Clustering Regional Ozone Concentrations to Reveal Meteorological Regimes Influencing Air Quality

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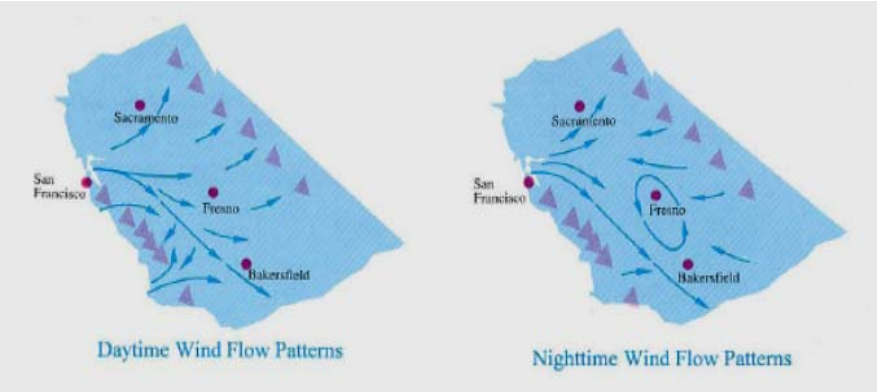
January 13, 2010

Motivations:

1. Meteorological Influences on AQ in Central California



(source: "San Joaquin Valley Air Basin Plan Demonstrating Attainment Of Federal 1-hour Ozone Standards", by San Joaquin Valley Air Pollution Control District, October 8, 2004.)

- Direct effects: ozone chemistry and transport
- Indirect effects: light and temperature sensitive emissions

Motivations:

2. Identify Association between Met and AQ

- Two approaches used in observational studies
  - Meteorological regimes → Pollutant concentrations
  - Pollution regimes → Met conditions
- Limitations in observational studies
  - Spatial representation of measurement locations
  - Local influences vs. regional perspective
  - Emission influences
- Applications to modeled data
  - Suitable for longer-term modeling period
  - Basis for study variability in ozone responses and inter-basin transport

Methods

1. Clustering Ozone → Met Conditions

- Cluster analysis

  Groups large amounts of data into smaller categories so that each subset share some common trait (Everitt, 1993)

- Principal component analysis (PCA)

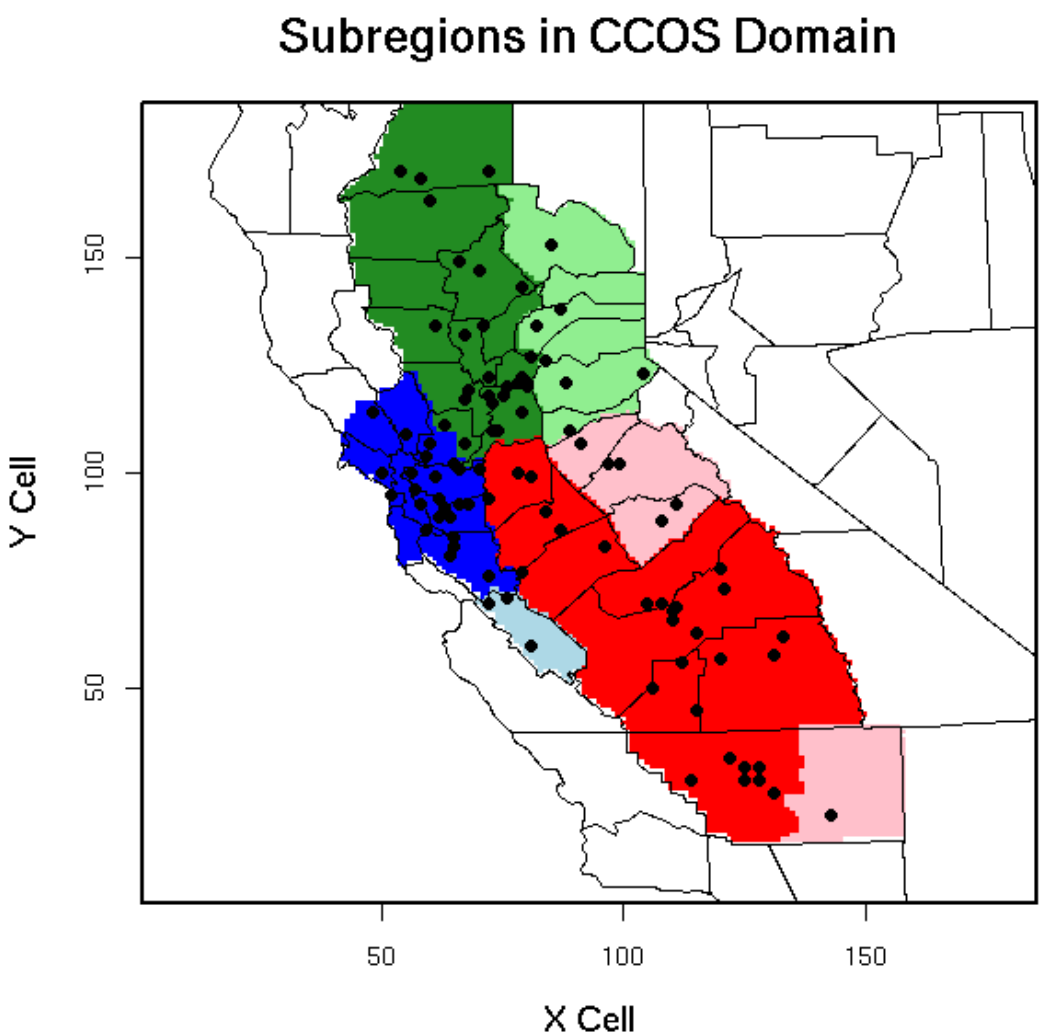
  - Converts data into a new coordinate system
    - Reduced dimension
    - Easier to interpret

- Ozone regimes → Met conditions

  - Cluster (k-means) summer days according to their ozone spatial distributions
    - consider magnitude and spatial extent
    - exclude clean days (< 1% grids exceed 8 h ozone standard)
  - Average met conditions for each ozone clusters

Methods

2. Subregions from CCOS domain



Three subregions in central California for clustering ozone spatial patterns:

SJV (red+pink),
SFB (blue+lightblue),
SV (green + lightgreen).

Black dots are actual ozone measurement sites.

Questions to Address

- Ozone regimes in each subregion
- Met conditions for each ozone cluster (temperature and winds)
- Overall cluster characteristics

  -Ozone and met

  - Inter-basin relationships
- Comparison of clustering results to historical data

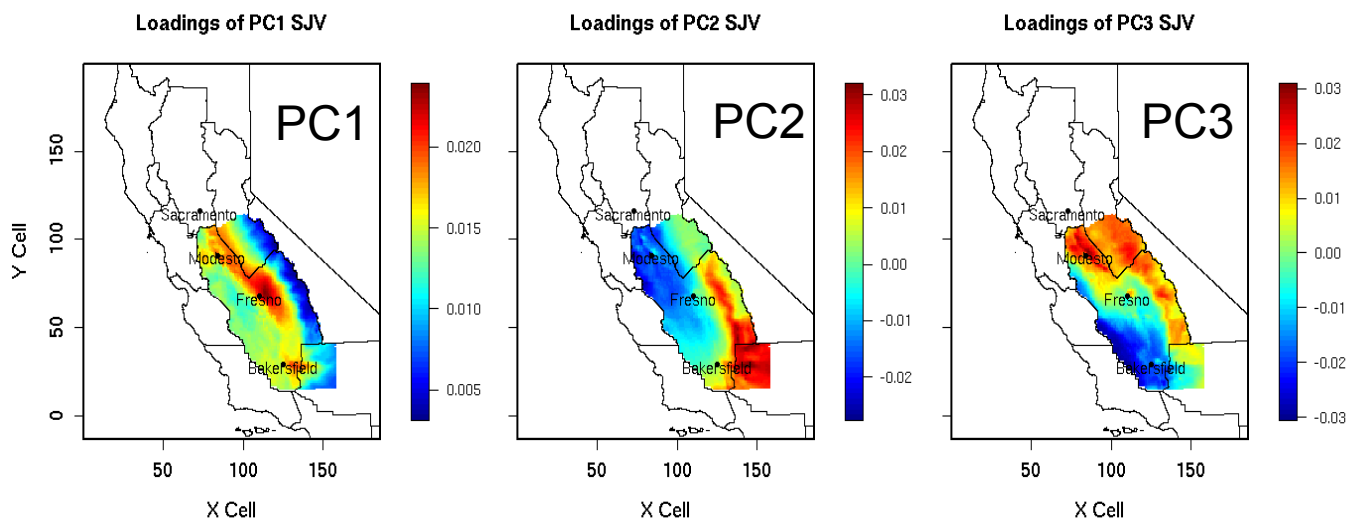
  - Spatial representativeness of measurement sites

