Quantifying local creation and regional transport using a hierarchical space-time model of ozone as a function of observed NO_x, a latent space-time VOC process, emissions, and meteorology.

Community Modeling and Analysis System Conference
Chapel Hill, NC

October 6, 2008

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Outline

1. Scientific and regulatory context → goals
2. The data
3. The models

   Original, Newmean, Metcov
4. Two different predictors for two different purposes
5. Model performance and CMAQ comparison
6. Discussion and future work

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Goals based on regulatory needs Formulate and assess the

ability of a **process-based** space-time **statistical** model of 8-hour ozone as a function of NO_x and VOC emissions and meteorology to allow:

1. Decomposition into local creation vs. regional transport
2. Space-time predictions backward in time (at *any* space-time point)
3. Assessment of past emission control programs
4. Assessment of future emission control programs
5. Quantification of uncertainty

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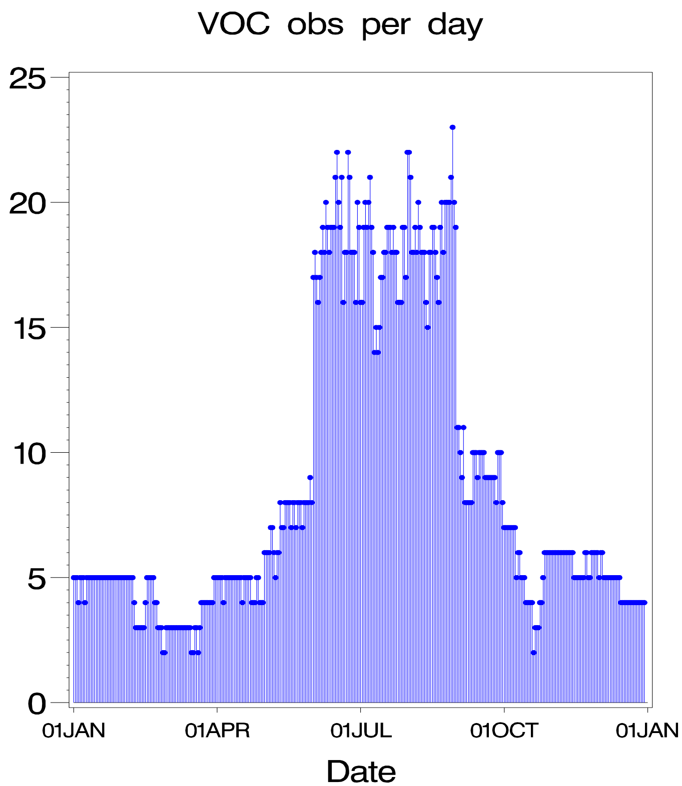
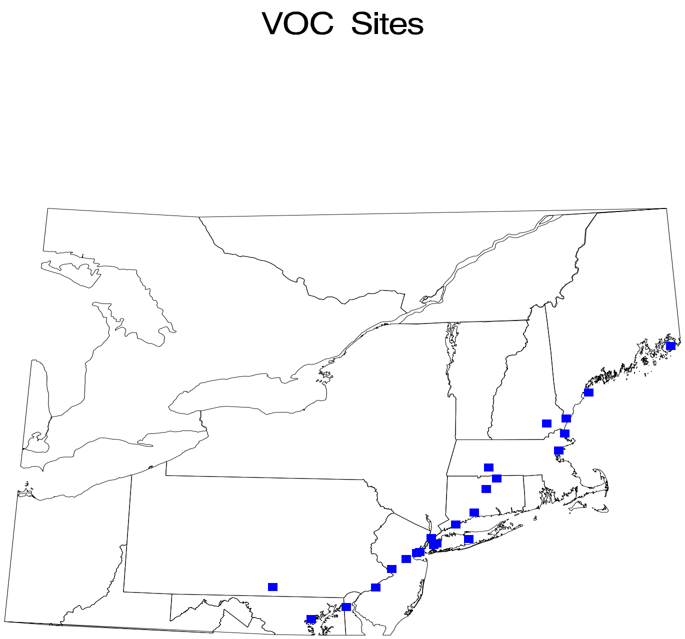
VOC: N=3k dataset



(a)

