Bayesian melding in the hunt for the elusive PRB level

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James V Zidek

U British Columbia

OUTLINE

- The problem of the PRB
- The melding approach
- Results
- Discussion

Acknowledgements: Zhong Liu(UBC), Nhu Le(BC Cancer Research Center), Prasad Kasibhatla(Duke U),

Genesis of the talk

I My 2003 **SAMSI** visit

II The **Pacific Institute for the Mathematical Science (PIMS)** Collaborative Research Group on "Climate Change and Georisk"

III The **EPA** CASAC panel on ozone

II:PIMS CRG Objectives

Long term

- To develop a distributed Pacific Northwest center on **Environmetrics** that builds on:
  - UW's **Northwest Center for Research in Statistics** & the Environment (NRCSE)
  - large PNW community of researchers in a variety of disciplines
  - available courses, etc

II:PIMS CRG Objectives

Long term

- to create
  - graduate/diploma program in environmetrics along with workshops, short courses, etc
  - a multi-center for research
  - a pool of experts for policy and societal concerns

II:PIMS CRG Objectives

Near Term: 2007-2008. To:

- integrate a number of existing research subgroups under a single umbrella &
  - forest fires and environmental risk
  - agroclimate risk management
  - integration of statistics into climate and weather models
- generate new research subgroups
- fund grad students and postdocs
- conferences, workshops & short courses
- develop strategic links with other groups, e.g. Pacific Rim

III: EPA's CASAC on ozone

- The CASAC core committee
- Augmented Committee for setting ozone standards
- The process & "postnormal science"

