Supporting Information for:

Application of PRIM for understanding patterns in carbon dioxide model-observation differences

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Supporting Methodology

Example for PRIM Trajectory

The PRIM algorithm seeks to find regions of high density for a specific target class within the entire parameter space of observations, by creating a trajectory of more restrictive rectangular boxes leading to a set of increasingly restricted dimensions associated with narrower parameter ranges for atmospheric variables associated with the target class. As the density of the target class inside the PRIM box increases, an increasing number of observations belonging to the target class will fall outside the box, such that coverage of the target class will decrease. Following along the density-coverage trajectory, parameter ranges can be retrieved for each restricted dimension at each coverage level.

In the illustration below (Figure S1), we find that 73.9% of Fair Weather ABL Observations during Summer 2016 can be found in only 6.4% of the entire parameter space (Mass), which is defined by the displayed restricted dimension range. The resulting box has a density of 52.9% target observations, indicating some overlap between the target class and other classes.

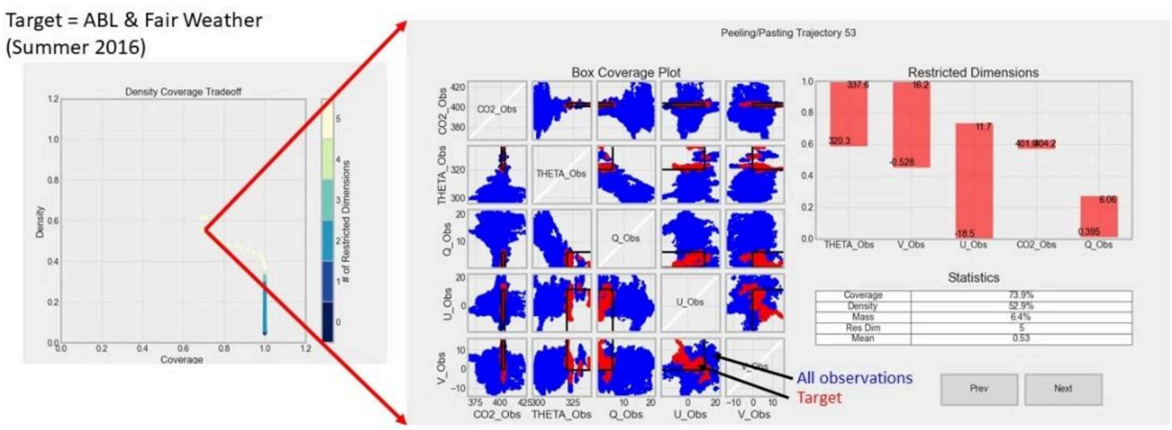

Figure S1: *Illustration of PRIM peeling trajectory to identify high density regions of a target class (Fair Weather ABL Observations during Summer 2016) within a parameter space*

Supporting Tables

Table S1: ACT-America flights considered in this manuscript (Table modified from Gerken et al. 2021)

Campaign	**Region**	**Start & End Dates**	**# Flight Days**[a]
Summer 2016	Northeast Mid-Atlantic	June 18-27	7
	Mid-West	August 1-14	10
	South Central	August 16-28	9
Winter 2017	Northeast Mid-Atlantic	January 30 to February 12	8
	Mid-West	February 13–26	9
	South Central	February 27 to March 10	9

[a] Transit flights between regions are attributed to their destination region

Table S2: *PRIM box limits for target coverage of 0.75 separated by season, level, and airmass. Values correspond to lines in Figure 2. See main text for details.*