  - Weekend effect influences

Result 1 Ozone Clusters:

Principal Components: SJV

- Variations seen in ozone spatial distribution governed by a few patterns: **SJV**



On any given day: **Ozone spatial distribution** =

summer average distribution +

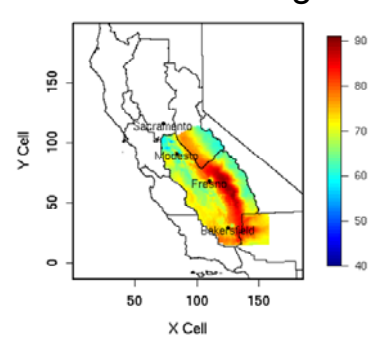
s1 * PC1 + s2 * PC2 + s3 * PC3 + …

si: scores, a scalar value

Summer average: Common to each day

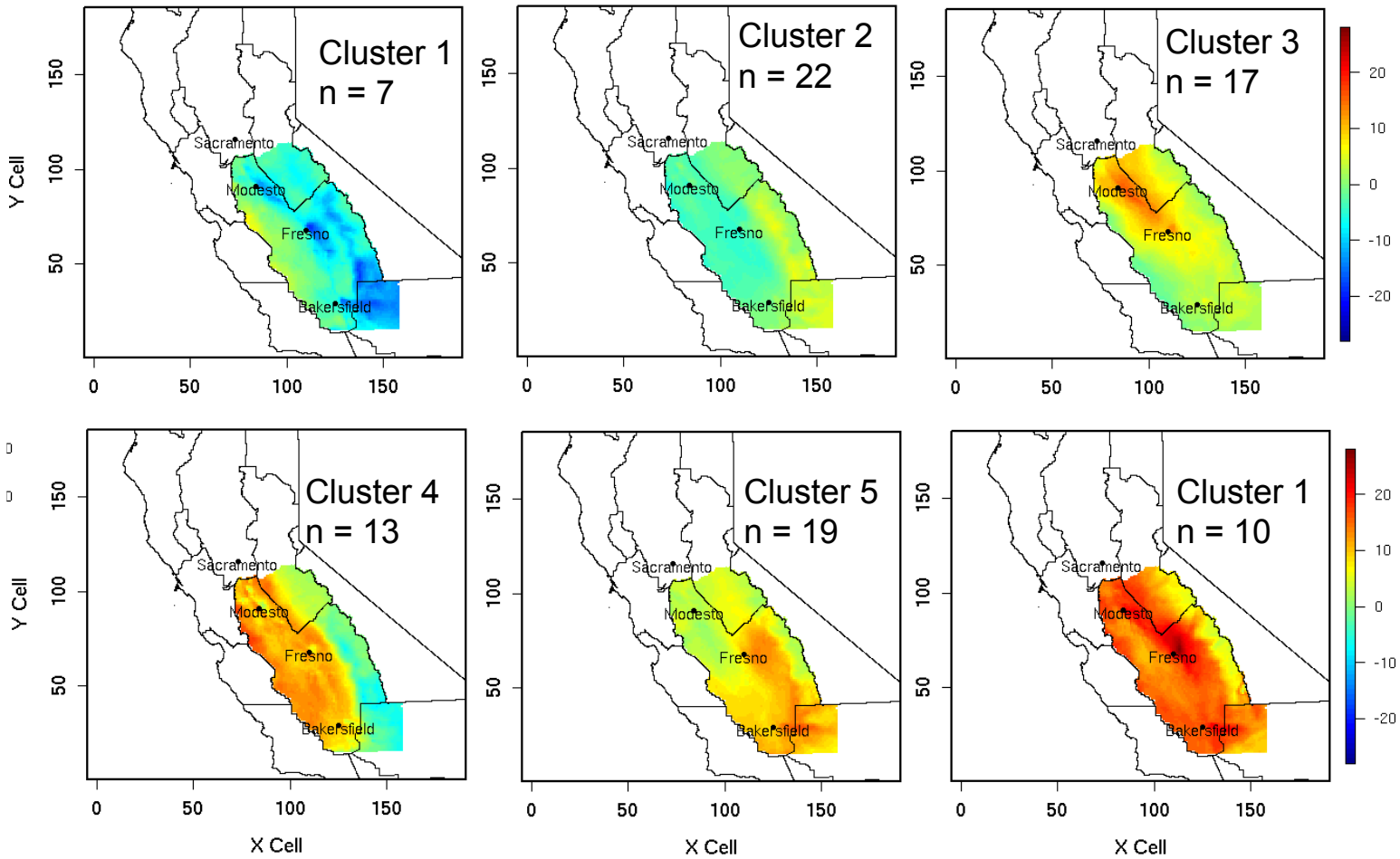
Ozone Anomaly: Distinctive features

Summer Average



Result 1 Ozone Clusters:

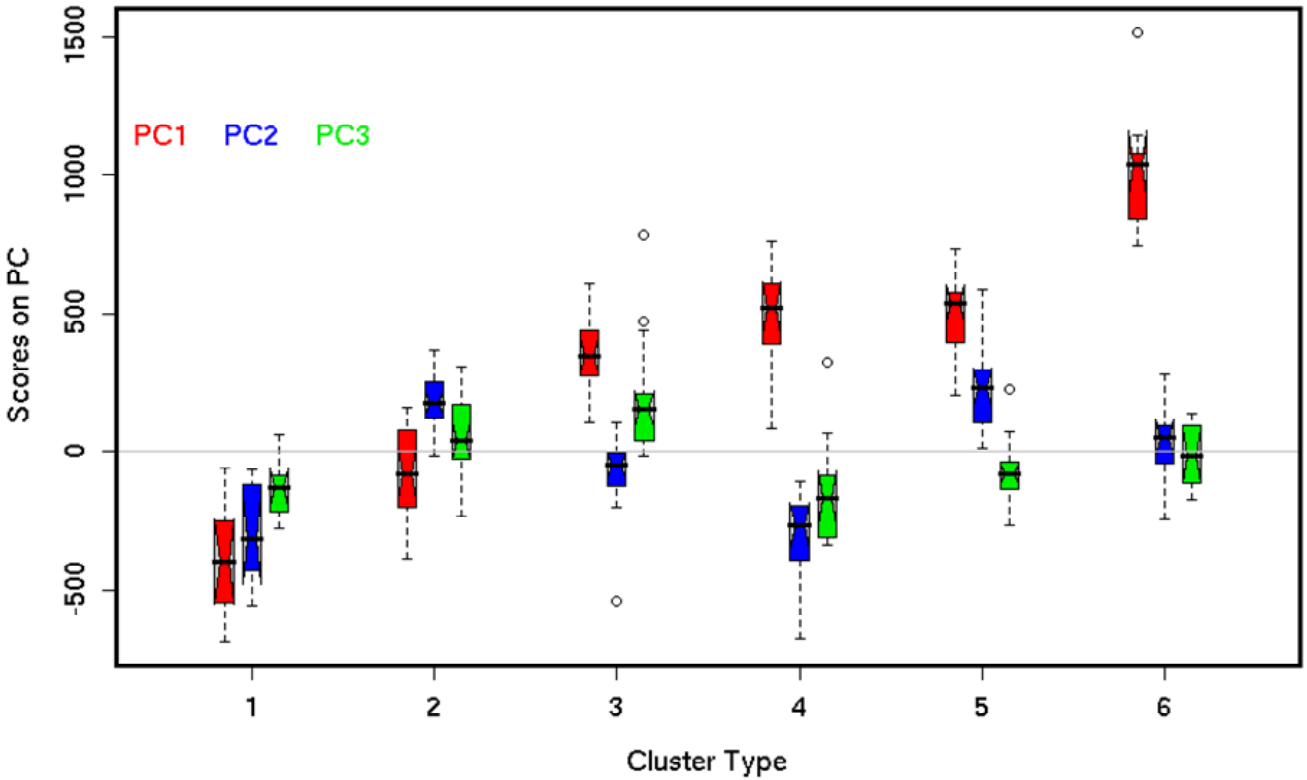
Ozone Clusters: SJV



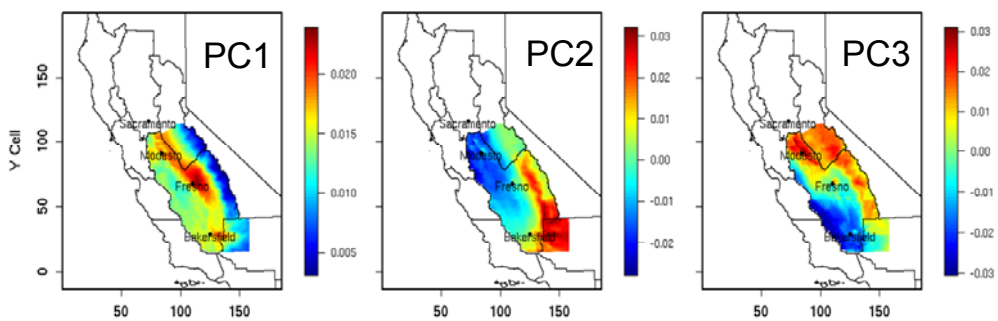
Ozone anomalies averaged over each cluster (= cluster mean – summer mean)