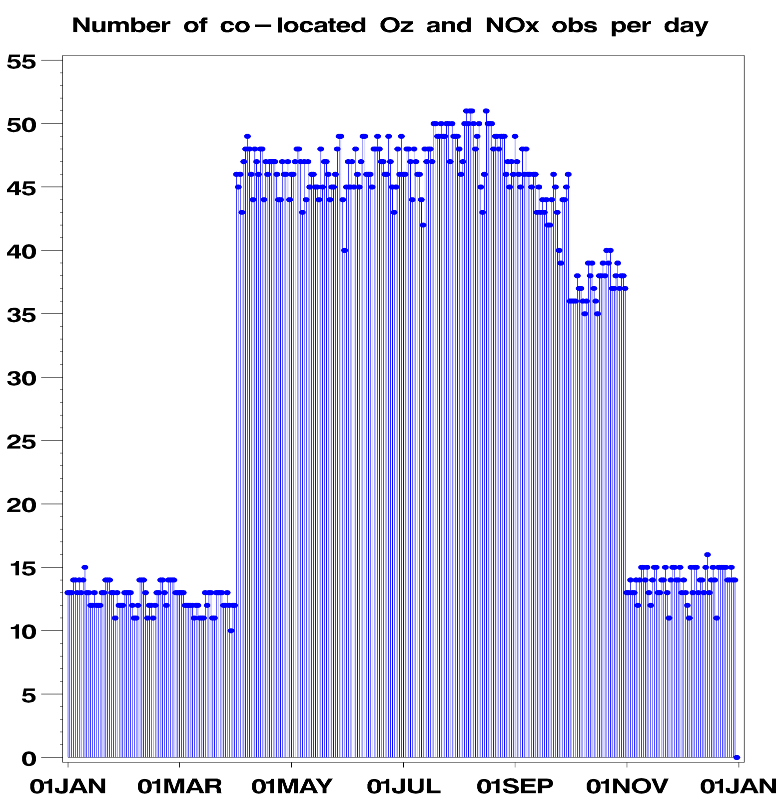


(b)

VOC Emissions data resolution before and after

	Resolution			
	In the data		In the model	
Dataset	**Time**	**Space**	**Time**	**Space**
Onroad	Year	County	Day	Lon, lat
Nonroad	Year	County	Day	Lon, lat
Storage & Transport	Year	County	Day	Lon, lat
Other area	Year	County	Day	Lon, lat
Biogenic	Month	County	Day	Lon, lat

Co-located O_3 and NO_x: N=11k dataset



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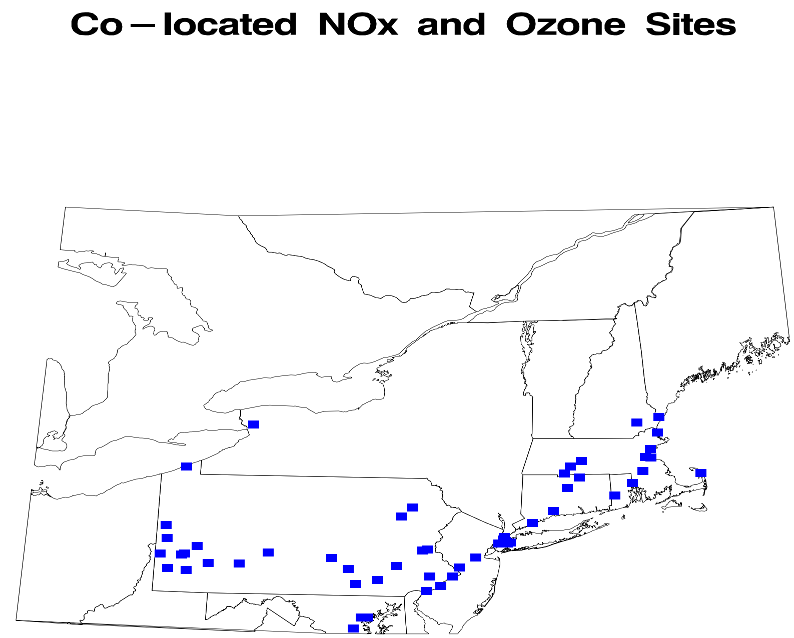

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The model (using N=11k dataset):

$$Y_{t,\,i} = Y^{C}_{t,\,i} + Y^{T}_{t,\,i} + \nu_{t,\,i}, \qquad \boldsymbol{\nu}_t \sim \begin{cases} N\{\,\mathbf{0}\,,\ V_t(\boldsymbol{\phi}^*_1)\,\} & t \text{ in Jan-Apr} \\ N\{\,\mathbf{0}\,,\ V_t(\boldsymbol{\phi}^*_2)\,\} & t \text{ in May-Sept} \\ N\{\,\mathbf{0}\,,\ V_t(\boldsymbol{\phi}^*_3)\,\} & t \text{ in Oct} \\ N\{\,\mathbf{0}\,,\ V_t(\boldsymbol{\phi}^*_4)\,\} & t \text{ in Nov-Dec} \end{cases}$$

$$\beta_1 + \beta_2\mathcal{N}_{t,\,i} + \beta_3\mathcal{N}^2_{t,\,i} + \beta_4\mathcal{N}_{t,\,i}(\mathcal{T}_{t,\,i} - 1.4) + \beta_5\mathcal{N}^2_{t,\,i}(\mathcal{T}_{t,\,i} - 1.4) + \beta_6\mathcal{N}_{t,\,i}\mathcal{V}_{t,\,i} + \beta_7\mathcal{N}_{t,\,i}\mathcal{T}_{t,\,i}\mathcal{V}_{t,\,i}$$

$$\delta\boldsymbol{\lambda}'_{t-1,i}\boldsymbol{Y}^*_{t-1}$$

$$f_1(\mathcal{V}^{N}_{m_t,C_i}, \mathcal{V}^{OR}_{C_i}, \mathcal{V}^{NR}_{C_i}, \mathcal{V}^{ST}_{C_i}, \mathcal{V}^{OA}_{C_i}, \mathcal{M}_{t,i}, \mathcal{W}_{t,i}, \gamma) + \omega_{t,\,i}$$

