

Estimating Biases for Regional Methane Fluxes

Employing Temporally Varying Random-Field Representations of Biases

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Introduction

- Top-down estimates of regional CH_4 emissions in the San Francisco Bay area are highly uncertain.
- Mismatch between measured and modeled receptor concentrations using inventories for CH_4 can vary greatly during an individual month
- Potential sources of model bias include inadequacies or errors in the atmospheric transport modeling and in the emissions inventory.
- Here we infer the model bias as time-varying parameter to improve estimates and help diagnose the sources of mismatch between measurements and our expectation based on an emissions inventory.

Site Information

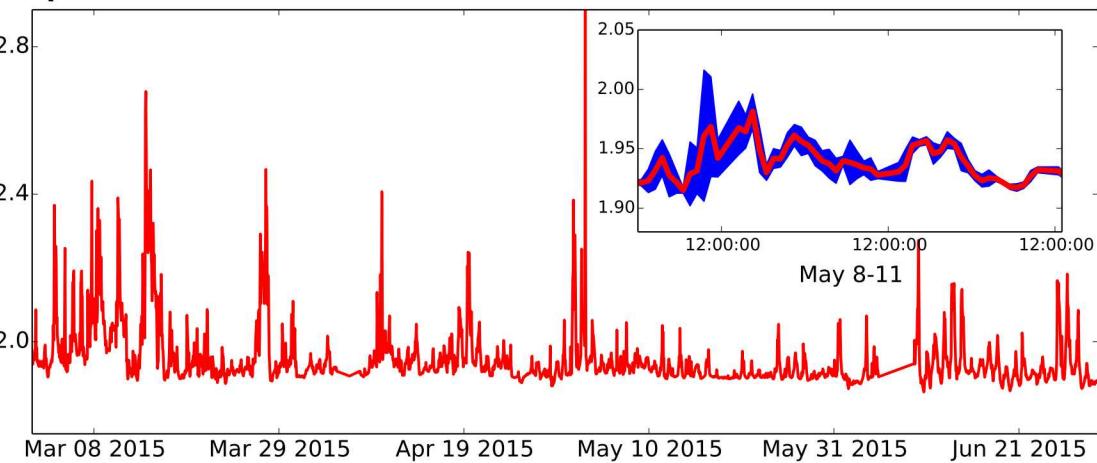
- Location:** Livermore, CA, ~150 m above sea level, 64 km south-east of San Francisco. Prevailing westerly winds provide frequent Pacific Ocean background



- Tower:** Inlet height: 27 m above ground level

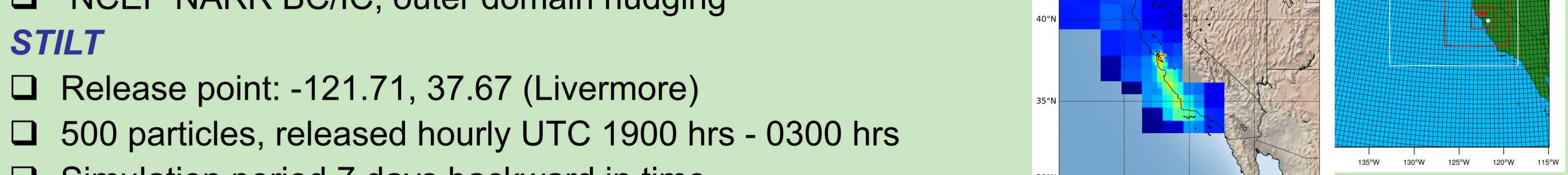
- Instrumentation:**
 - Climate-controlled 30-ft mobile laboratory
 - Cavity ringdown spectrometer for CH_4 , CO_2 , H_2O (Picarro, Inc.)
 - Various other instruments are available but were not used in this study

