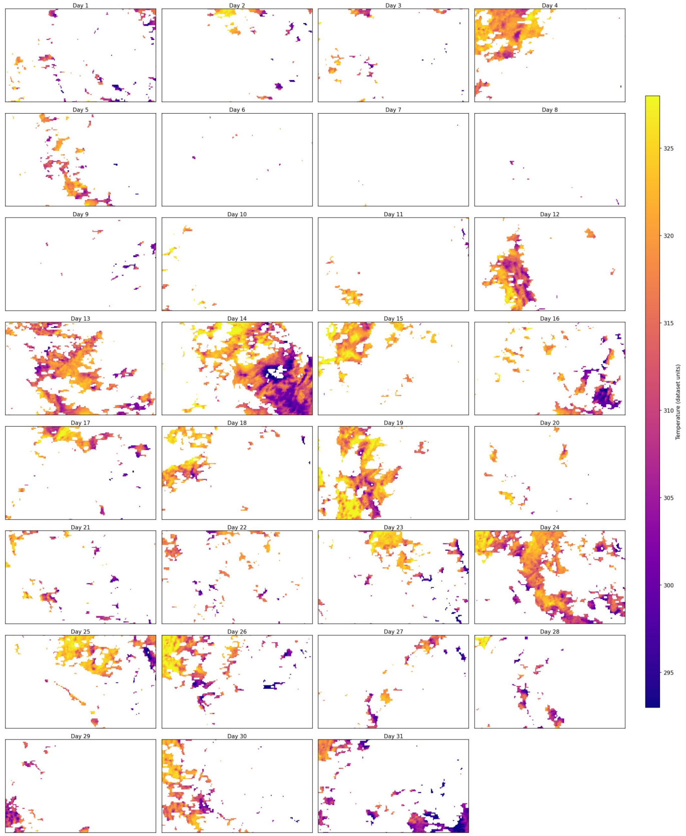
1. Background and Introduction



Training set



Test set

Objective of the project:
Develop probabilistic interpolation models for land surface temperature (LST) data collected from the MODIS satellite platform.

Dataset: $100 \times 200 \times 31$ (latitude $\times$ longitude $\times$ days)

- Latitude: 35° to 40° (100 grid points)
- Longitude: -115° to 105° (200 grid points)
- Time: 31 consecutive days
- 494,762 training points
- 85,942 test points
- No overlap between training and test sets.

2. Project Questions & Objectives

Q1. Model Performance

How well do models reconstruct MODIS LST?

IDW, Random Forest (RF), Sparse Gaussian Process (SVGP)

Q2. Kernel Design

Which covariance kernels best capture LST structure in (lon, lat, time)?

Linear, RBF, Matern 3/2, Matern 5/2, RQ-Like, RBF+Linear, Periodic × Time, Space × Time

Q3. Role of Additional information (Elevation)

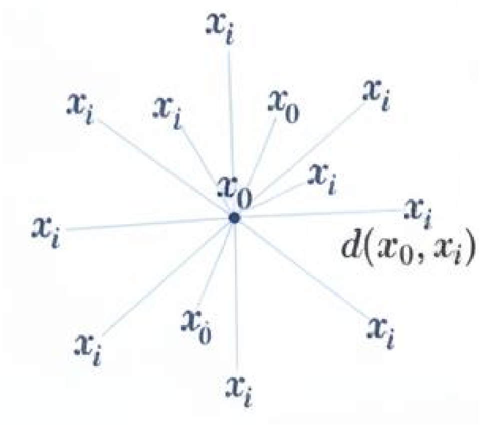
How does elevation improve LST interpolation? What is the best integration strategy?

Strategy 1: SVGP+Elevation as input feature Strategy 2: Multi-output SVGP (Elevation + Temperature)

3. Model choice

3.1 Baseline Models: IDW & Random Forest

Model 1: Inverse Distance Weighting (IDW)



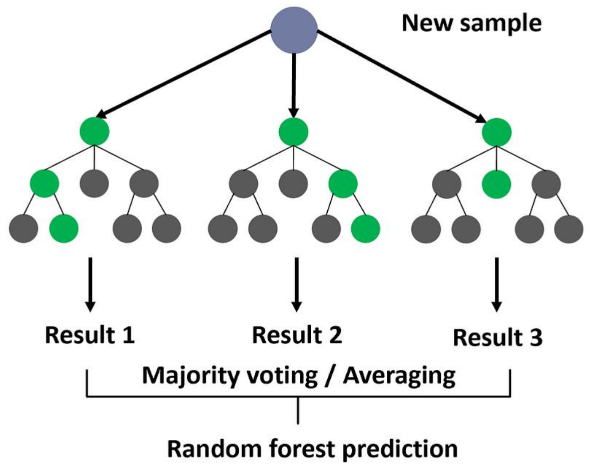
$$\hat{y}(x_0) = \frac{\sum_i w_i y_i}{\sum_i w_i}$$

$$\text{where} \quad w_i = \frac{1}{d(x_0, x_i)^p}.$$

- Deterministic spatial interpolation
- Local weighted averaging of nearby observations
- Weights decay with distance
- Applied independently for each day → no temporal modeling
- No uncertainty quantification
- Simple, fast, and widely used as a baseline method

Model 2: Random forest model

- Ensemble of many decision trees (bagging)
- Captures nonlinear relationships effectively
- Treats (row,col,time) as regular features
- Robust to noise and requires little tuning
- No uncertainty quantification
- Not a spatiotemporal model → may produce non-smooth spatial patterns



3.2 Sparse Gaussian Process (SVGP)

Start

1. Data preparation

2. Inducing Point Selection
Randomly Sample M=800 Points
Initialize variational posterior

3. Kernel Construction
Choose Kernel
Apply Scale kernel + White noise kernel

4. Model Setup
Configure Variational Strategy
Set Constant Mean +Kernel Covariance
Define Gaussian Likelihood

5. Variational Training
Maximize the variational ELBO
Mini-batch: 8192
Adam optimizer
30 Epochs

6. Evaluation

End

SVGP Kernel Designs and Structures

Base Kernels

K1: Linear

$$k_{lin}(x,x') = \sigma_\ell^2 (x^\top x')$$

K2: RBF

$$k_{RBF}(x,x') = \sigma^2 \exp\left(-\frac{1}{2}\sum_{d=1}^{3}\frac{(x_d - x'_d)^2}{\ell_d^2}\right)$$