$$f_2(ws_{t,\,i}, wd_{t,\,i})$$

N=54k dataset

$$\boldsymbol{\omega}_t \sim \begin{cases} N\{\,\mathbf{0}\,,\ W_t(\boldsymbol{\psi}^*_1)\,\} & t \text{ in Jan-Apr} \\ N\{\,\mathbf{0}\,,\ W_t(\boldsymbol{\psi}^*_2)\,\} & t \text{ in May-Sept} \\ N\{\,\mathbf{0}\,,\ W_t(\boldsymbol{\psi}^*_3)\,\} & t \text{ in Oct} \\ N\{\,\mathbf{0}\,,\ W_t(\boldsymbol{\psi}^*_4)\,\} & t \text{ in Nov-Dec} \end{cases}$$

"Newmean" model improvement

1. Separate NO_x into NO and NO_2
2. Include pressure
3. Include dewpoint as a measure of humidity
4. Include yesterday's ozone at the same site (nighttime transport)
5. Better transformation of maximum temperature

“Metcov” model improvement

Before: covariance parameters based on “season”

Now: covariance parameters based on windspeed and temperature

“Metcov” model:

$$Y_{t,\,i} = Y^C_{t,\,i} + Y^T_{t,\,i} + \nu_{t,\,i}, \qquad \boldsymbol{\nu}_t \sim \begin{cases} N\{\,\mathbf{0}\,,\ V_t(\boldsymbol{\phi}_1^*)\,\} & ws \geq 4.6 \text{ m/s} \\ N\{\,\mathbf{0}\,,\ V_t(\boldsymbol{\phi}_2^*)\,\} & maxtemp < 55 \\ N\{\,\mathbf{0}\,,\ V_t(\boldsymbol{\phi}_3^*)\,\} & 55 \leq maxtemp < 75 \\ N\{\,\mathbf{0}\,,\ V_t(\boldsymbol{\phi}_4^*)\,\} & maxtemp \geq 75 \end{cases}$$

$$\beta_1 + \beta_2 \mathcal{N}_{t,\,i} + \beta_3 \mathcal{N}^2_{t,\,i} + \beta_4 \mathcal{N}_{t,\,i}(\mathcal{T}_{t,\,i} - 1.4) +$$
$$\beta_5 \mathcal{N}^2_{t,\,i}(\mathcal{T}_{t,\,i} - 1.4) + \beta_6 \mathcal{N}_{t,\,i}\mathcal{V}_{t,\,i} + \beta_7 \mathcal{N}_{t,\,i}\mathcal{T}_{t,\,i}\mathcal{V}_{t,\,i}$$

$$f_1(\mathcal{V}^N_{m_t,C_i}, \mathcal{V}^{OR}_{C_i}, \mathcal{V}^{NR}_{C_i}, \mathcal{V}^{ST}_{C_i}, \mathcal{V}^{OA}_{C_i},$$
$$\mathcal{M}_{t,i}, \mathcal{W}_{t,i}, \gamma) + \omega_{t,\,i}$$

$$\delta \boldsymbol{\lambda}'_{t-1,i} \boldsymbol{Y}^*_{t-1}$$

$$f_2(ws_{t,\,i}, wd_{t,\,i})$$

N=54k dataset

$$\boldsymbol{\omega}_t \sim \begin{cases} N\{\,\mathbf{0}\,,\ W_t(\boldsymbol{\psi}_1^*)\,\} & ws \geq 4.6 \text{ m/s} \\ N\{\,\mathbf{0}\,,\ W_t(\boldsymbol{\psi}_2^*)\,\} & maxtemp < 55 \\ N\{\,\mathbf{0}\,,\ W_t(\boldsymbol{\psi}_3^*)\,\} & 55 \leq maxtemp < 75 \\ N\{\,\mathbf{0}\,,\ W_t(\boldsymbol{\psi}_4^*)\,\} & maxtemp \geq 75 \end{cases}$$

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Predicting unobserved ozone conditional on observed

$$\begin{pmatrix} \boldsymbol{Y}_t^o \\ \boldsymbol{Y}_t^u \end{pmatrix} \mid \boldsymbol{\beta}, \delta, \boldsymbol{\phi}_t, \boldsymbol{\gamma}, \boldsymbol{\psi}_t \sim N\left\{ \begin{pmatrix} \mu_{Y_t}^o \\ \mu_{Y_t}^u \end{pmatrix}, \begin{pmatrix} \Sigma_{Y_t}^o & \Sigma_{Y_t}^{ou} \\ \Sigma_{Y_t}^{uo} & \Sigma_{Y_t}^u \end{pmatrix} \right\}$$