Air Pollution: historical perspective

1952 London Fog

1952-Onwards Environmental cleanup begins in Britain

1970 USA's Clean Air Act

1971 USA EPA formed

1973 First SIMS group setup - dawn of “environmetrics”

1980-1990 NAPAP program to tackle “acid rain” problem

1990 Clean Air Act Amendments: **Accountability**

AIR POLLUTION

AIR POLLUTION

DISEASE/DEATH

NEED TO REGULATE

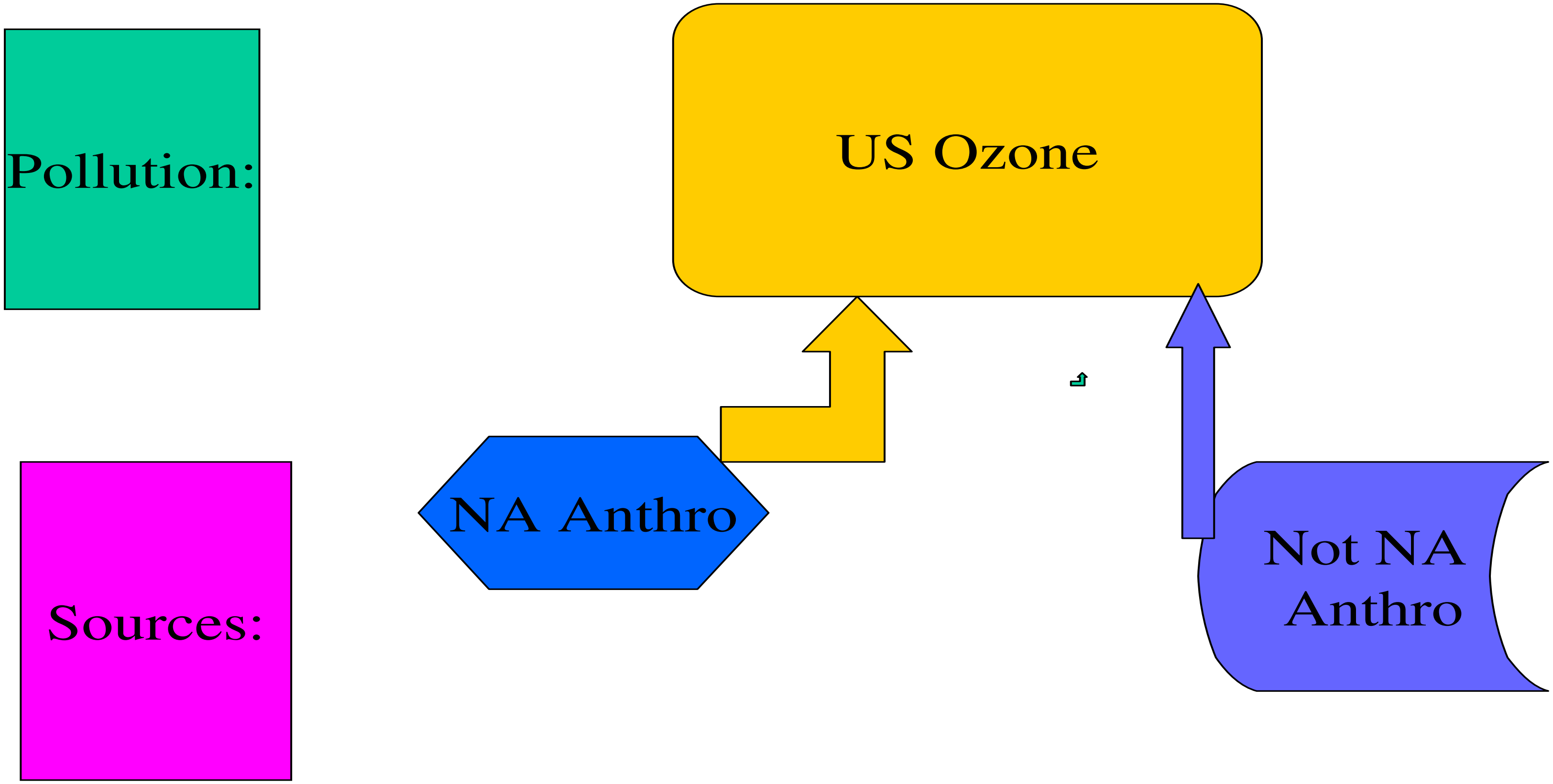
NEED TO MONITOR

NEED TO RELATE AMBIENT TO
PERSONAL EXPOSURES