K3: Matern-3/2

$$k_{M32}(x,x') = \sigma^2 \prod_{d=1}^{3}\left(1+\frac{\sqrt{3}|x_d - x'_d|}{\ell_d^2}\right)\exp\left(-\frac{\sqrt{3}|x_d - x'_d|}{\ell_d^2}\right)$$

K3: Matern-5/2

$$k_{M52}(x,x') = \sigma^2 \prod_{d=1}^{3}\left(1+\frac{\sqrt{5}r}{\ell_d^2}+\frac{5r^2}{3\ell_d^2}\right)\exp\left(-\frac{\sqrt{5}r}{\ell_d}\right), r = |x_d - x'_d|$$

Additive Kernels

K5: RQ-Like

$$k_{\mathrm{RQlike}}(x,x') = \sum_{q=1}^{3}\sigma_q^2 \exp\left(-\frac{1}{2}\sum_{d=1}^{3}\frac{(x_d - x'_d)^2}{\ell_{q,d}^2}\right)$$

K6: RBF + Linear

$$k(x,x') = k_{\mathrm{RBF}}(x,x') + k_{\mathrm{lin}}(x,x')$$

Separable Kernels

K7: Periodic ×RBF
Periodic kernel × RBF

$$k(t,t') = k_{\mathrm{per}}(t,t') \cdot k_{\mathrm{RBF}}(x,x')$$

K8: Space ×Time
Matern-3/2 over space×
RBF over time

$$k((s,t),(s',t')) = k_{\mathrm{space}}(s,s') \cdot k_{\mathrm{time}}(t,t')$$

Plus

White Noise Kernel

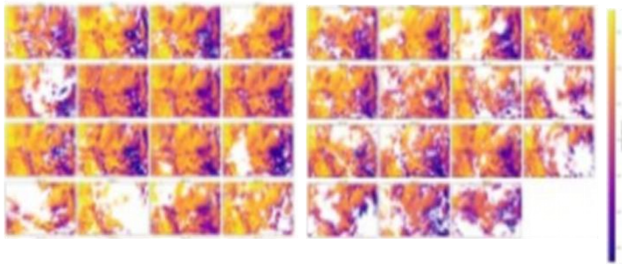
$$k_{\mathrm{noise}}(x,x') = \sigma_n^2\,\delta(x,x')$$

$$k_{\mathrm{total}}(x,x') = \underbrace{\mathrm{outputscale}\cdot k_{\mathrm{base}}(x,x')}_{\mathrm{ScaleKernel}} + \underbrace{\sigma_n^2\,\delta(x,x')}_{\mathrm{WhiteNoiseKernel}}$$

3.3 SVGP with elevation

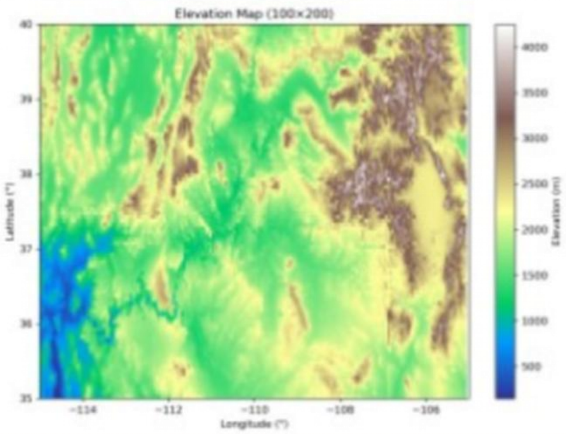
Data source

MODIS LST (100 × 200 × 31)



+

Elevation grid (100 × 200)



Processing

- Reshape LST tensor to training samples
- Split training vs test data
- Normalize inputs (row, col, day)
- Align elevation grid with spatial coordinates
- Produce training X, y

Strategy 1 : SVGP + Elevation as Input Feature

- Input: X = [row, col, day, elevation]
- Kernel design:
- k_total = k_spacetime + k_elev
- (RBF / Matérn5/2 / Space×Time)
- Sparse Variational GP (SVGP)
- Complexity $O(NM^2)$

Strategy 2 — Multi-output SVGP

- Input: X = [row, col, day]
- Outputs:

y_1 = LST (temperature), y_2 = elevation

- Shared inducing points Z
- Shared kernel hyperparameters
- (lengthscale & outputscale for RBF/Matérn)
- Joint ELBO = ELBO_temp + ELBO_elev

Evaluation

Data source: OpenTopography- NASADEM Global Digital Elevation Model

4. Metrics Design (Evaluation Criteria)

Model Evaluation Metrics

Error-based Metrics

[1] Root Mean Squared Error (RMSE)

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}$$

[2] Mean Absolute Error (MAE)

$$\mathrm{MAE} = \frac{1}{N}\sum_{i=1}^{N}|y_i - \hat{y}_i|$$

[3] Coefficient of Determination

$$\mathrm{R}^2 = 1 - \frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{N}(y_i - \bar{y})^2}$$

Probabilistic Metrics

[4] Continuous Ranked Probability Score (CRPS)

$$\mathrm{CRPS}(y, \mu, \sigma) = \sigma[z(2\Phi(z) - 1) + 2\phi(z)] - \frac{\sigma}{\sqrt{\pi}}$$

Interval Metrics

[5] Prediction Interval Coverage Probability (PICP)

$$PICP = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

[6] Mean Prediction Interval Width (MPIW)