$$\begin{aligned}
\mu_{Y_t}^o &\equiv X_t^{Ao}\boldsymbol{\beta}^A + M_t^o Z_t^o \boldsymbol{\gamma} + \delta \Lambda_{t-1}^o \boldsymbol{Y}_{t-1}^* \\
\mu_{Y_t}^u &\equiv X_t^{Au}\boldsymbol{\beta}^A + M_t^u Z_t^u \boldsymbol{\gamma} + \delta \Lambda_{t-1}^u \boldsymbol{Y}_{t-1}^* \\
\Sigma_{Y_t}^o &\equiv V_t^o(\phi_t) + M_t^o W_t^o(\phi_t) M_t^o \\
\Sigma_{Y_t}^u &\equiv V_t^u(\phi_t) + M_t^u W_t^u(\phi_t) M_t^u \\
\Sigma_{Y_t}^{ou} &\equiv V_t^{ou}(\phi_t) + M_t^o W_t^{ou}(\phi_t) M_t^u .
\end{aligned}$$

$$\boldsymbol{Y}_t^u \mid \boldsymbol{Y}_t^o, \boldsymbol{\beta}, \delta, \boldsymbol{\phi}_t, \boldsymbol{\gamma}, \boldsymbol{\psi}_t \sim$$

$$N\Big\{ \underbrace{\underbrace{\mu_{Y_t}^u}_{\text{Meanhat}} + \Sigma_{Y_t}^{uo}[\Sigma_{Y_t}^o]^{-1}\big(\boldsymbol{Y}_t^o - \mu_{Y_t}^o\big)}_{\text{Yhat}},\ \Sigma_{Y_t}^u - \Sigma_{Y_t}^{uo}[\Sigma_{Y_t}^o]^{-1}\Sigma_{Y_t}^{ou} \Big\}.$$