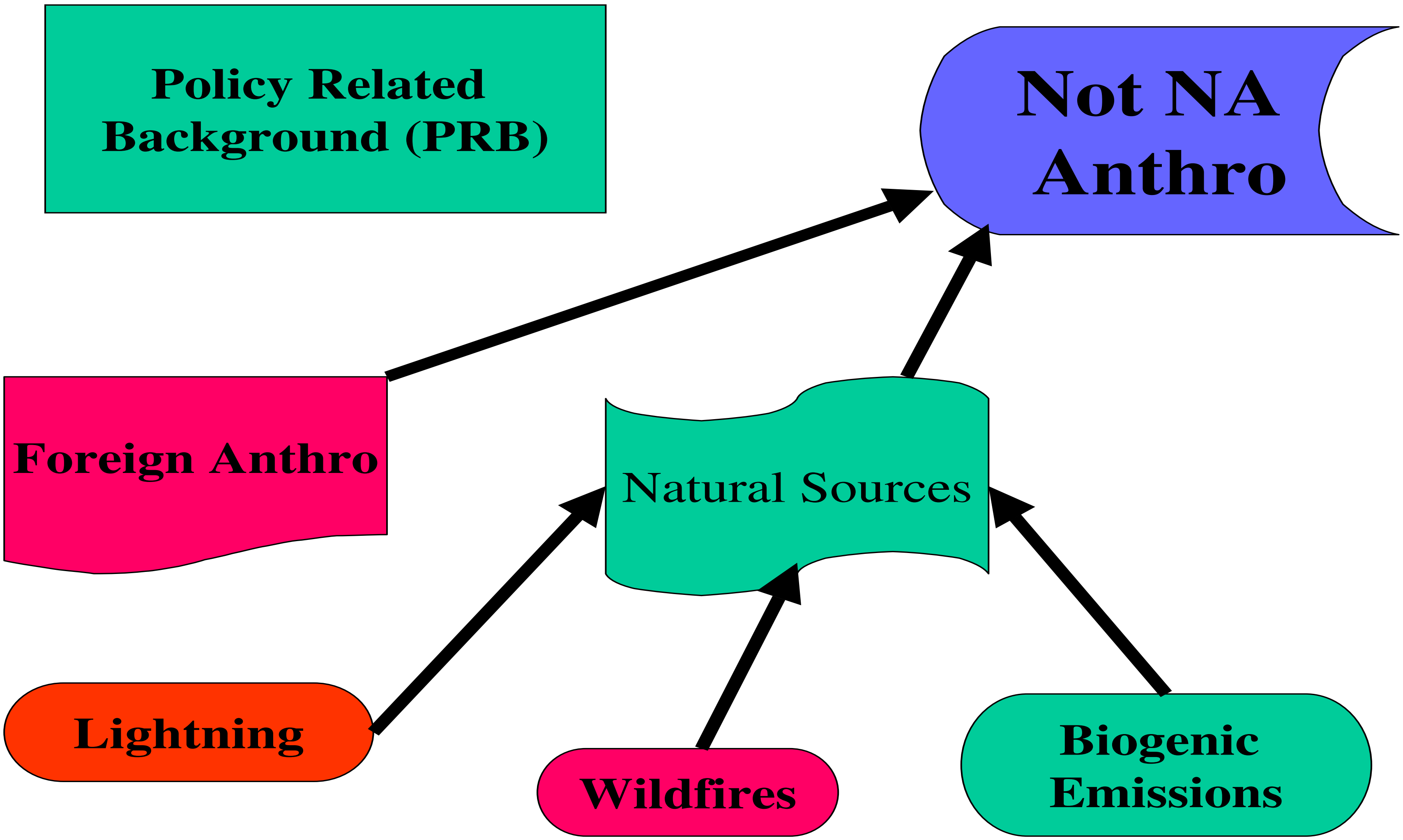
NEED DOSE RESPONSE MODELS

IMPACT ESTIMATES/CONTROL!!!

Ozone example



Ozone example



Estimating the PRB

- Not measurable
  - urban pollution spreads to rural areas
  - few pristine sites left
  - not likely representative of contaminated areas
- points to the need to use deterministic chemical transport models
  - GEOS-CHEM used for ozone
  - outputs similar to MAQSIP seen below
- need to calibrate against ground measurements