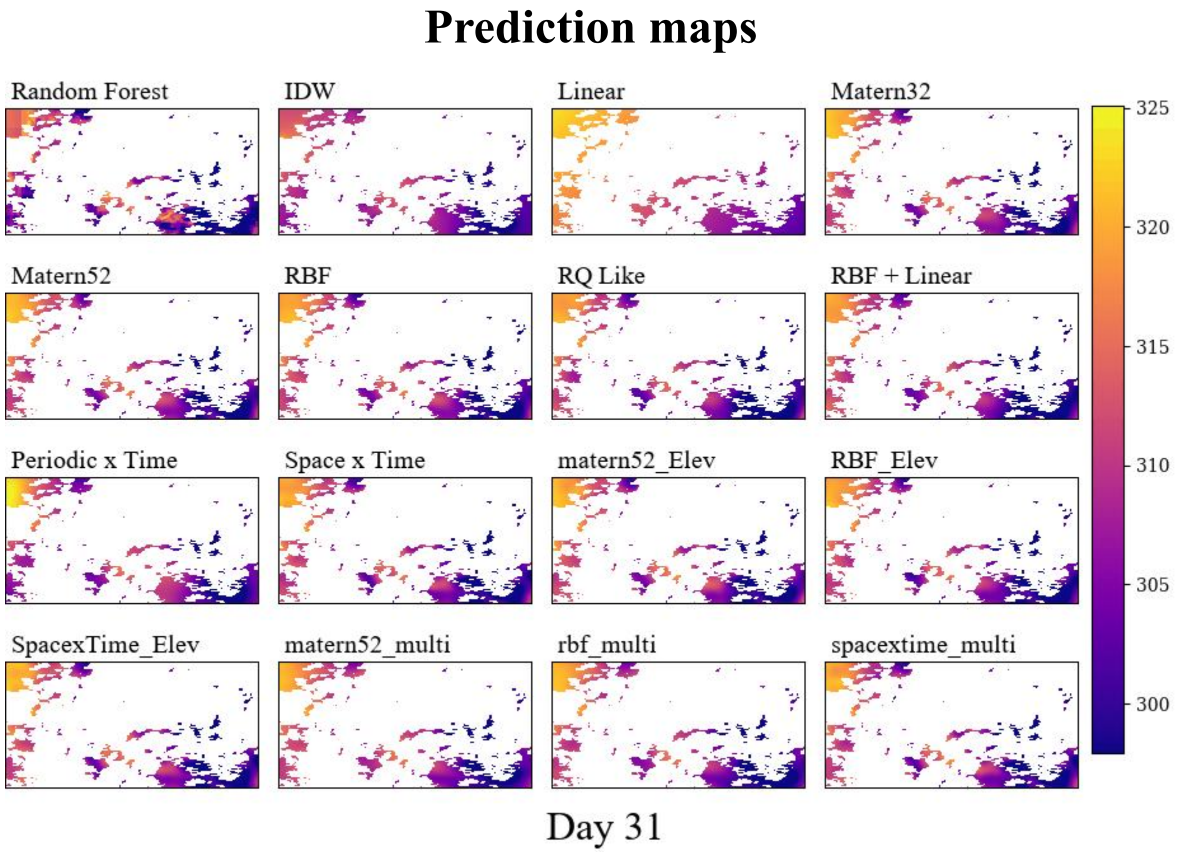
$$\mathrm{MPIW} = \frac{1}{n}\sum_{i=1}^{n}(U_i - L_i)$$