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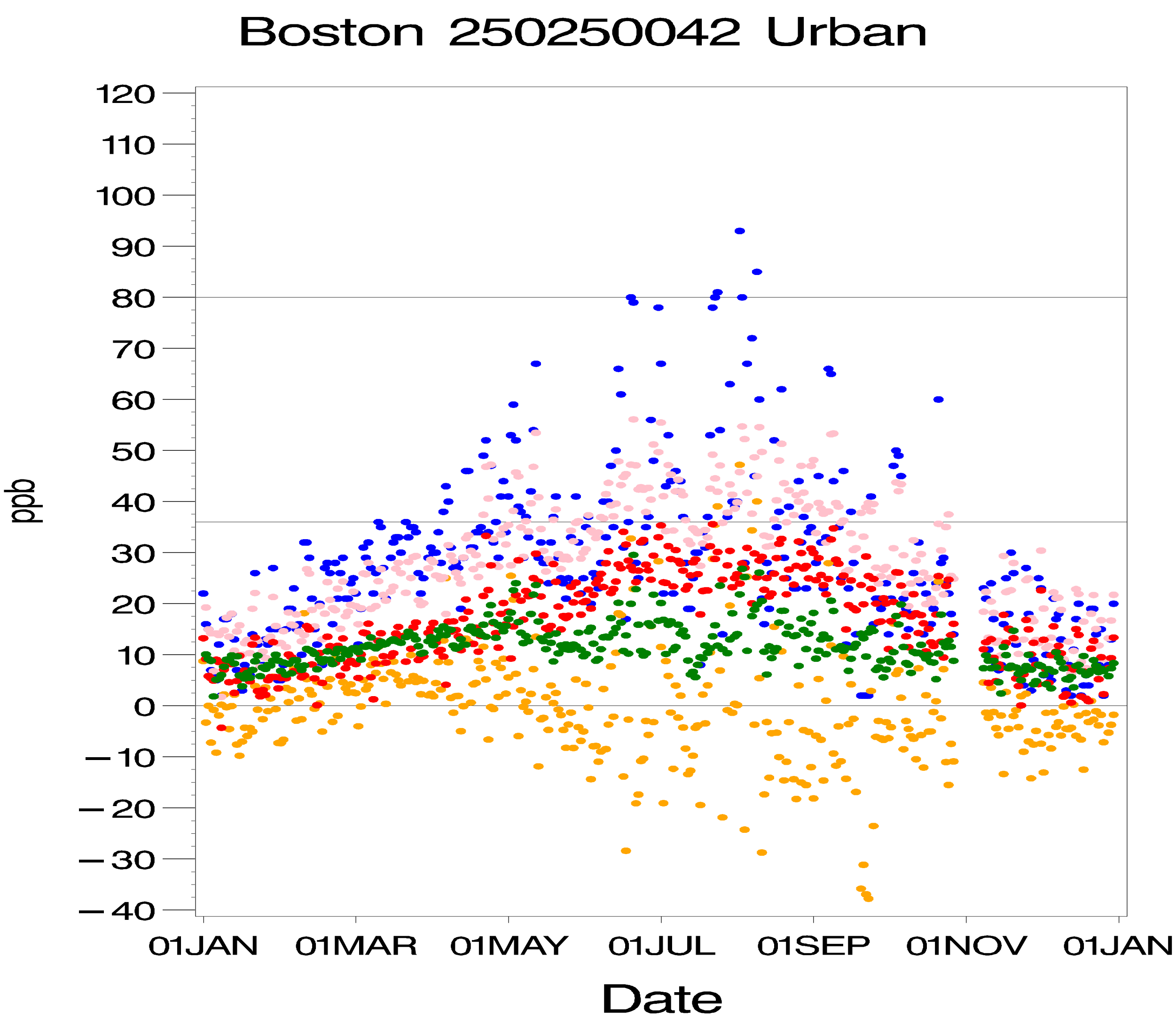
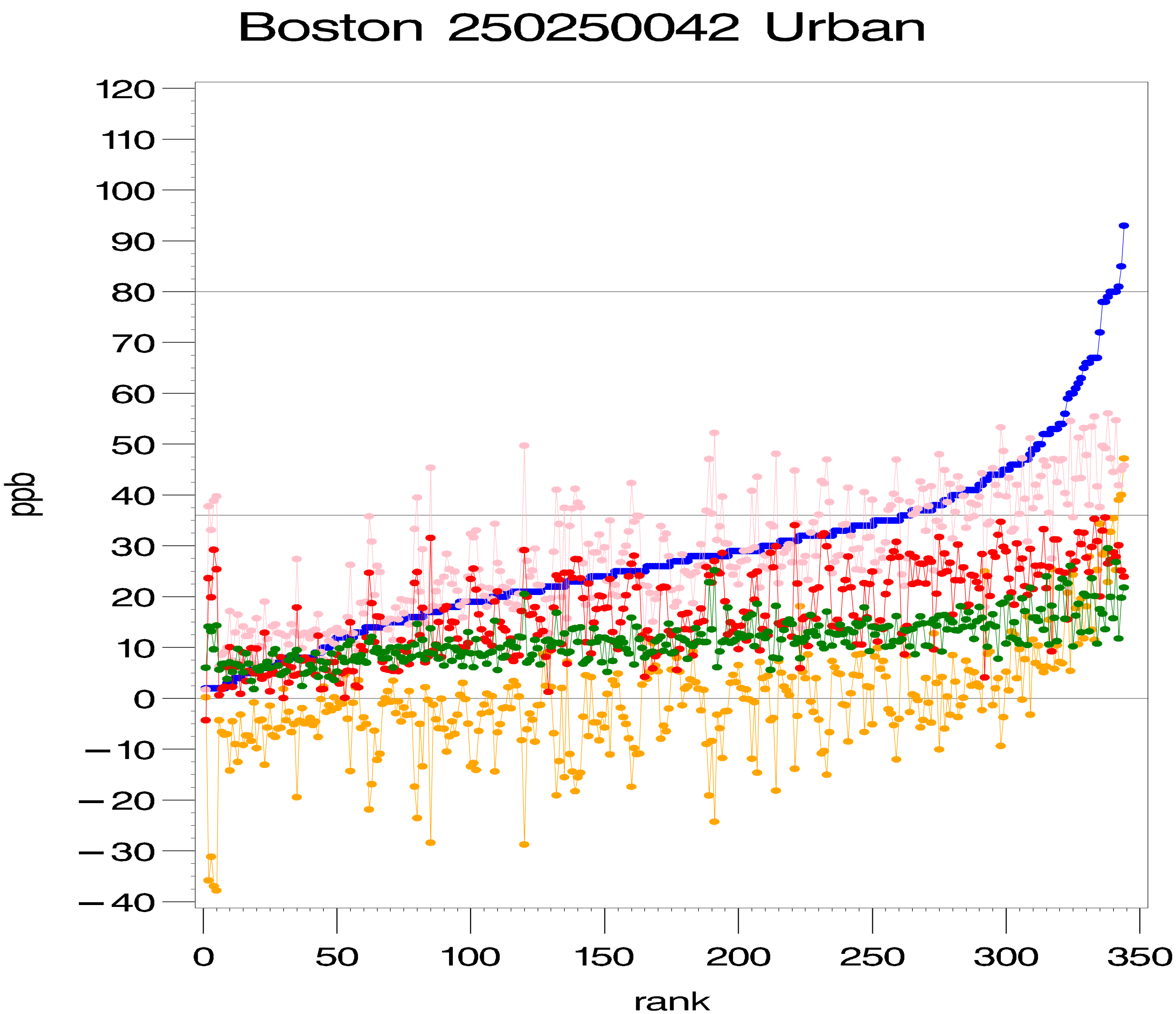
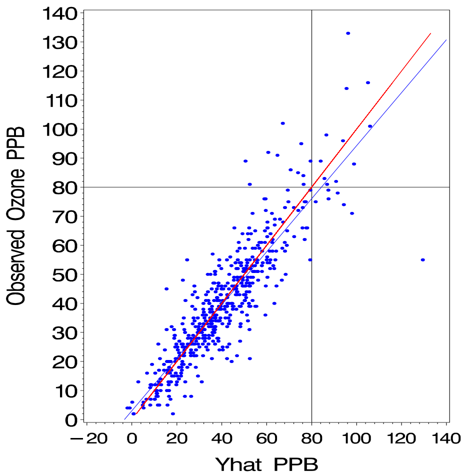
Decomposition of ozone (by day)



Decomposition of ozone (by rank)



Leave out ten percent scatterplots and residuals



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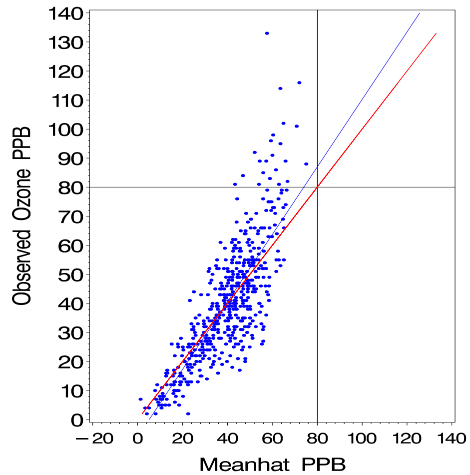