Result 1 Ozone Clusters:

Interpret SJV ozone clusters by PCs



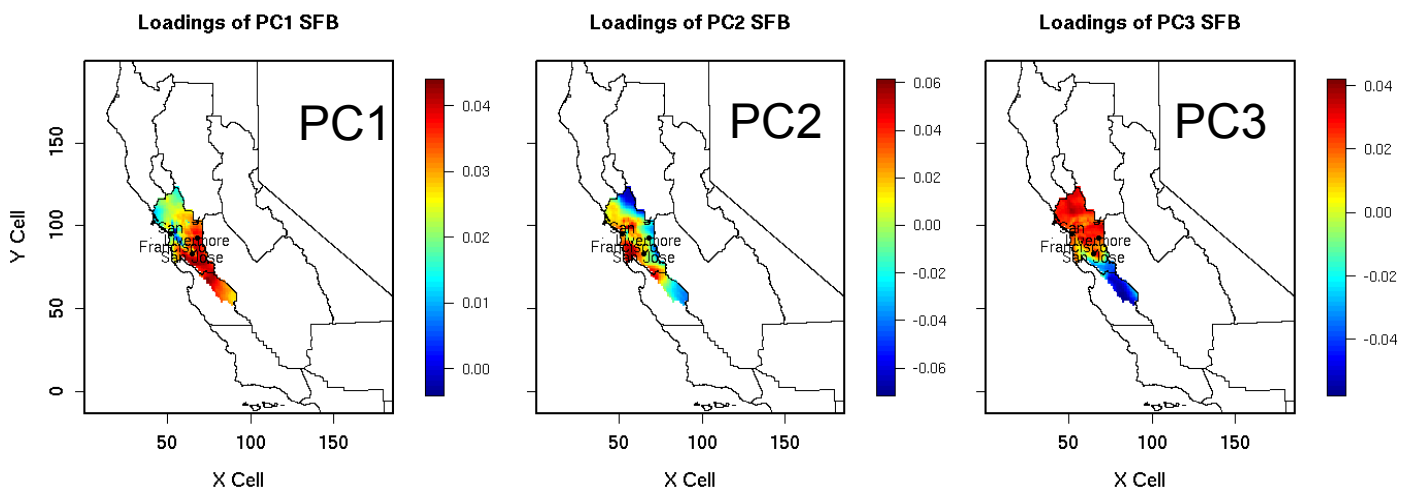
Scores represent how much each component there is in the data.



Result 1 Ozone Clusters:

Principal Components: SFB

- Variations seen in ozone spatial distribution governed by a few patterns: **SFB**



On any given day: **Ozone spatial distribution** =

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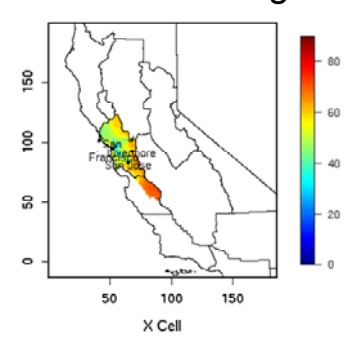
s1 * PC1 + s2 * PC2 + s3 * PC3 + …

si: scores, a scalar value

Common to each day

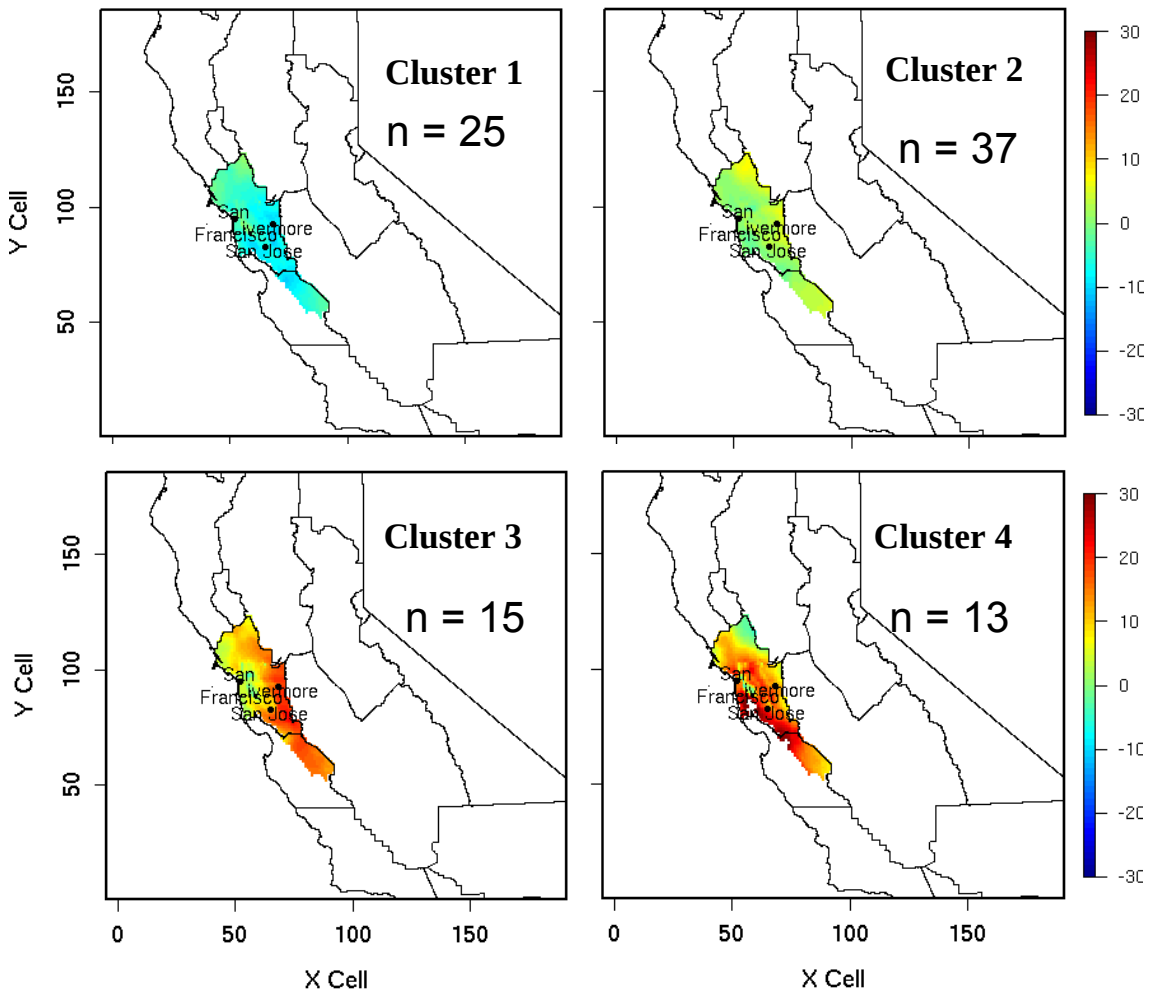
Distinctive features

Summer Average



Result 1 Ozone Clusters:

Ozone Clusters: SFB

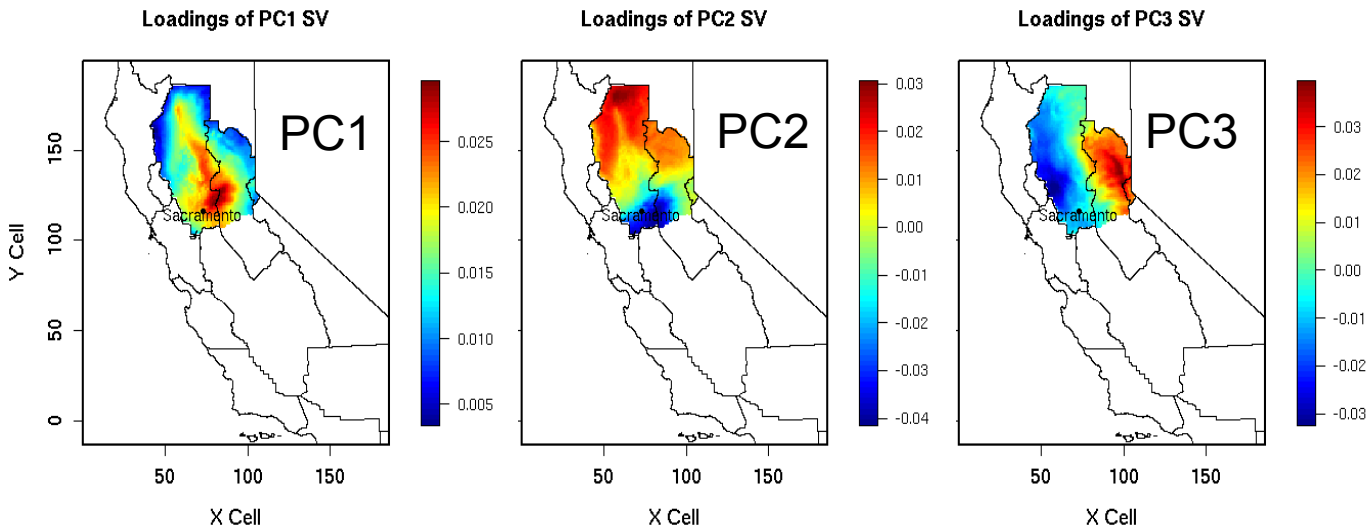


Ozone anomalies averaged over each cluster (= cluster mean – summer mean)

Result 1 Ozone Clusters:

Principal Components: SV

- Variations seen in ozone spatial distribution governed by a few patterns: **SV**



On any given day: **Ozone spatial distribution** =

summer average distribution +

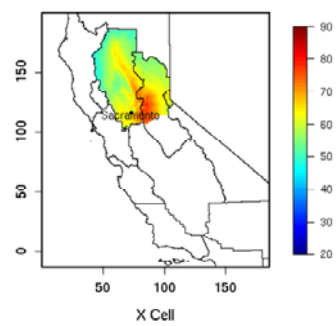
s1 * PC1 + s2 * PC2 + s3 * PC3 + …

si: scores, a scalar value

Common to each day

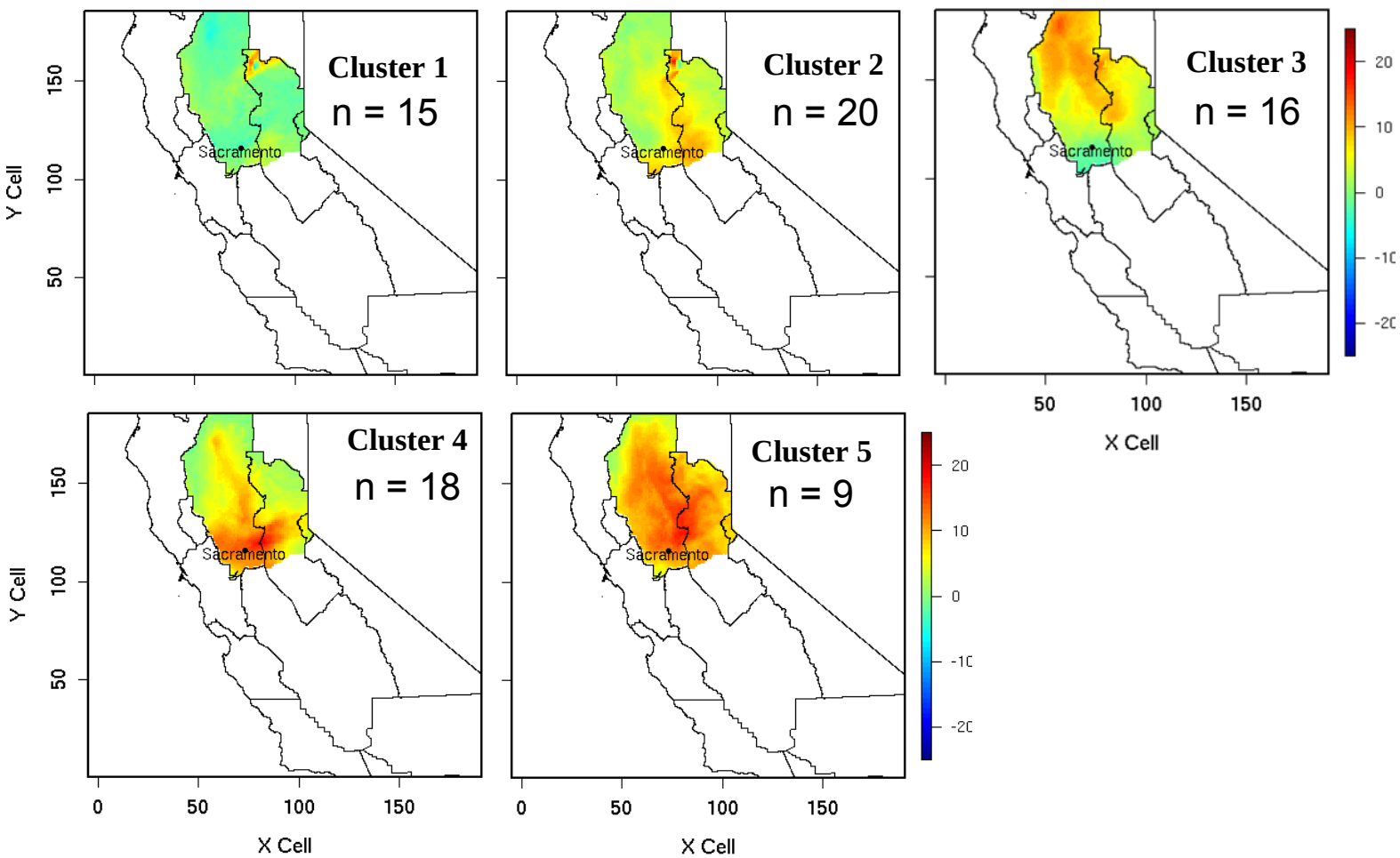
Distinctive features

Summer Average



Result 1 Ozone Clusters:

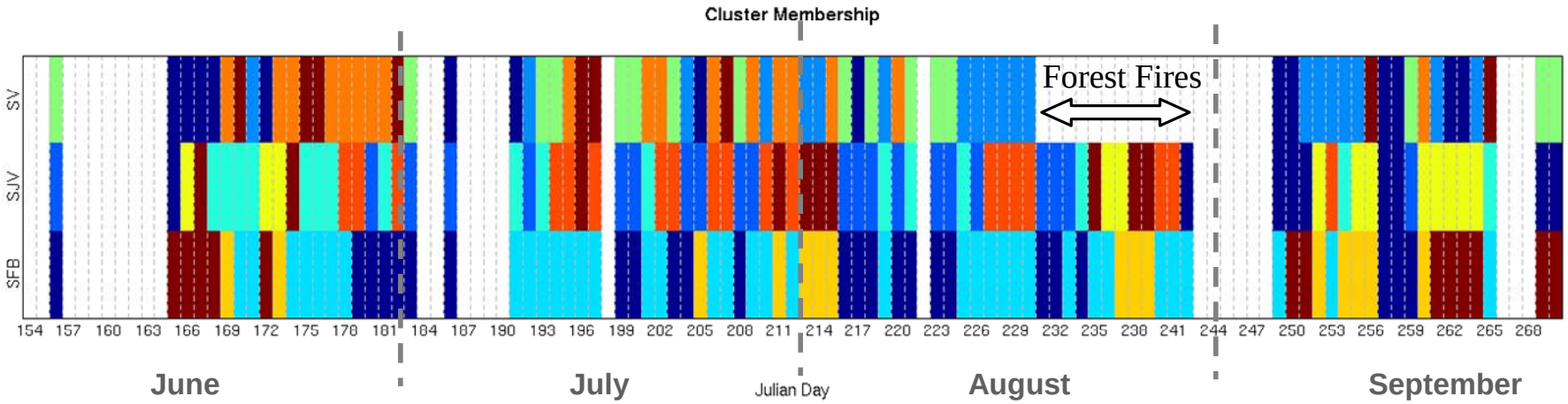
Ozone Clusters: SV



Ozone anomalies averaged over each cluster (= cluster mean – summer mean)

Result 1 Ozone Clusters:

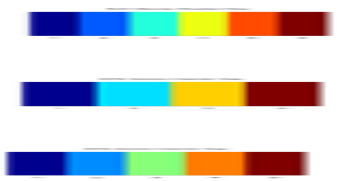
Cluster Membership



SJV Key (cluster type from 1 to 6)

SFB Key (cluster type from 1 to 4)

SV Key (cluster type from 1 to 5)



"Clean Days" in blank. Days affected by large fire emissions are excluded for SV clustering.