Example time series in Livermore



Transport Models

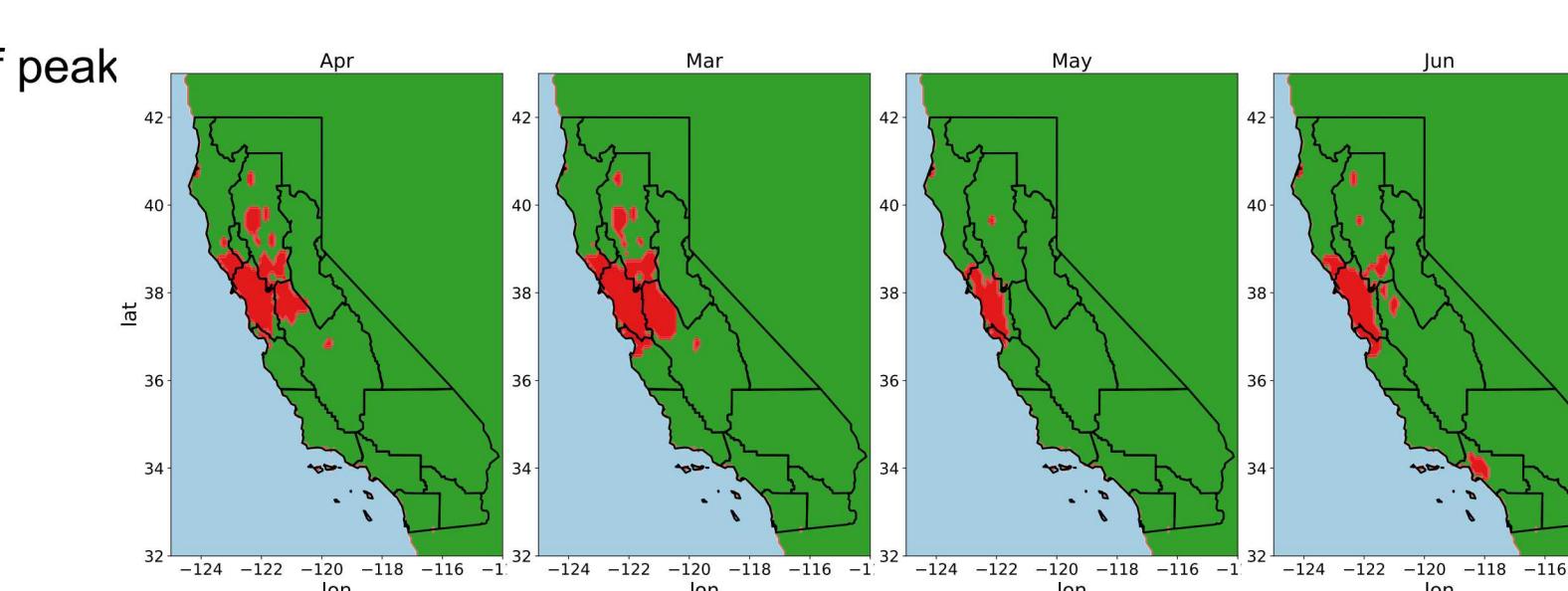
- WRF** v3.9 with 36, 12, 4, 1.3km domains, 50 vertical layers.
- NCEP NARR BC/IC**, outer domain nudging