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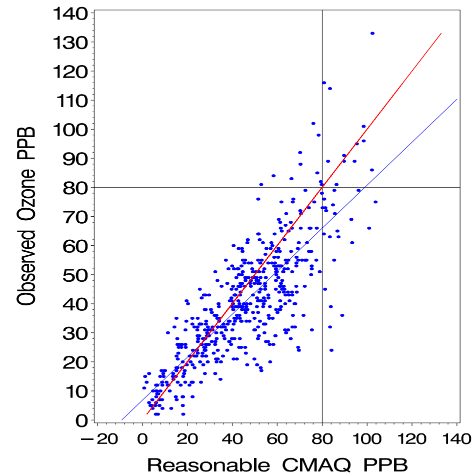

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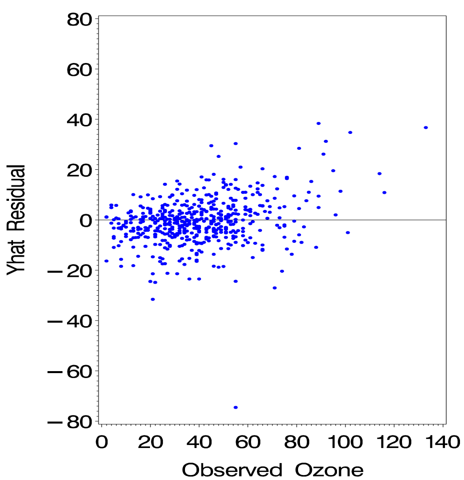

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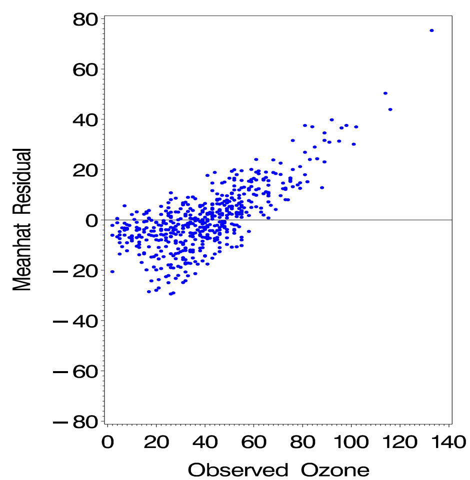

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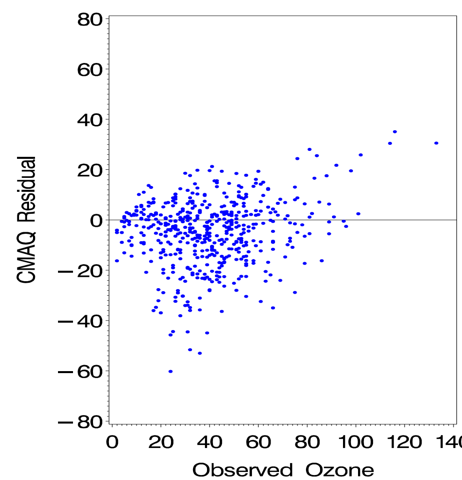


(j)

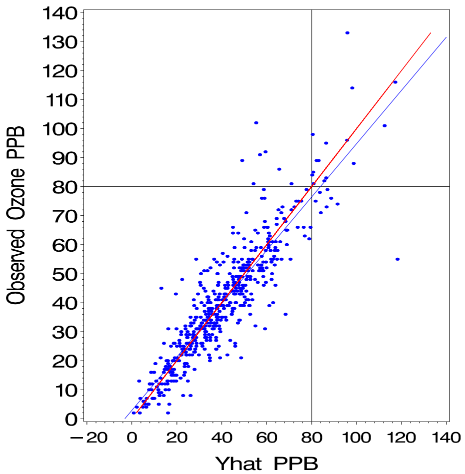
Leave out ten percent regression diagnostics

	N	R^2	RMSE	Slope	Intercept
Yhat	508	.78	9.6	**.91**	**3.0**
				.022	**.98**
Meanhat	508	.64	12	**1.2**	**-6.0**
				.039	**1.6**
Reasonable	508	.64	12	**.74**	**6.8**
CMAQ				**.025**	**1.2**
CMAQ	532	2.0E-4	21	-3.8E-5	**40**
				1.1E-4	**.91**

New mean improvements

	N	Model	R^2	RMSE	Slope	Intercept
Yhat	508	Original	.78	9.6	**.91**	**3.0**
					(.022)	**(.98)**
Yhat	508	Newmean	.79	9.4	**.92**	**2.9**
					(.021)	**(.95)**
Meanhat	508	Original	.64	12	**1.2**	**-6.0**
					(.039)	**(1.6)**
Meanhat	508	Newmean	.66	12	**1.1**	**-3.1**
					(.035)	**(1.5)**
Reasonable	508		.64	12	**.74**	**6.8**
CMAQ					**(.025)**	**(1.2)**