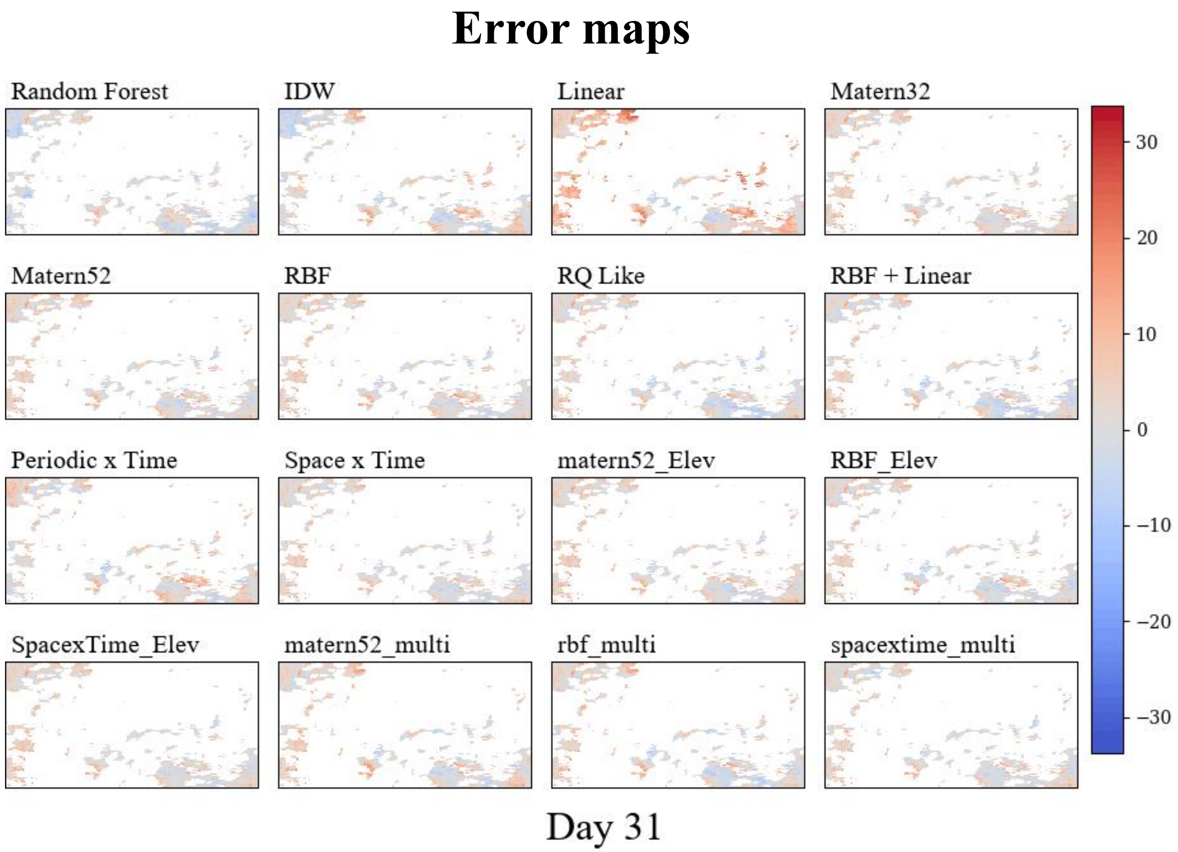
Efficiency

Training Time

5. Results

5.1 Results OveRview





5.2 Metrics Results

Model	Kernel	RMSE	MAE	R2	CRPS	PICP	MPIW	Time(s)
IDW	/	6.20	4.73	0.47	/	0.00	0.00	47.09
Random Forest	/	3.56	2.53	0.83	/	0.00	0.00	4.90
SVGP	Linear	7.39	5.96	0.25	4.17	0.95	28.02	263.32
	RBF	4.73	3.72	0.69	2.65	0.96	19.23	282.76
	Matern3/2	4.60	3.59	0.71	2.58	0.96	19.41	311.14
	Matern5/2	4.59	3.58	0.71	2.56	0.95	18.79	303.28
	rq_like(Mixture of RBFs)	4.99	3.91	0.66	2.79	0.95	20.13	329.13
	RBF + Linear	5.03	3.91	0.65	2.80	0.95	20.26	300.58
	Periodic× time	5.47	4.24	0.59	3.04	0.94	20.39	324.39
	Space×time Matern3/2(x, y)×RBF(t)	4.40	3.43	0.73	2.46	0.96	18.27	314.06
SVGP+ Elevation (input feature)	RBF_Elev	4.76	3.73	0.69	2.67	0.96	19.52	398.81
	Matern5/2_Elev	4.62	3.62	0.71	2.59	0.96	19.13	381.83
	Space×time_Elev	4.44	3.46	0.73	2.48	0.96	18.45	347.45
Multi-output SVGP	RBF_multi	5.34	4.18	0.61	2.98	0.94	20.64	690.73
	Matern5/2_multi	5.26	4.12	0.62	2.94	0.94	20.36	592.98
	Space×time_multi	4.44	3.47	0.73	2.48	0.95	18.23	630.96

5.3 Comparaison of different models

Model	Kernel	RMSE	MAE	R2	CRPS	PICP	MPIW	Time(s)
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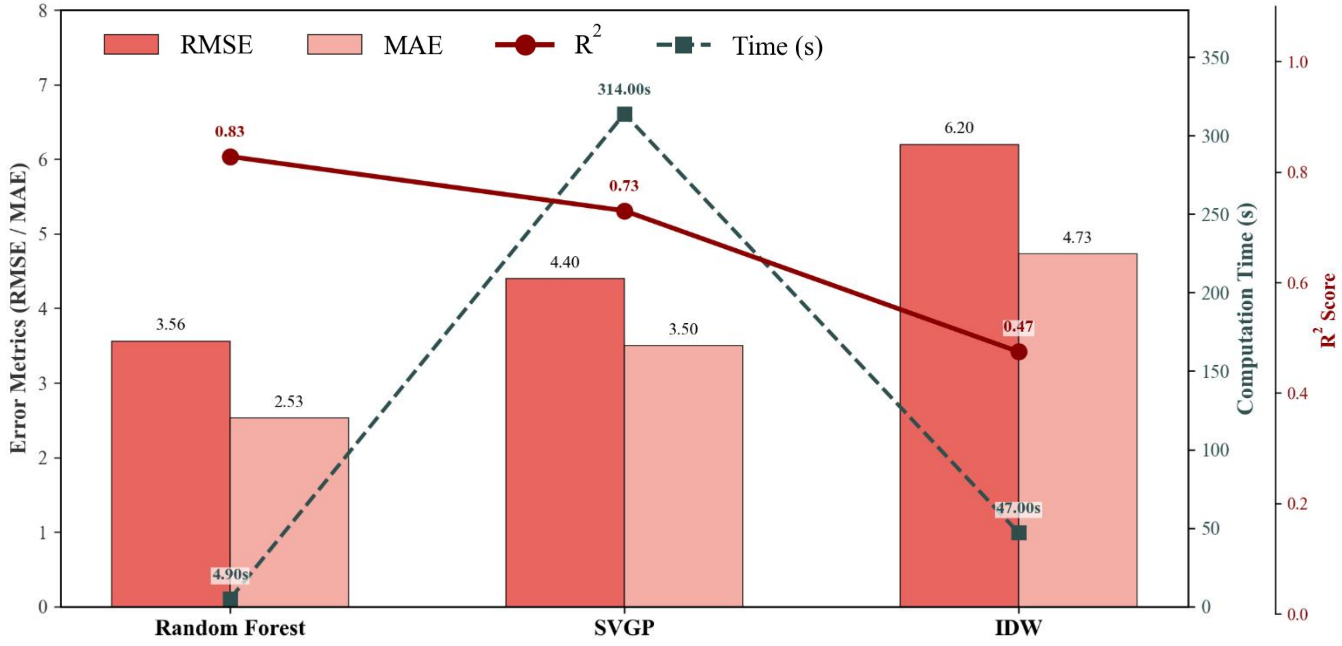

1. Random Forest (Best Accuracy)
Lowest RMSE, Highest R^2, Fastest model
Limitation: No uncertainty estimates

2. SVGP (Best Probabilistic Performance)
Good accuracy
Provides **well-calibrated uncertainty**
Trade-off: Highest computational cost (314 s)