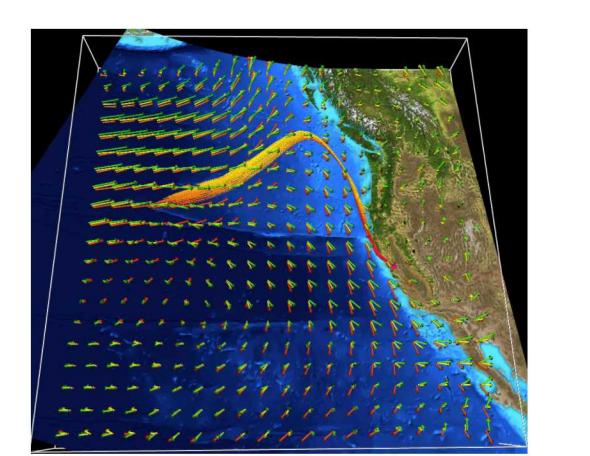
Regions of influence

Threshold for (Footprint) \times (Emissions Inventory) > 0.1% of peak

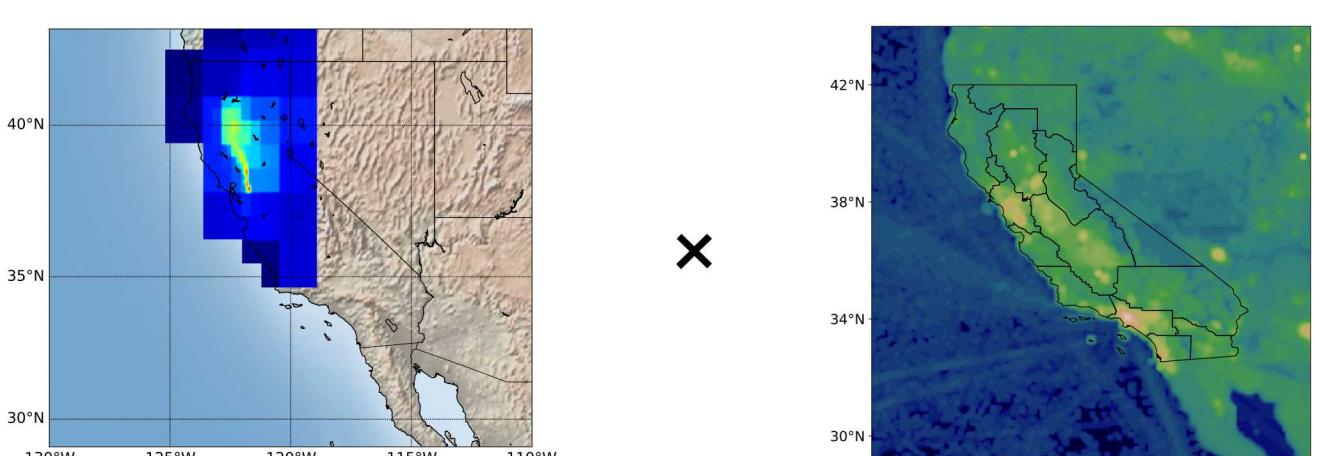
- In the maps (right) red areas indicate land influence above threshold
- Regional air districts and state border shown
- Retain only footprints with >80% marine boundary layer (mbl) influence prior to landfall to select times with an identifiable mbl background.



Forward Model



Trace emissions for 7 days prior using Lagrangian model



Integrated 7 day influence (for a single measurement hour)

Uncalibrated Model
Prior Model for observations: $X_{\text{CH}_4}(t)$
Predicted mixing ratio at our measurement location (before bias correction)

EDGAR v4.3.2, $(0.1^\circ \times 0.1^\circ)$
2012 anthropogenic methane

Bayesian Inference

- Traditional representation for mixing ratio at time i , X_i**

$$X_i = F^{(i)} \cdot \left(\sum_{k=1}^3 \lambda_k E_k \right) + b_i + \epsilon_{d,i} + \epsilon_{m,i} + \epsilon_{b,i}$$