Result 1 Ozone Clusters:

Cluster Membership

- Ozone dynamics
  - SJV and SV highest ozone days do not follow the “clean days” or low ozone days (cluster 1), but evolve over multiple days.
  - SFB adjusts its ozone more quickly: a clean day followed by a high ozone day (cluster 3 or 4).
- Inter-basin relationships

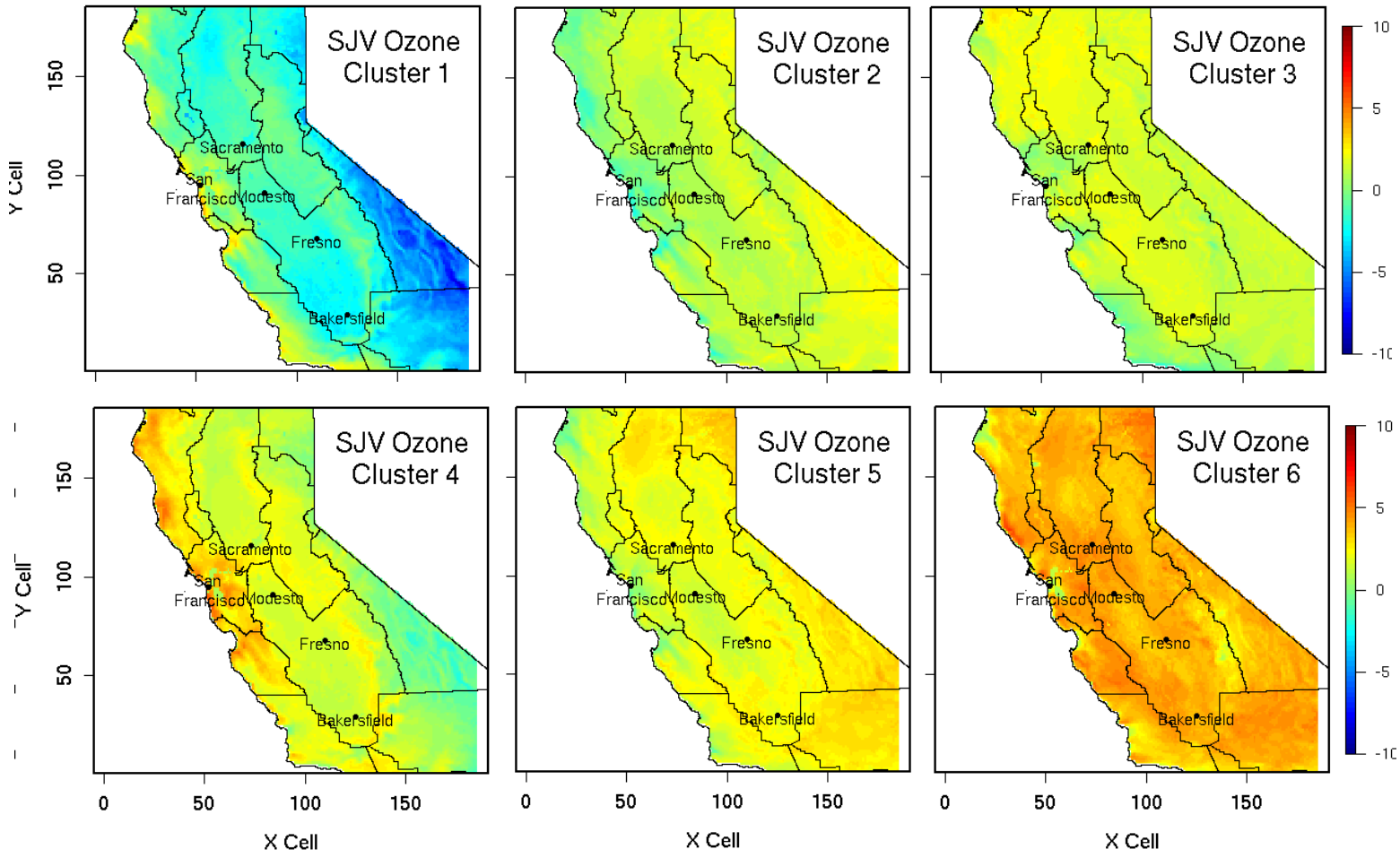
		SJV cluster type					
SFB		**1**	**2**	**3**	**4**	**5**	**6**
cluster	**1**	2	17	3	0	3	0
type	**2**	2	4	11	1	16	3
	3	0	1	2	6	0	6
	4	5	0	1	6	0	1

		SJV cluster type					
SV		**1**	**2**	**3**	**4**	**5**	**6**
cluster	**1**	5	3	2	4	0	1
type	**2**	1	3	4	4	6	2
	3	2	10	2	0	2	0
	4	0	3	4	2	6	3
	5	0	0	4	1	3	1

  - SJV cluster 4 associated with high ozone in SFB (cluster 3,4); SJV cluster 5 associated with lower ozone in SFB (cluster 1 and 2).
  - Less clear association between SV and SJV, lower SJV ozone clusters do not occur on high SV ozone days.

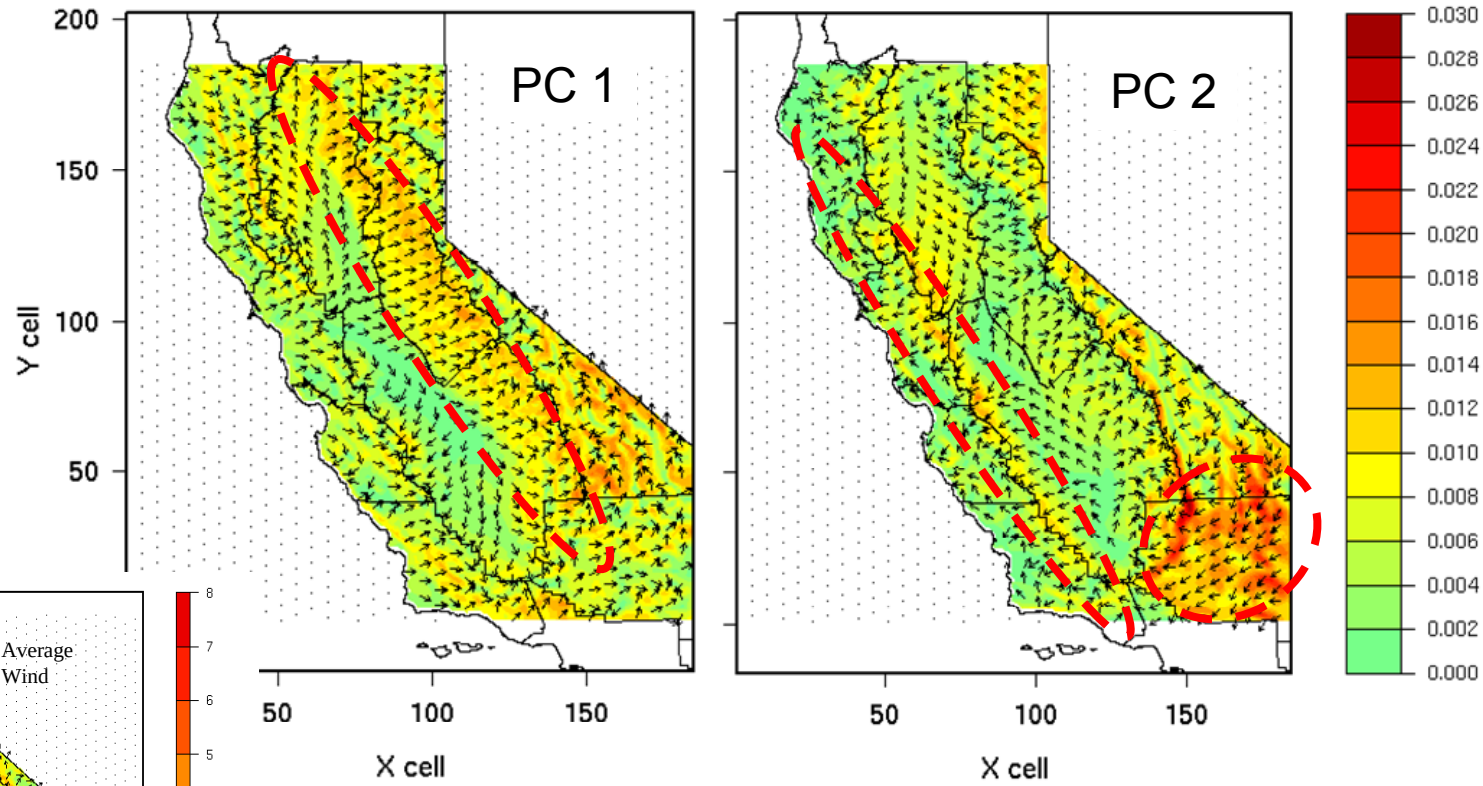
Result 2 Met Conditions:

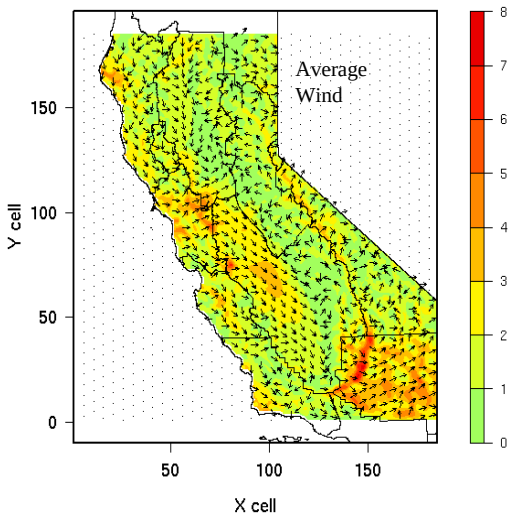
Daily Max Temperature Anomalies



Result 2 Met Conditions:

Diurnal Wind Flows

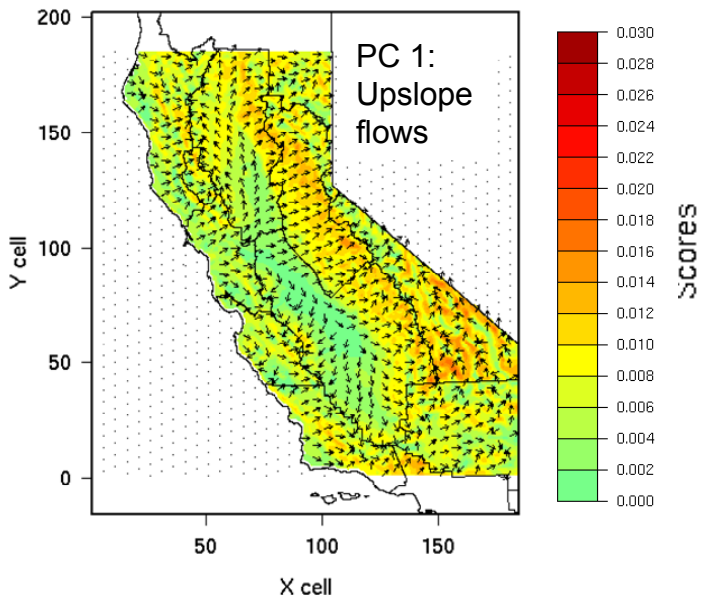


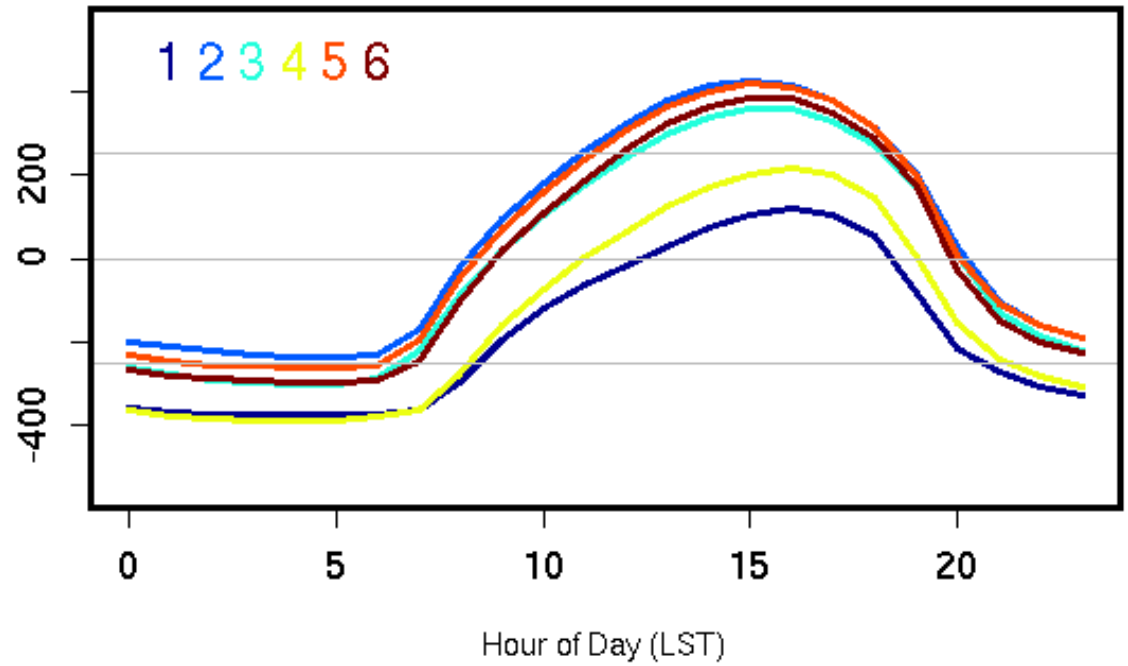


Variations in hourly wind fields are characterized by the strengths of upslope flows (PC1), and off-shore component & transport from MD to Kern (PC2).

Result 2 Met Conditions:

Diurnal Wind Flow Variations: Hourly Wind Scores on PC1

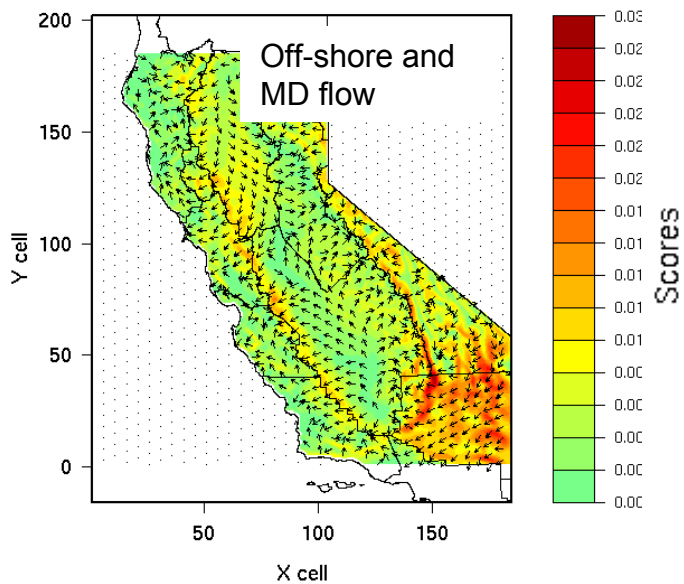


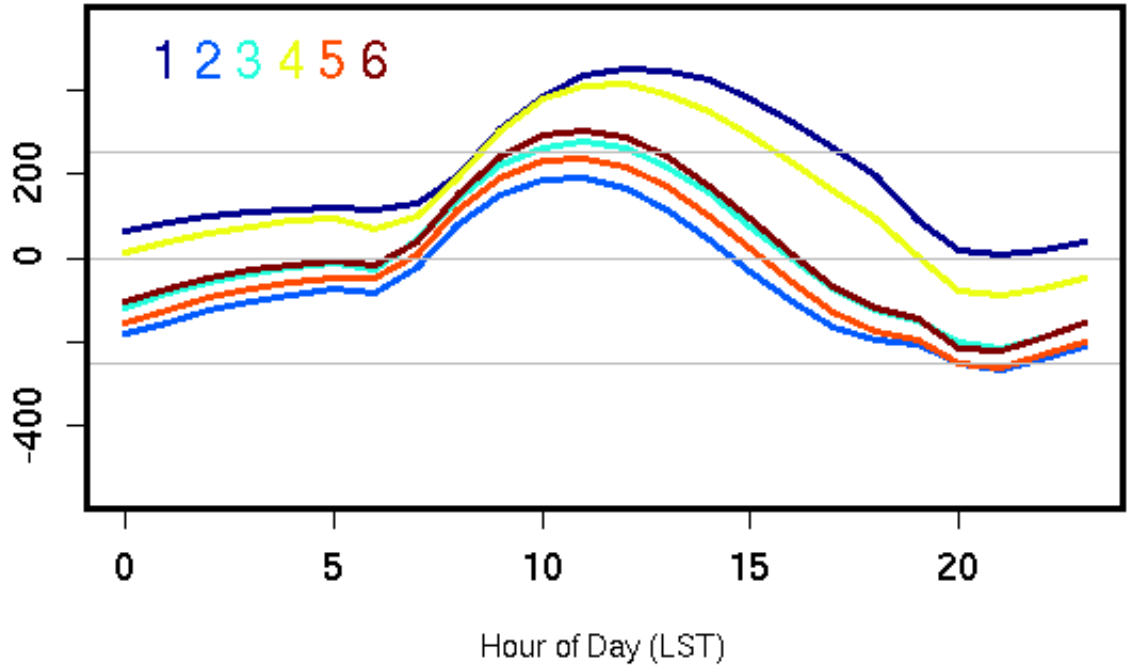


- **Similar diurnal patterns**: upslope flows increase from 7 AM until reaching max around 3 PM, then decrease and reverse at night.
- **Different strengths and durations**: weakest upslope flow in clusters 1 and 4, and strongest in clusters 2 and 5 (differ by ~2.5 m/s at 3 PM). Duration of positive upslope flow is shortest in clusters 1 and 4, and longest in clusters 2 and 5.

Result 2 Met Conditions:

Diurnal Wind Flow Variations: Hourly Wind Scores on PC2

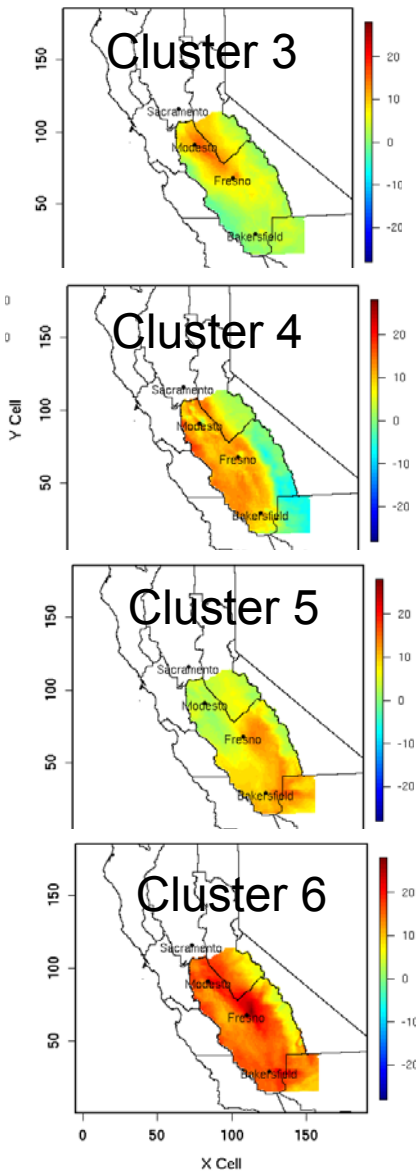




- **Similar diurnal patterns**: the off-shore component starts to decrease around 10 AM – noon (i.e. sea breezes increase) until ~ 8 PM, when sea breezes reach max. Then sea breezes start to decrease throughout the night.
- **Different strengths and durations**: weakest sea breezes in clusters 1 and 4, and strongest in clusters 2 and 5 (differ by ~2.5 m/s in the afternoon). Duration of positive off-shore component is shortest in clusters 2 and 5, and longest in clusters 1 and 4.

Characteristics of SJV Clusters

SJV Cluster 3	Ozone Distributions	SJV	Moderate to High
		SFB	Generally Low
		SV	Moderate to High
	Meteorological conditions	Temperature	High in SV
		Flow Patterns	Moderate
SJV Cluster 4	Ozone Distributions	SJV	High (western part)
		SFB	High
		SV	Moderate to Low
	Meteorological Conditions	Temperature	High along the coast
		Flow patterns	Weakest westerly
SJV Cluster 5	Ozone Distributions	SJV	High (southeast part)
		SFB	Low
		SV	Moderate
	Meteorological Conditions	Temperature	High (inland)
		Flow patterns	Strongest (westerly)
SJV Cluster 6	Ozone Patterns	SJV	Highest
		SFB	High
		SV	Moderate to High
	Meteorological Conditions	Temperature	Highest
		Flow Patterns	Moderate



Influence of Emission Changes

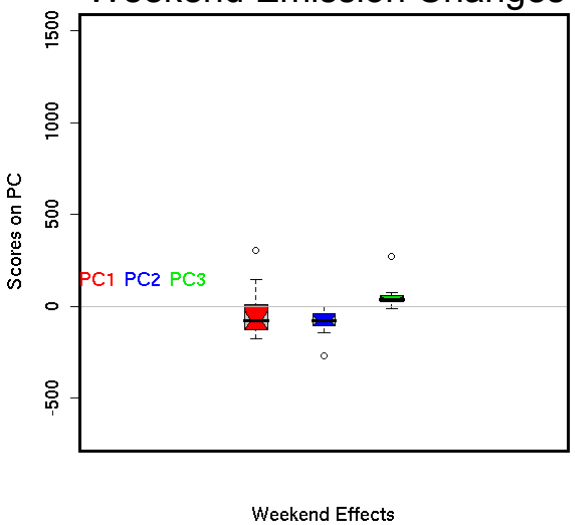
$$\Delta O_{3wnd} = O_{3a} - O_{3h}$$

O_{3a} Sunday ozone concentrations simulated using actual Sunday emissions.

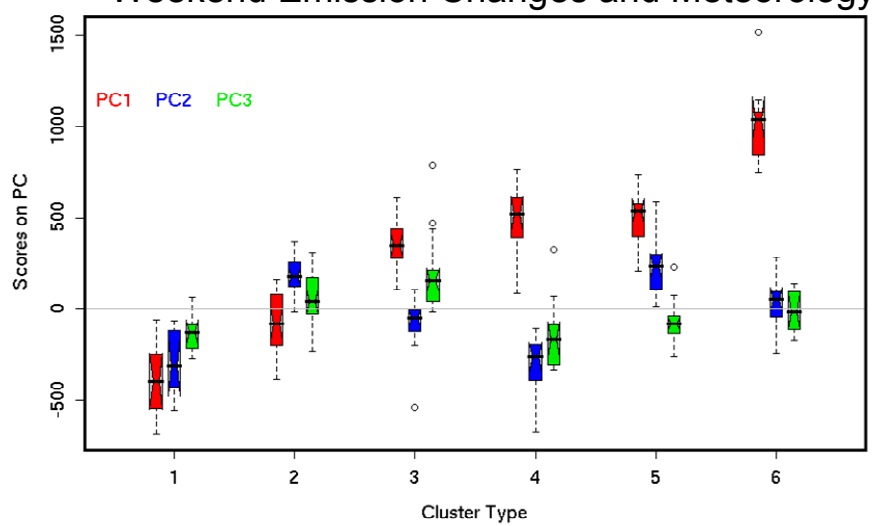
O_{3h} Sunday ozone concentrations simulated using typical weekday emissions.

Saturdays are excluded from the analysis because they can be affected by carryover of Friday emissions.

Variations induced by Weekend Emission Changes



Variations induced by both Weekend Emission Changes and Meteorology



Influence of Emission Changes

SJV clusters (c1~c6)	Meteorology induced variation
Meteorology + Emission	

	c1	c2	c3	c4	c5	c6
c1	8	0	0	0	0	0
c2	0	15	3	0	4	0
c3	0	1	14	1	0	0
c4	1	0	0	12	0	0
c5	0	0	4	0	12	3
c6	0	0	1	0	0	9

- Weekend emission changes produce minor effects, especially for SFB and SV.
- Lowering overall ozone and increasing spatial imbalance in SJV → small changes in assignment of ozone days.