3. IDW (Weakest Performance)
Highest error, Lowest R^2, No uncertainty estimation
Moderate runtime (47 s)

5.4.1 Comparaison of different kernels

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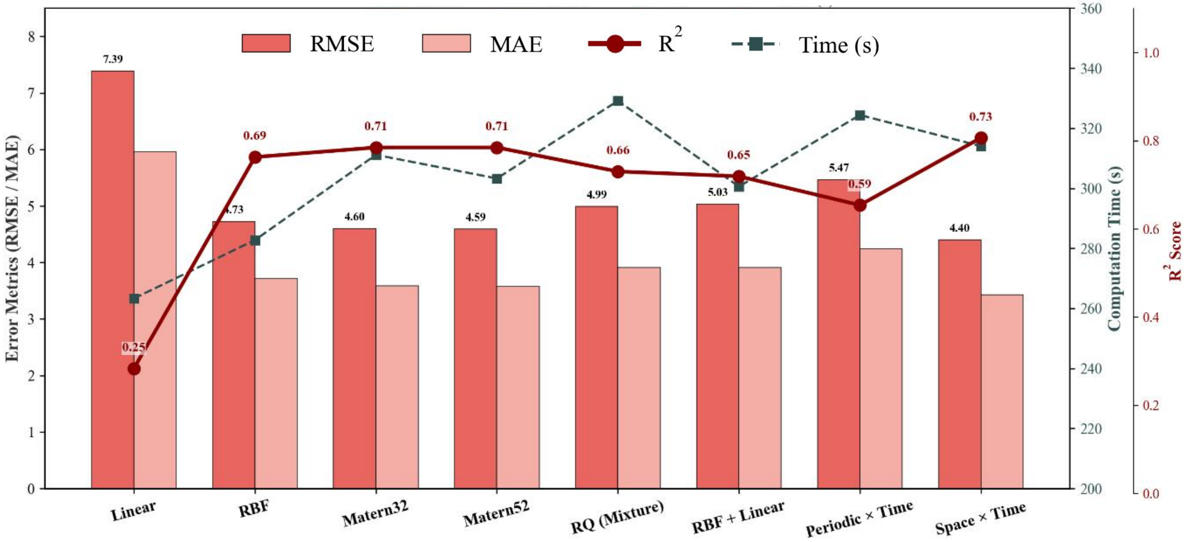
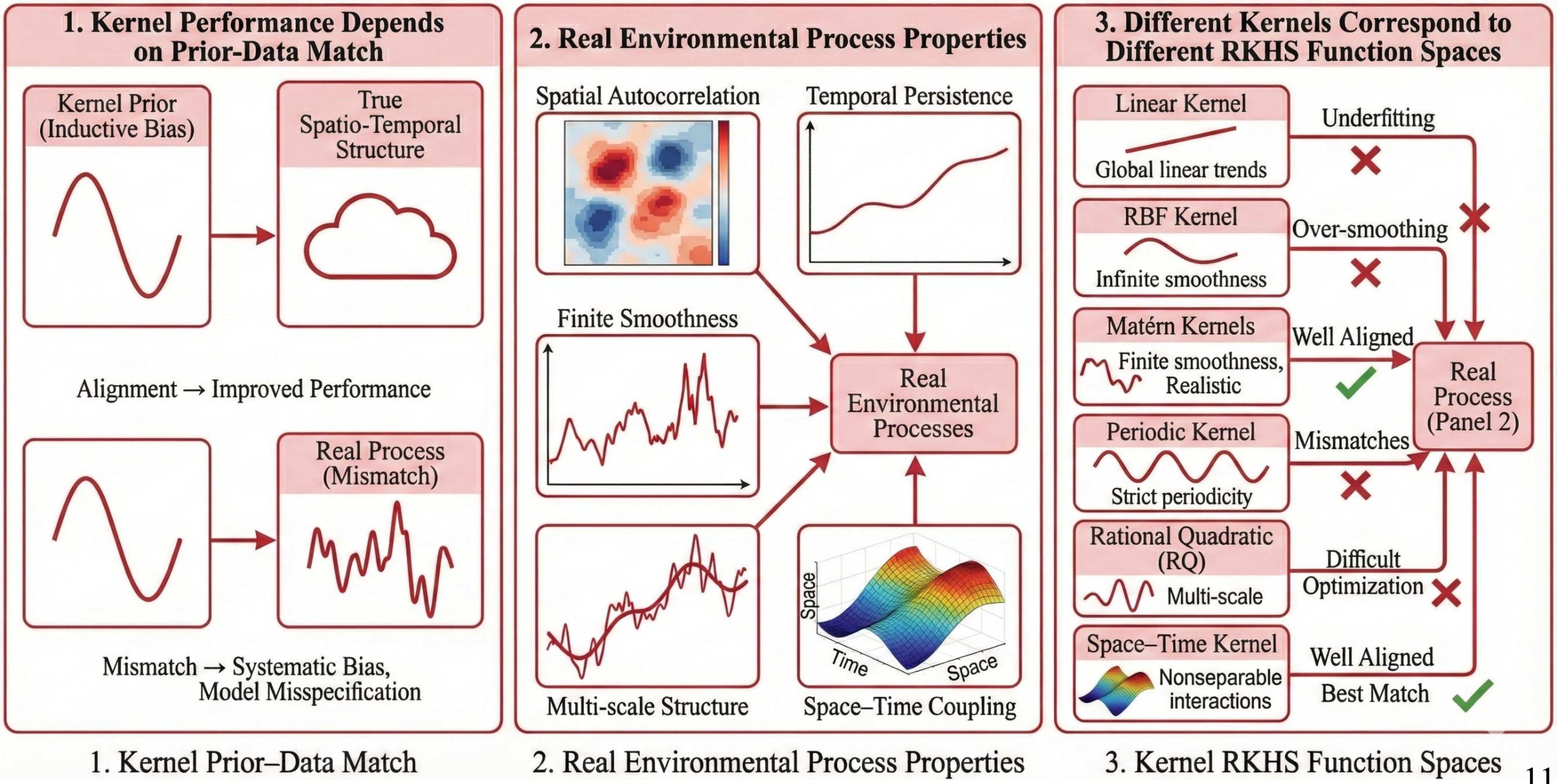