Newmean improvements



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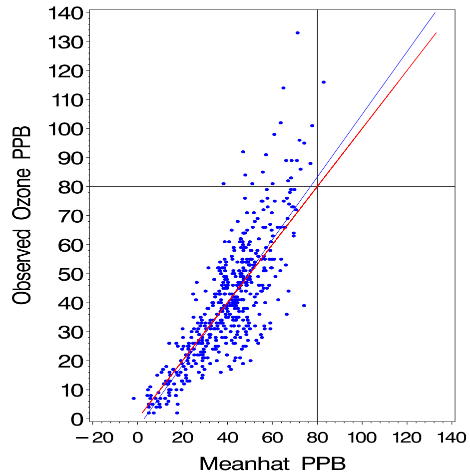

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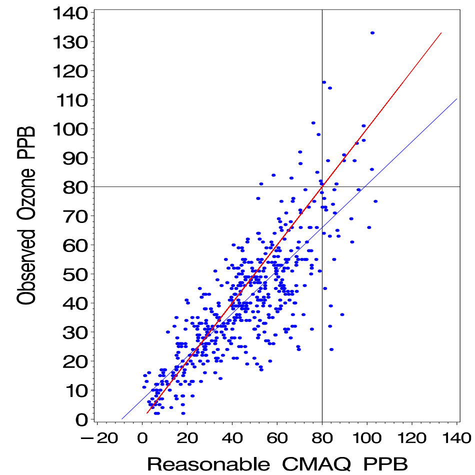

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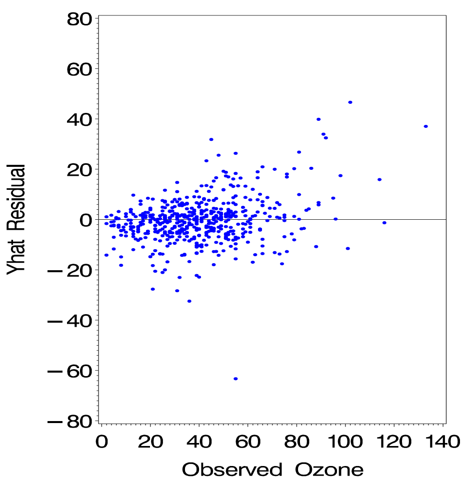

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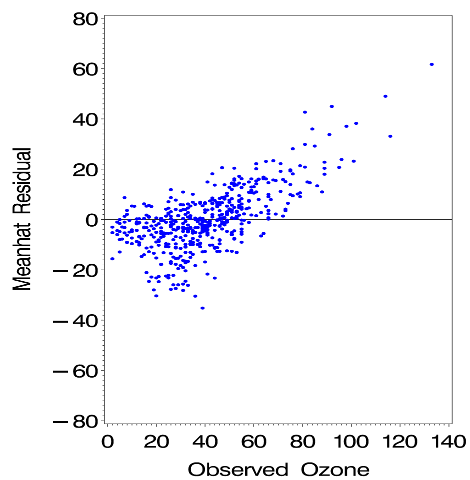

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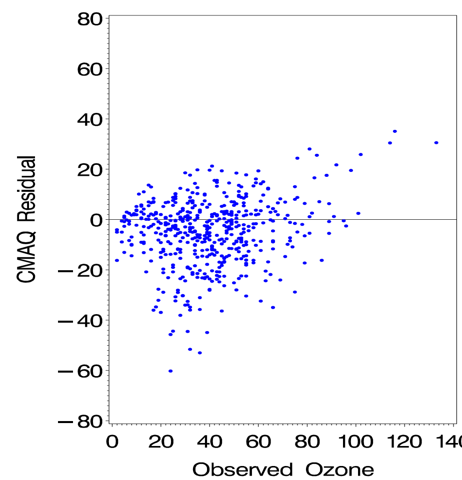
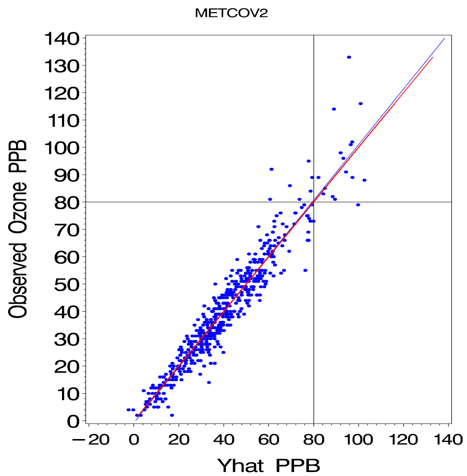


(p)

Metcov Improvements

	N	Model	R^2	RMSE	Slope	Intercept
Yhat	508	Original	.78	9.6	**.91**	**3.0**
					(.022)	**(.98)**
Yhat	508	Newmean	.79	9.4	**.92**	**2.9**
					(.021)	**(.95)**
Yhat	508	Metcov	.92	5.9	**1.0**	**-.68**
					(.014)	**(.61)**
Meanhat	508	Original	.64	12	**1.2**	**-6.0**
					(.039)	**(1.6)**
Meanhat	508	Newmean	.66	12	**1.1**	**-3.1**
					(.035)	**(1.5)**
Meanhat	508	Metcov	.65	12	**1.2**	**-6.4**
					(.039)	**(1.6)**
Reasonable	508		.64	12	**.74**	**6.8**
CMAQ					**(.025)**	**(1.2)**