Measurement Footprint Bias Emissions Background Discrepancy terms

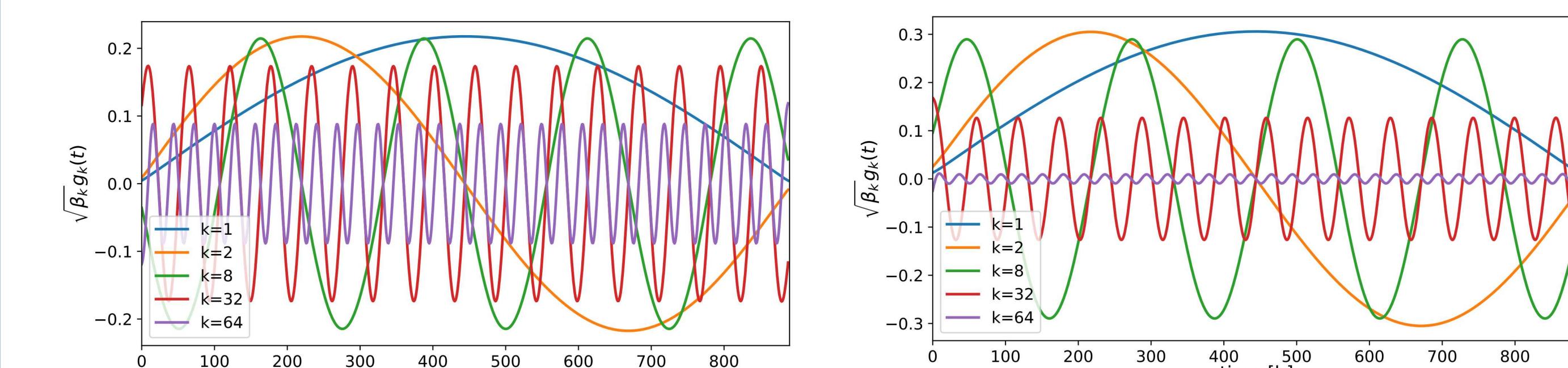
- New representation for mixing ratio at time i , X_i**

- Use Karhunen-Loeve Expansion to capture time dependence of the bias, assuming square exponential covariance:

$$X(t) = b(t) + \sum_{i=-(N_t-1)}^0 \left(\lambda_0 + \sum_k c_k \frac{1}{\delta t} \int_{t_{i-1}}^{t_i} \sqrt{\beta_k} g_k(t) d\tau \right) \sum_j F_{t,i}(x_j) E(x_j), \text{ where } \sqrt{\beta_k} g_k(t)$$

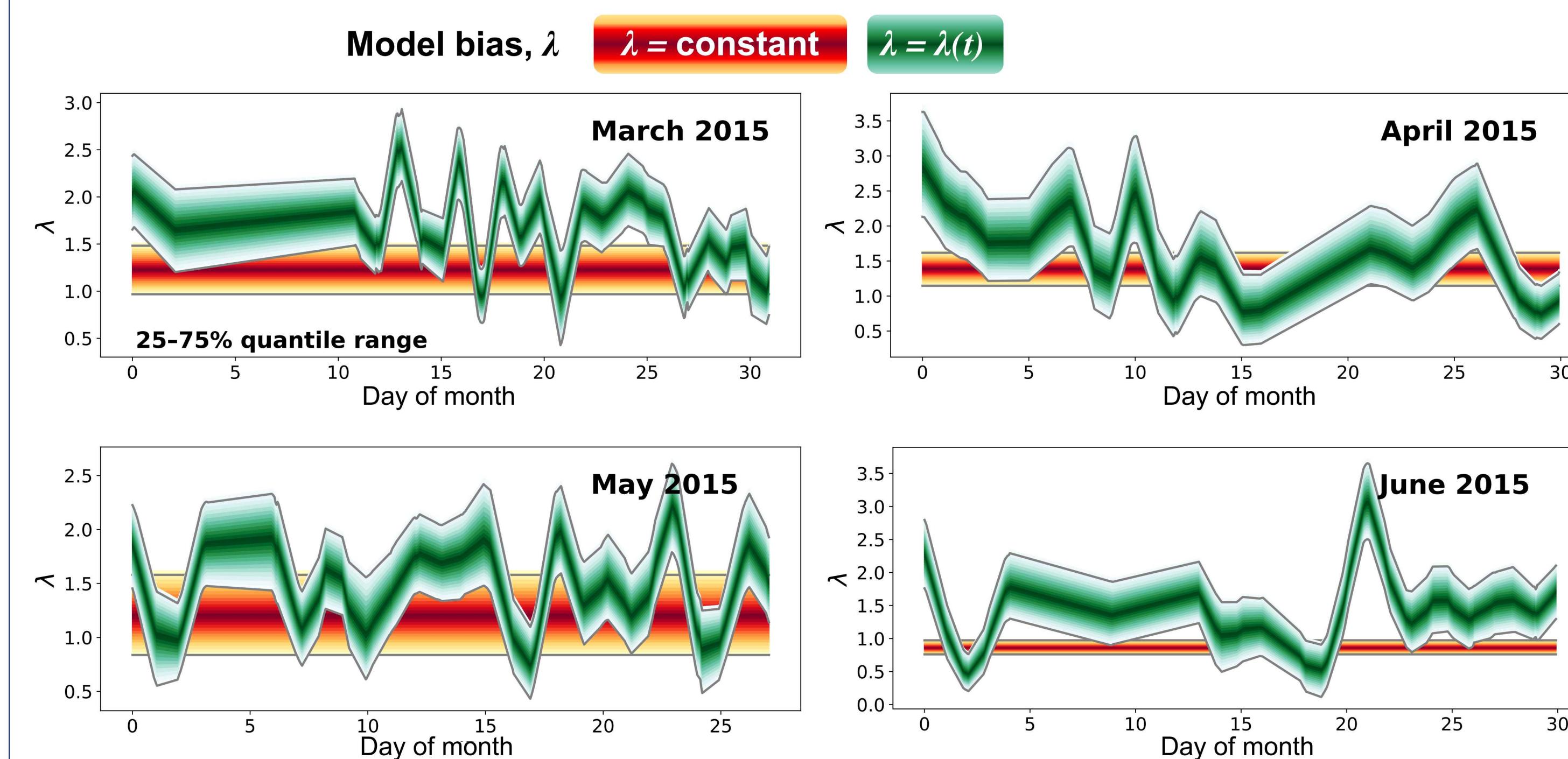
are the Karhunen-Loeve Expansion functions, and c_k are the coefficients to be inferred