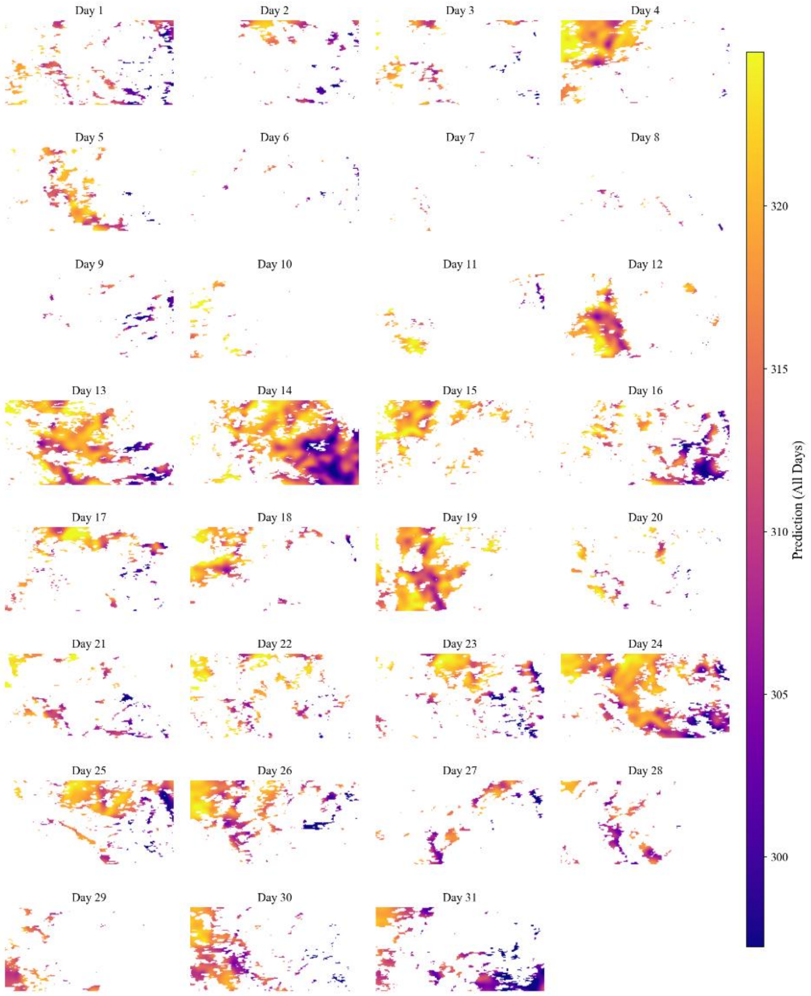
1. **Space–Time kernel**
   → most effective and best calibrated
2. **Matern kernels**
   → reliable, strong alternatives
3. **RBF**
   → moderate models
4. **Composite and Linear kernels**
   → significantly less effective