Metcov improvements



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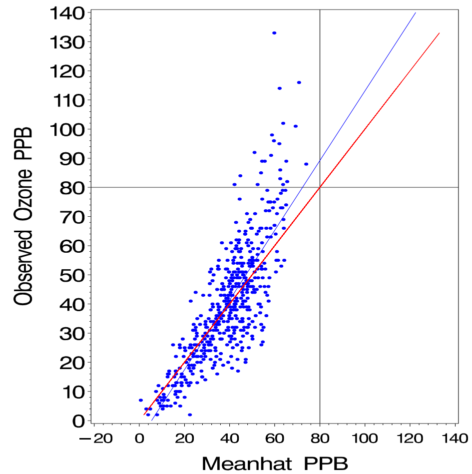

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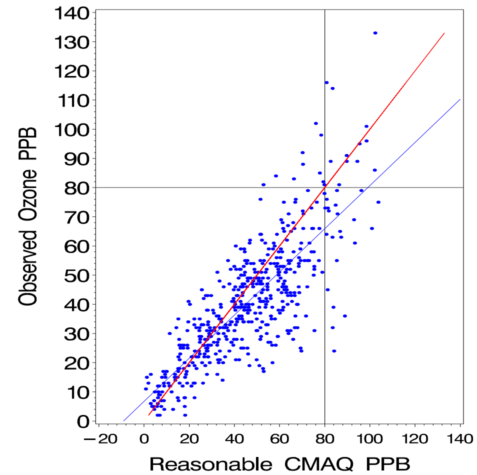

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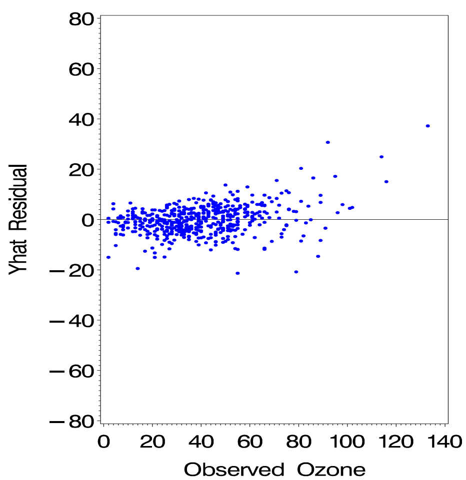

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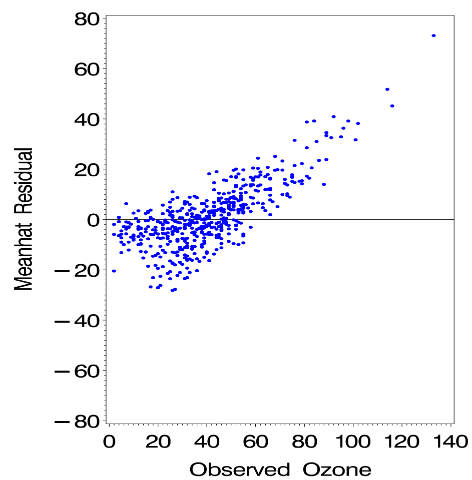

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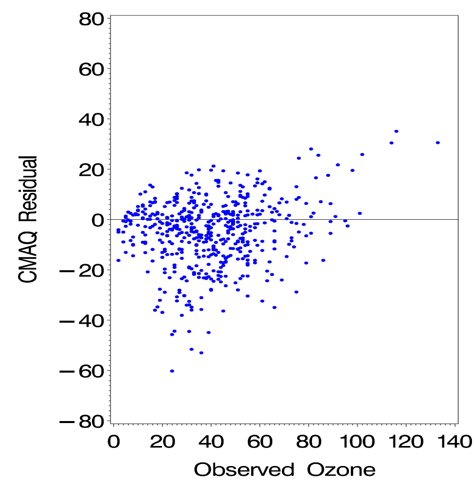

(v)

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Bottom line:

- **The good news**

  Metcov Yhat predictor performs very well for backward-in-time prediction

  Meanhat predictor allows us to decompose ozone into created + transported

- **The bad news**

  We underestimate high ozone values with the meanhat predictor

Future work:

- Different models for different goals:

  Build model from ground up based on ozone season for assessment of future emission programs.

- New explanatory variables? Solar radiation? Cloud cover?

- Explore nonparametric techniques for meanhat predictor.

- Expand model to two latent space-time fields (VOC and NO_x) via Bayesian framework

Acknowledgements:

Daniel Tong, Brian Eder

Lance McCluney, Rhonda Thompson, Doug Soloman, Wyatt Appel, Alice Gilleland, Fred Dimmick

Shelly Eberly, Bill Cox, Ellen Baldridge

Tesh Rao, David Mintz, James Hemby, Neil Frank

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Thank you!