KLE basis sets: correlation length = 12 hrs



correlation length = 24 hrs

- Employ Bayes formula and Adaptive-Metropolis Markov Chain Monte Carlo sampling to explore the posterior
- $p(\lambda, \sigma_m, \mu_\lambda, \sigma_\lambda, \delta_b, \tau_c | y) \sim p(y | \lambda, \delta_b, \sigma_m, \tau_c) p(\lambda | \mu_\lambda, \sigma_\lambda) p(\mu_\lambda) p(\sigma_\lambda) p(\tau_c) p(\sigma_m) p(\delta_b)$
- Construct posterior probability for model bias, $\lambda(t)$, and compare to constant bias assumption:



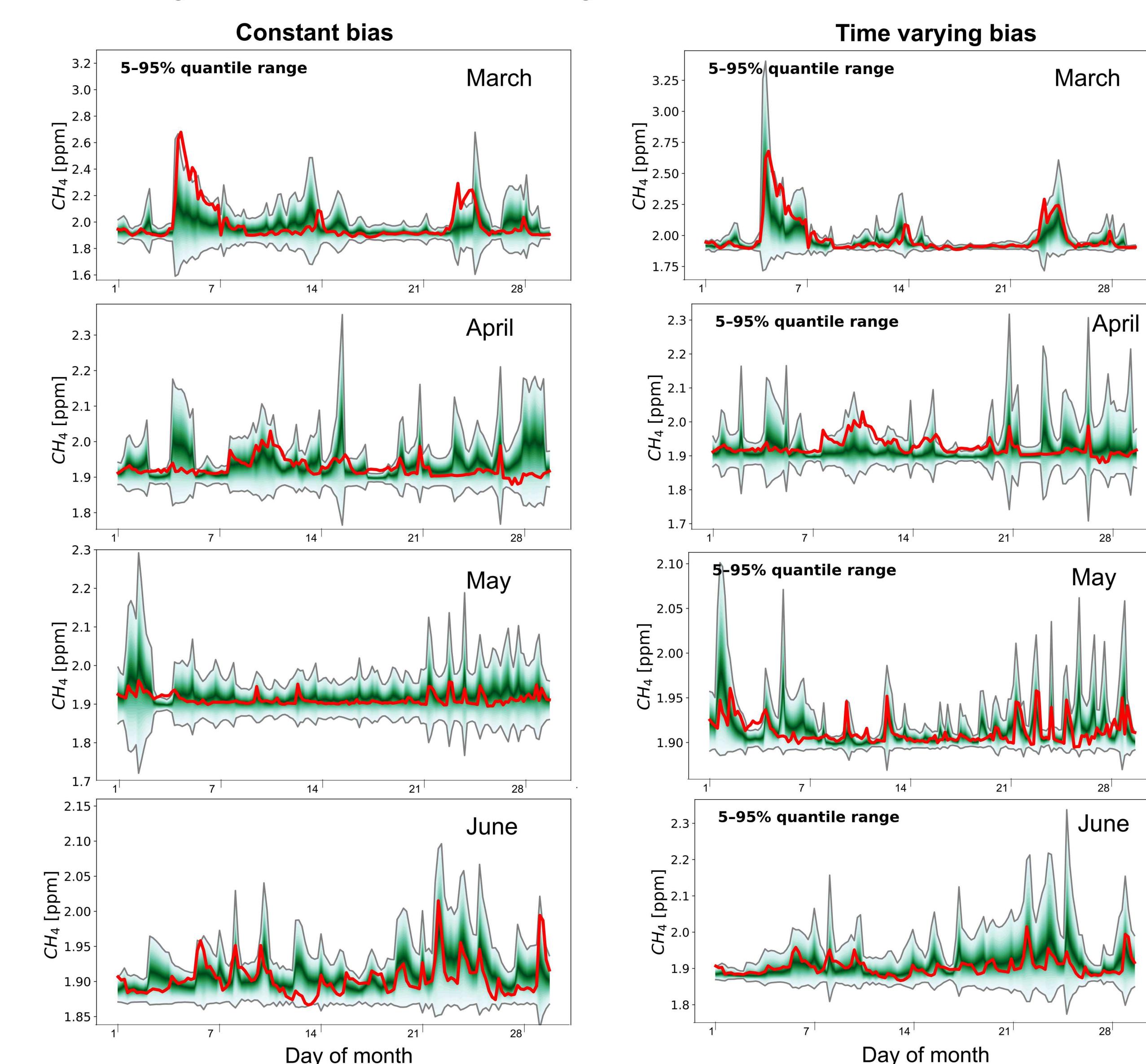
Acknowledgements

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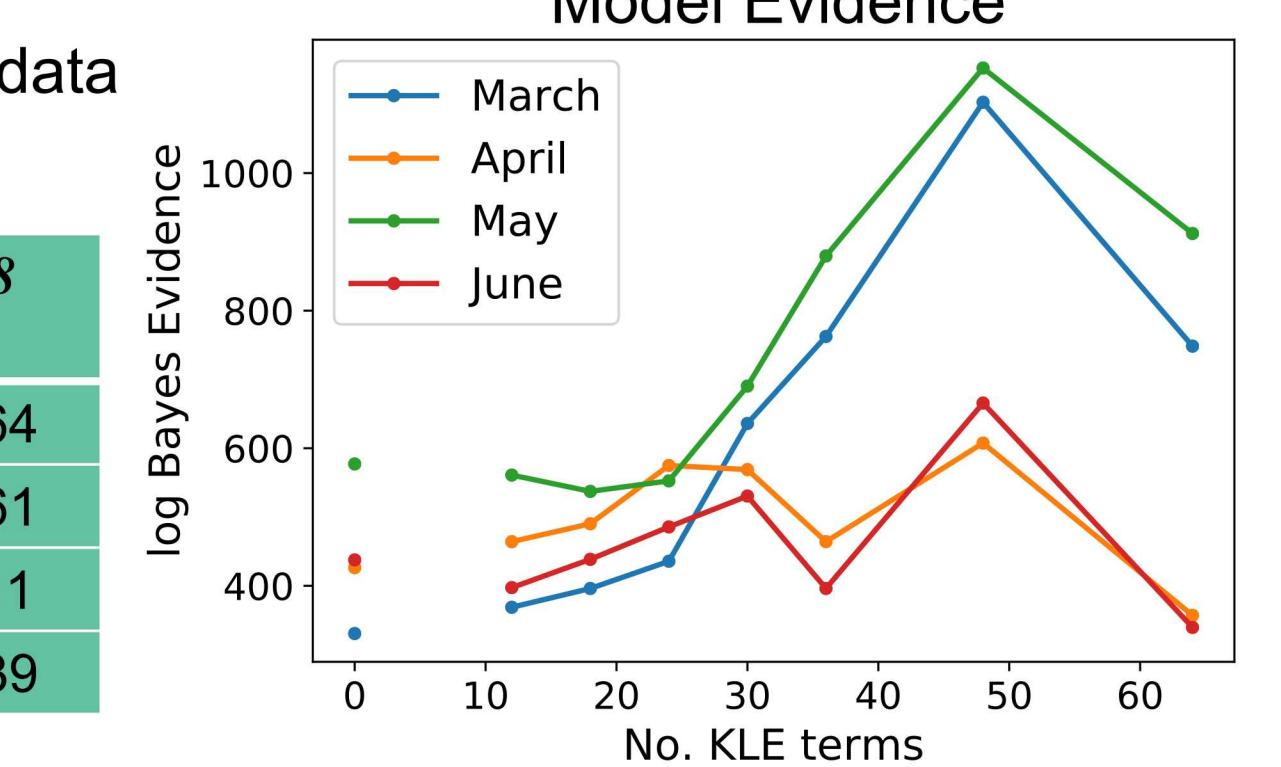
Comparing Assumptions for Model Bias

- Compute the model calibrated to observations (posterior predictive) and compare model assuming constant bias with model using 48 KLE modes:



- Compare marginal likelihoods (probability of data given model) to determine "optimal" model

	$k=0$	$k=0$	$k=30$	$k=30$	$k=48$	$k=48$
	λ	σ_λ	λ	σ_λ	λ	σ_λ
March	1.241	0.448	1.342	0.286	1.713	0.264
April	1.382	0.384	1.523	0.347	1.696	0.661
May	1.260	0.635	1.101	0.186	1.537	0.311
June	0.875	0.191	1.057	0.239	1.461	0.439



Conclusions and Next Steps