	ABL						LFT						HFT					
Season	Sector	Variable	Min	Max	Cov	Density	Sector	Variable	Min	Max	Cov	Density	Sector	Variable	Min	Max	Cov	Density
Summer 16	Fair	θ	296.24	307.20	0.76	0.79	Fair	$[CO2]$	367.83	402.70	0.74	0.74	Fair	θ	319.40	337.57	0.98	0.41
		v	-3.26	5.72				θ	305.48	317.03				$[CO_2]$	400.28	404.54		
		$[CO_2]$	367.83	403.34				q	0.16	11.64				u	-18.50	15.80		
		u	-18.50	7.87				u	-18.50	9.18				v	-7.64	43.68		
		q	4.57	21.67				v	-37.28	4.68				q	0.38	7.16		
	Warm	q	5.89	21.67	0.75	0.20	Warm	u	1.79	22.41	0.74	0.43	Warm	$[CO_2]$	394.68	403.88	0.84	0.59
		θ	300.18	322.10				θ	306.55	321.90				θ	317.76	332.86		
		v	-0.30	43.68				q	3.86	17.08				u	-2.19	27.14		
		u	-4.94	57.63				$[CO_2]$	398.12	404.98				q	0.15	8.74		
		$[CO_2]$	384.98	427.20														
	Cold	θ	296.10	303.38	0.75	0.36	Cold	θ	306.97	318.48	0.77	0.13						
		q	6.69	16.13				q	1.01	7.36								
		$[CO_2]$	367.83	405.98				$[CO_2]$	395.56	405.70								
		u	-5.55	14.77				v	-6.56	43.68								
		v	-37.28	7.72														
Winter 17	Fair	$[CO_2]$	408.68	416.86	0.76	0.86	Fair	$[CO_2]$	404.24	412.06	0.75	0.66	Fair	q	0.03	0.47	0.76	0.60
		q	0.92	9.02				θ	273.68	308.20				$[CO_2]$	404.36	412.02		
		u	-18.50	14.25				u	5.18	31.82				θ	283.76	337.57		
		v	-6.63	13.91				q	0.03	5.81				v	-37.28	18.44		
		θ	264.25	303.58														
	Warm	θ	285.76	297.88	0.75	0.38	Warm	$[CO_2]$	405.38	412.72	0.76	0.25						
		q	4.06	15.35				θ	296.02	313.42								
		v	0.97	43.68				v	-0.77	43.68								
		u	-3.35	16.16				q	0.16	8.26								
		$[CO_2]$	404.90	427.20				u	-18.50	24.18								
	Cold	q	2.12	18.01	0.76	0.52	Cold	q	0.95	4.76	0.74	0.25						
		v	-37.28	-0.87				$[CO_2]$	406.64	410.56								
		θ	272.23	297.62				θ	293.26	308.64								
		$[CO_2]$	404.46	427.20				u	-18.50	18.59								
		u	-18.50	21.19														

Units are: $[CO_2]$: ppm; θ: K; q: g kg^{-1}; u-wind: m s^{-1}; v-wind: m s^{-1}

Supporting Figures

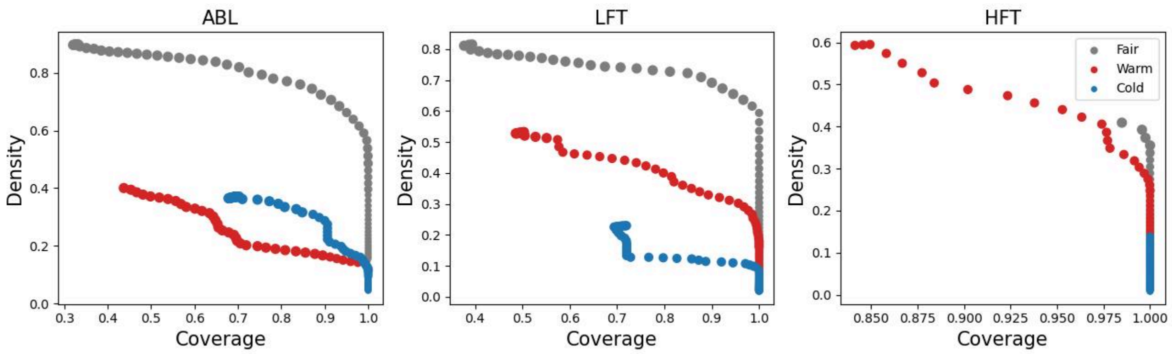

Figure S2: *PRIM Coverage-Density-Tradeoff curve (i.e. peeling trajectory) for Summer 2016 ABL (left), LFT (center), and HFT (right) separated by fair weather, warm, and cold airmasses.*

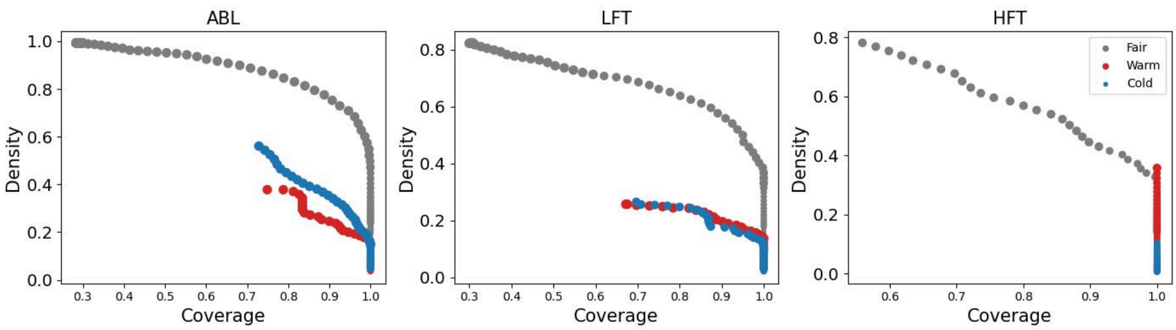

Figure S3: *PRIM Coverage-Density-Tradeoff curve (i.e. peeling trajectory) for Winter 2017 ABL (left), LFT (center), and HFT (right) separated by fair weather, warm, and cold airmasses.*