5.4.2 Why Different Kernels Perform Differently

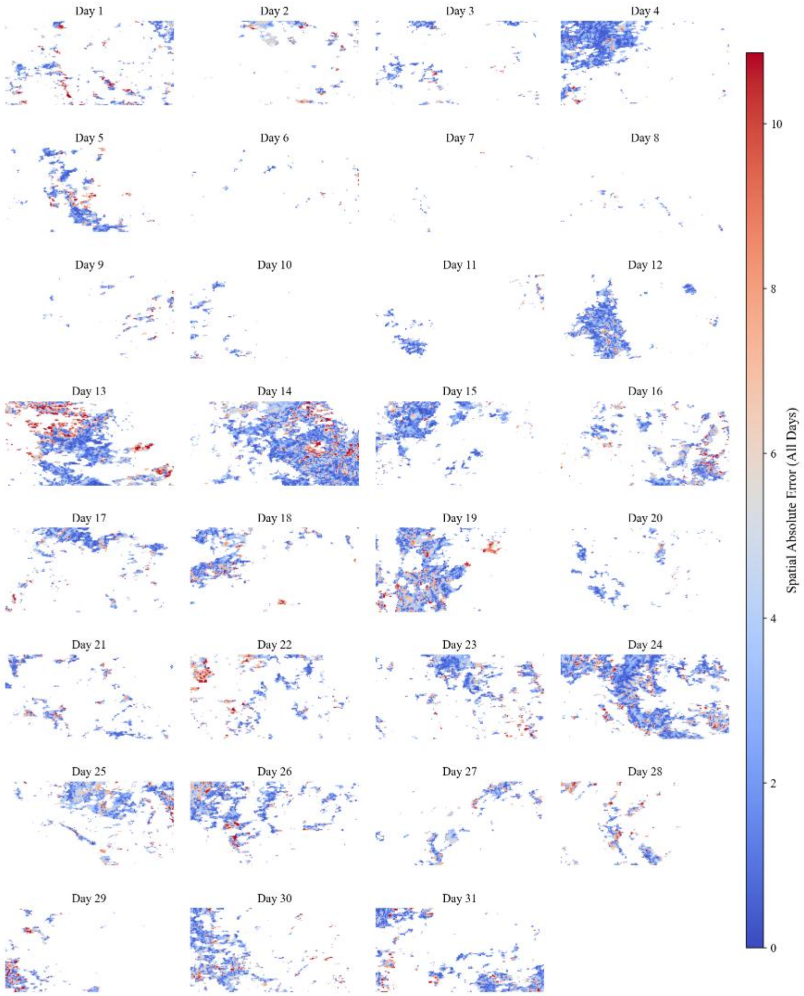


5.4.3 Spatio-Temporal Results of the Space × Time Kernel

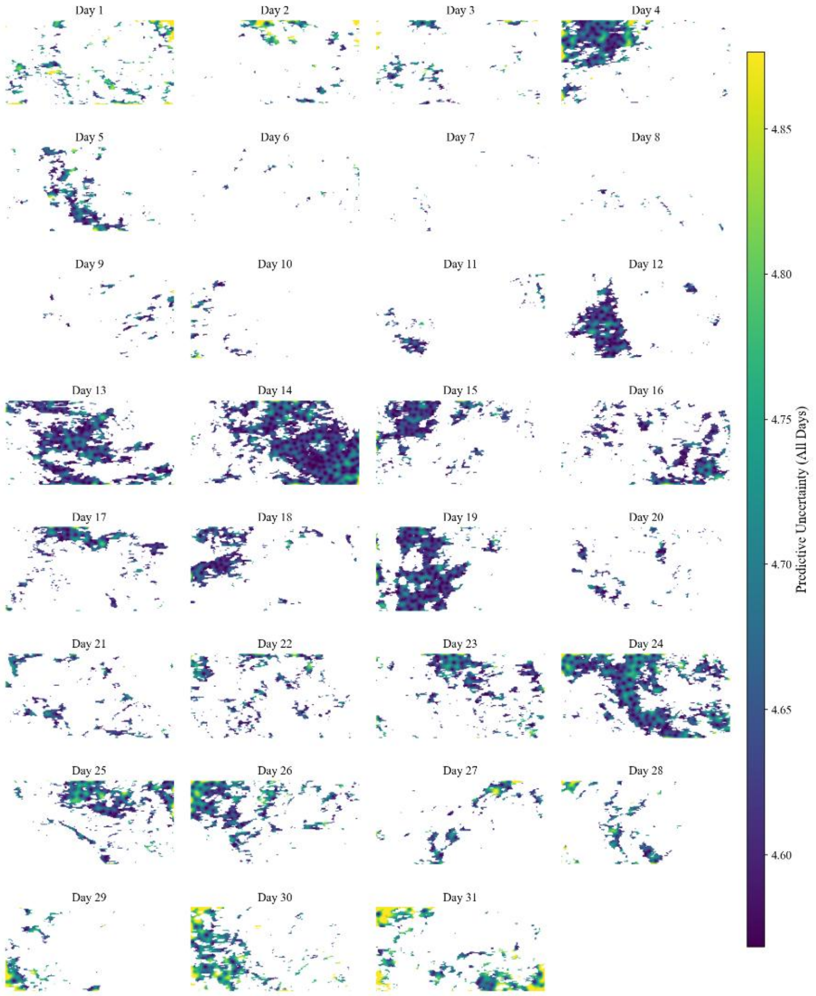
Space × Time Kernel: Prediction



Space × Time Kernel: Spatial Absolute Error



Space × Time Kernel: Predictive Uncertainty



5.4.4 Interpreting the Space × Time Kernel Performance

1. Prediction Maps: Strong Spatio-Temporal Coherence

- Smooth spatial gradients and temporally consistent evolution patterns across all 31 days.
- Capture nonseparable spatio-temporal dependencies (broad patterns & localized transitions)

2. Spatial Error: Concentrates in High-Variability Regions

- Errors remain mostly low, consistent with strong RMSE/R^2 performance.
- Discrepancies localize in areas with:

-Rapid temporal changes
-Strong spatial gradients
-Dynamic boundaries

3. Predictive Uncertainty: Well-Calibrated & Interpretable Patterns

Spatially structured (Not noise)

- Forms coherent patterns representing systematic epistemic uncertainty

Physically Meaningful:

- Uncertainty increases in:

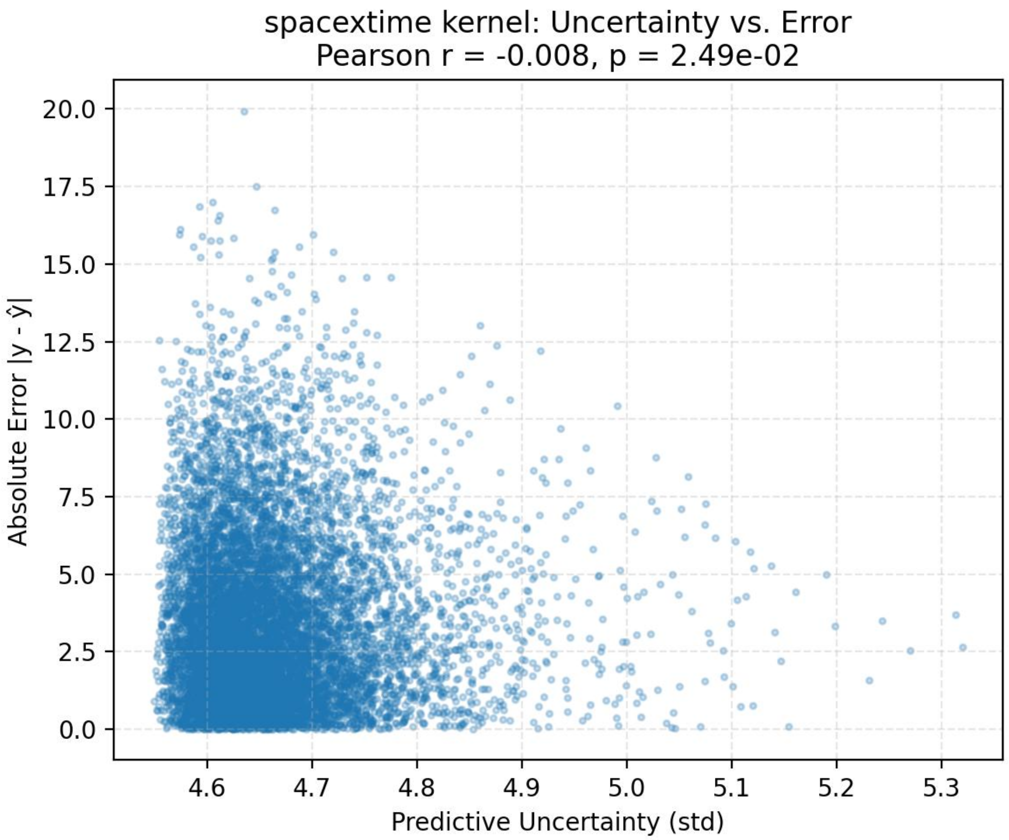
-Data-sparse regions
-Complex dynamics or rapid changes

Excellent Calibration
High sharpness (narrow intervals) + correct coverage (PICP=0.96) indicates an exceptionally well-calibrated GP.

4. Integrated Interpretation: Model Validation

Accurate mean predictions, spatially coherent and interpretable residual patterns, well-structured, meaningful uncertainty estimates aligned with both data density and physical complexity.

5.4.5 Relationship Between Predictive Uncertainty and Error



Key Finding: Predictive uncertainty (std) from the Space–Time SVGP is almost uncorrelated with actual prediction error.