- Employing a temporally varying bias improves representativeness of the posterior predictive model
- Uncertainty in the posterior model may increase in certain cases and may indicate other model inadequacies
- Inversions will be performed on additional months to examine an entire year
- Temporal structure will be analyzed to diagnose the source of the variations
- Alternative emissions inventories to EDGAR will be analyzed

UQToolkit: <http://www.sandia.gov/UQToolkit/>
NOAA flask measurements: <https://www.esrl.noaa.gov/gmd/dv/data/>
EDGAR priors: <http://edgar.jrc.ec.europa.eu/overview.php?v=42FT2010>
Olivier, J.G.J. and Janssens-Maenhout, G., CO2 Emissions from Fuel Combustion -2016 Edition, IEA CO2 report 2016, Part III, Greenhouse-Gas Emissions, ISBN 978-92-64-25856-3, 2016b.
Ganesan, A. L. et al. (2014), Characterization of uncertainties in atmospheric trace gas inversions using hierarchical Bayesian methods. Atmos. Chem. Phys., 14, 3855-3864, doi:10.5194/acp-14-3855-2014.
Jeong, S., et al. (2016), Estimating methane emissions in California's urban and rural regions using multi-tower observations, J. Geophys. Res. Atmos., 121, doi:10.1002/2016JD025404.

References