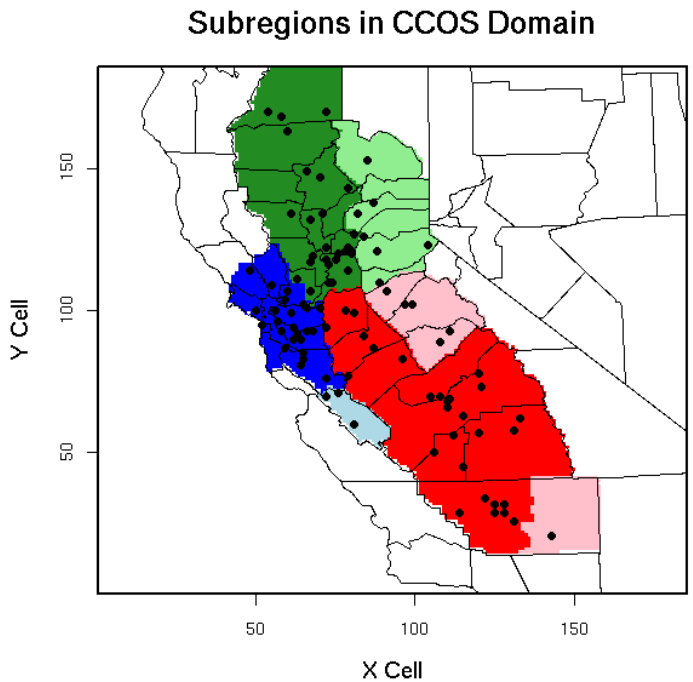
SFB clusters (c1~c4)	Meteorology induced variation
Meteorology + Emission	

	c1	c2	c3	c4
c1	24	1	0	0
c2	0	35	1	0
c3	0	2	13	0
c4	0	0	0	13

SV (c1~c5)	Meteorology induced variation
Meteorology + Emission	

	c1	c2	c3	c4	c5
c1	14	0	0	0	0
c2	2	17	0	1	0
c3	0	1	15	0	0
c4	0	1	0	17	0
c5	0	0	0	1	8

Representation of Measurement Sites



- Good spatial representation in SFB and SV
- Measurement sites cannot distinguish spatial distributions of cluster 1 from cluster 2, and cluster 4 from cluster 5.
  - Under-representation on the western side of SJV
- SJV Clusters 4 and 5 are associated with high and low SFB ozone levels, respectively, pooling SJV and SFB data will help distinguish the two clusters.

SJV

grids \ sites	0	1	2	3	4	5	6
0	*25*	2	0	0	0	0	0
1	3	*4*	0	2	0	0	0
2	1	9	*8*	4	0	0	0
3	0	0	0	*11*	1	5	0
4	0	0	0	1	*3*	8	1
5	0	0	2	0	0	*17*	0
6	0	0	0	0	1	1	*8*

SFB

grids \ sites	0	1	2	3	4
0	*25*	0	2	0	0
1	3	*15*	7	0	0
2	1	2	*32*	2	0
3	0	0	1	*12*	2
4	0	0	0	0	*13*

SV

grids \ sites	0	1	2	3	4	5
0	*24*	0	1	1	0	0
1	4	*10*	1	0	0	0
2	0	4	*16*	0	0	0
3	0	1	1	*14*	0	0
4	0	0	2	0	*12*	4
5	0	0	0	1	0	*8*

Comparison to Historical Data

- Clustering of observed ozone from 1996 to 1999 (reported by Fujita et al. 1999)

  Three spatial patterns of "very high ozone days"

  Most frequent

  (1) the SFB has its highest ozone, while SJV ozone is also very high, which is characterized by the weakest sea breeze;

  (2) the SJV has its highest basin-wide ozone, while SFB and SV are relatively clean, which is characterized by a stronger sea breeze, moving pollutants from SFB and SV to SJV;

  (3) SV is at its highest ozone values, which, similar with the second cluster, has a stronger sea breeze but higher temperature in the Sacramento Valley; SJV ozone in this cluster is also high.

Clustering from this study

SJV Cluster 3	Ozone Distributions	SJV	Moderate to High
		SFB	Generally Low
		SV	Moderate to High
	Meteorological conditions	Temperature	High in SV
		Flow Patterns	Moderate
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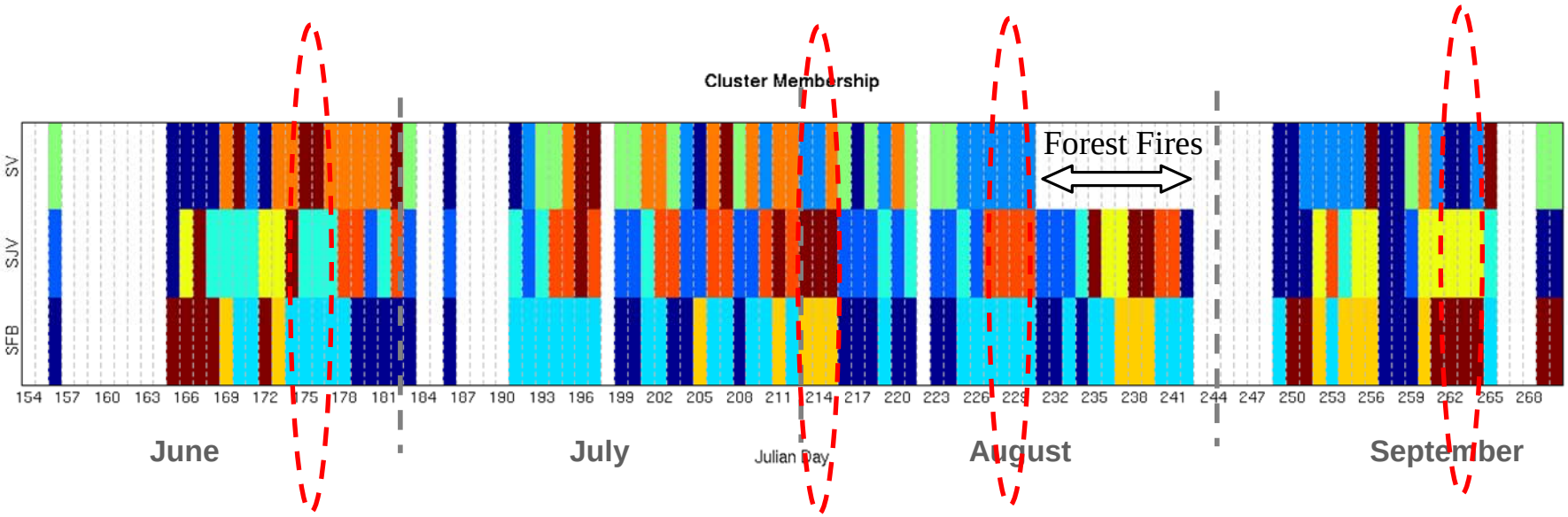
SJV Cluster 5	Ozone Distributions	SJV	High (southeast part)
		SFB	Low
		SV	Moderate
	Meteorological Conditions	Temperature	High (inland)
		Flow patterns	Strongest (westerly)
SJV Cluster 6	Ozone Patterns	SJV	Highest
		SFB	High
		SV	Moderate to High
	Meteorological Conditions	Temperature	Highest
		Flow Patterns	Moderate

Most frequent

Qualitatively: SJV cluster 3 ←→ Historical Cluster 3
SJV cluster 4 ←→ Historical Cluster 1
SJV cluster 5 ←→ Historical Cluster 2

SJV cluster 6: not identified.

Ozone Episodes and CCOS IOPs



- Representative ozone episodes:

  Jun 23rd to 25th : Historical Cluster 3 (SJV cluster 3)

  Aug 14th to 17th: Historical Cluster 2 (SJV cluster 5)

  Sep 17th to 20th: Historical Cluster 1 (SJV cluster 4)

  Jul 29th to Aug 2nd: highest ozone

  Aligning with IOPs, except the June episode.

Summary and Conclusions

- Ozone distributions in the SJV can be explained by associated meteorology and in relation to ozone in upwind regions.

  - need both temperature and winds.

- Ozone buildup in the SJV and SV occur on multiple days, SFB ozone transition occurs faster.

- Variations in modeled ozone are mostly induced by meteorology; weekend emission changes produce minor effects.

- Measurement sites have good spatial coverage in SFB and SV, under-representation on the western side of SJV.

- Historical clusters seen in model clusters with different frequencies. Most stagnant condition occurs least frequently.

  - Summer 2000 is cooler than usual.

- IOP days largely align with representative ozone episodes.