Why This Happens:

- Variational Posterior Variance Collapse

→ predictive std falls within a very narrow range

- Homoscedastic Gaussian Likelihood

→ predictive uncertainty is largely dominated by data geometry (distance to training samples) rather than the intrinsic difficulty of the prediction task.

- Strong Smoothness Imposed by the Space–Time Kernel
- Environmental Data Are Highly Smooth

Implications:

Uncertainty Does Not Track Error
Globally Calibrated but Not Locally Calibrated
Uncertainty Reflects Data Density, Not Epistemic Risk

5.5.1 Effect of Incorporating Elevation into the SVGP Model

Model	Kernel	RMSE	MAE	R2	CRPS	PICP	MPIW	Time(s)
SVGP	RBF	4.73	3.72	0.69	2.65	0.96	19.23	282.76
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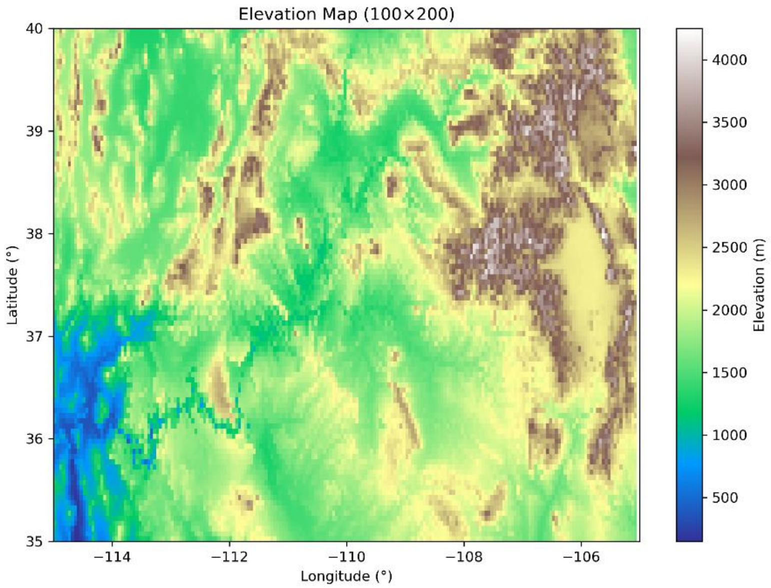
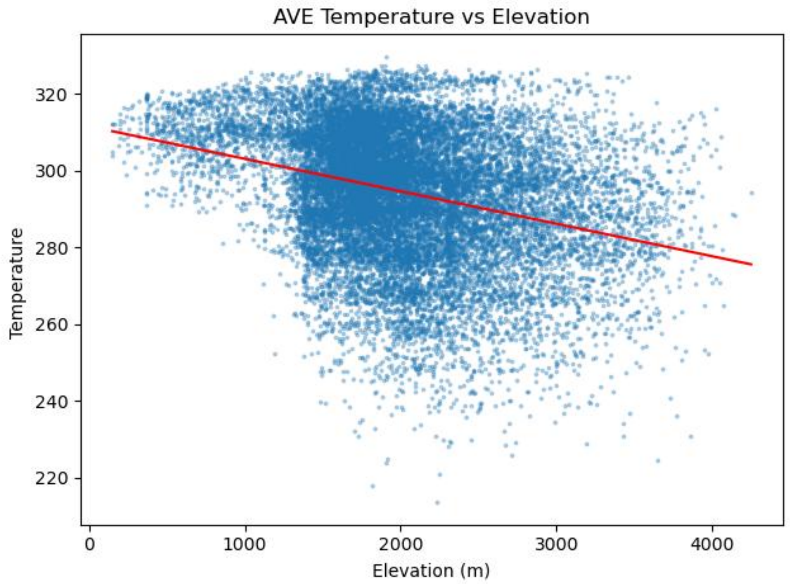
- **Adding Elevation as an input yields only marginal gains**
  Minimal improvement (e.g., 4.40 → 4.44)
  20–30% higher computation
  Indicates elevation effect is mostly absorbed by spatial coordinates
- **Multi-output SVGP increases cost but not accuracy**
  Training time nearly doubles
  Very similar RMSE and R^2
  Cross-output correlation too weak to offer benefit

5.5.2 Why Elevation Fails to Improve Prediction Accuracy





Insights from Temperature–Elevation Scatter Plot

- Clear global negative trend → elevation matters
- But large vertical spread → strongly nonstationary & heteroscedastic effect
- Elevation strongly collinear with spatial coordinates
- Sparse high-elevation samples

Why Elevation Adds Little Benefit?

- Elevation–temperature relationship is nonstationary
- Spatial coordinates already encode major elevation trends
- Uneven elevation distribution impairs uncertainty learning
- Model ends up capturing only a weak global trend

Why Multi-output SVGP Fails to Improve Performance?

- Cross-output correlation is weak → limited information sharing
- Shared inducing points lead to underfitting each output
- Increased complexity does not increase representation power
- High computational cost with minimal benefit

6. Conclusion

1. SVGP provides a principled probabilistic framework

- Balances predictive accuracy and uncertainty quantification.
- More suitable for environmental modeling than deterministic methods (RF/IDW).

2. Space × Time kernel achieves the best performance

- Captures spatial autocorrelation and temporal continuity.
- Best results in RMSE, spatial coherence, and probabilistic metrics (CRPS/PICP).

3. Elevation contributes limited improvement

- Temperature–elevation relationship is highly non-stationary.
- Latitude/longitude already encode most terrain structure → marginal gain.
- Multi-output GP increases computational cost with little benefit.

4. Key limitation: local uncertainty does not track error

- Variational inference leads to variance collapse and narrow predictive std.
- Global calibration is good, but uncertainty ≠ local error.

7. Future work

1. Improved uncertainty modeling

•Heteroscedastic or non-Gaussian likelihoods for adaptive local uncertainty.

2. More expressive kernels

•Deep Kernel Learning (DKL), non-stationary kernels, spatially varying length-scales.

3. Enhanced calibration

•Conformal Prediction for locally reliable prediction intervals.

Course project presentation

Thanks for your listening!

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