15

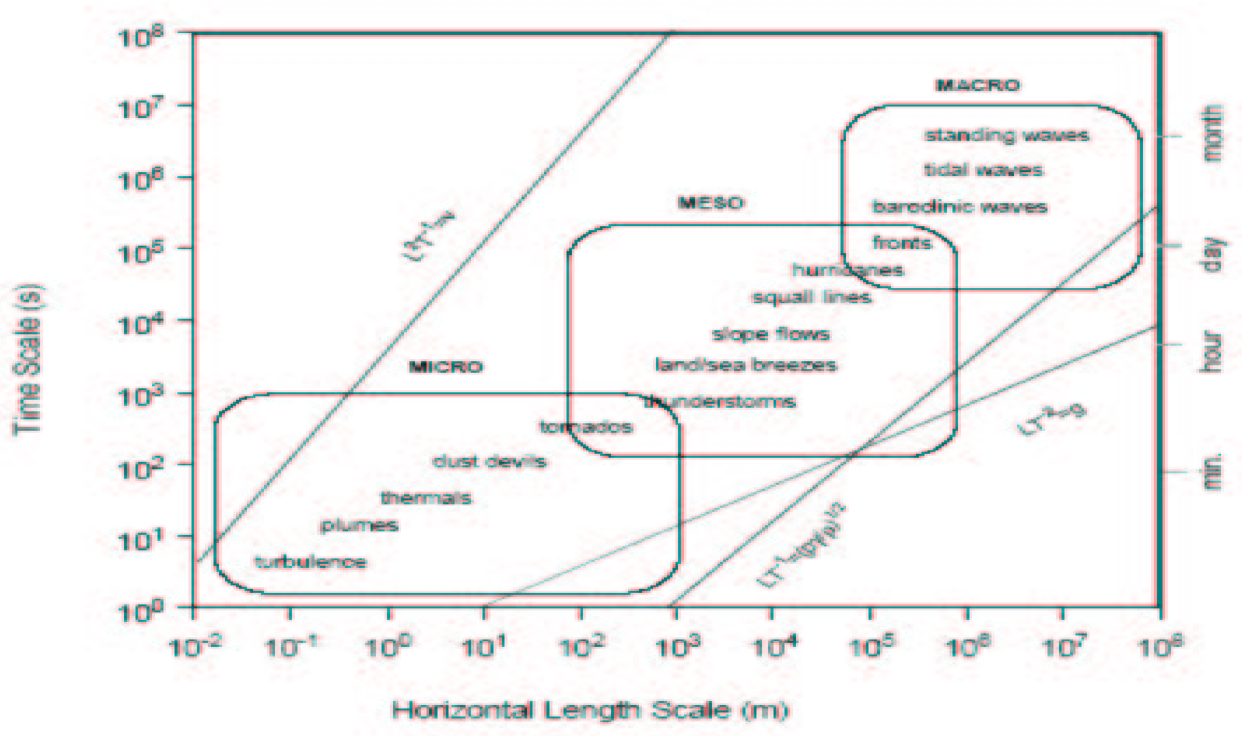
Calibrating CTMs

Must confront the differential scaling.

- CTMs are meso-scale models
- field measurements are made at the microscale

Problem: incomparable scales

Steyn & Galmarini 2003.



Models: mesoscale. **Real data:** just $m^2 \times$ few minutes $\rightarrow$ lower left hand corner!!

11

Solution: Bayesian Melding

- Instrument ensemble $i = 1, \ldots, D$
- Model ensemble $i = 1, \ldots, M$
- s = spatial location
- Measured values $\hat{Z}_i(s), \; i = 1, \ldots, D$
- $Z(s)$ = true value
- B = grid cell
- Simulated values $\tilde{Z}_i(B), \; i = 1, \ldots, M$

Extends Montserrat Fuentes and Adrian E. Raftery 2005 Biometrics

Solution: Bayesian Melding

Case of a single model, single instrument:

$$
\begin{aligned}
\hat{Z}(s) &= Z(s) + e(s) \leftarrow N(0, \sigma_e^2) \perp Z(s) \\
Z(s) &= \mu(s) + \epsilon(s) \leftarrow N(0, \Sigma) \\
\tilde{Z}(s) &= a(s) + b(s)Z(s) + \delta(s) \leftarrow N(0, \sigma_\delta^2) \perp Z(s), e(s) \\
\tilde{Z}(B) &= \mathbf{[} \int_B a(s)ds + \int_B b(s)Z(s)ds + \int_B \delta(s)ds \mathbf{]} / |B|
\end{aligned}
$$

Dealing with the integrals

$Z(B)$ can be approximated by the average of the values of process evaluated at the sampling points within B:

$$\tilde{Z}(B) \approx \frac{1}{L} \sum_{j=1}^{L} Z(\boldsymbol{s}_{j,B}). \tag{1}$$

The covariance field

local stationarity Spatial covariance given by:

$$C(s_1, s_2; \theta) = \int_D K(s_1 - s)K(s_2 - s)C_{\theta(s)}(d)ds$$

- $d = s_1 - s_2$
- D = whole region
- Matern covariance kernel with parameters
  - $\theta(s) = (\nu_s, \sigma_s, \rho_s)$
- Approximation: D replaced by regular grid - $\theta(s)$ has ANOVA model without interaction - independent normal main effects fitted in MCMC.

Prior - posterior modelling

- Joint posterior distribution stationary case:

$$
\begin{aligned}
& p(\hat{\boldsymbol{Z}}, \tilde{\boldsymbol{Z}}, \boldsymbol{Z}, \boldsymbol{\beta}, \boldsymbol{\theta}, a, b, \sigma_e^2, \sigma_\delta^2) \\
= \;& p(\hat{\boldsymbol{Z}}|\boldsymbol{Z}, \sigma_e^2) p(\tilde{\boldsymbol{Z}}|\boldsymbol{Z}, a, b, \sigma_\delta^2) p(\boldsymbol{Z}|\boldsymbol{\beta}, \boldsymbol{\theta}) \pi(\sigma_e^2, \sigma_\delta^2, \boldsymbol{\beta}, \boldsymbol{\theta}) \\
= \;& \Phi_{\sigma_e^2 \boldsymbol{I}}(\hat{\mathbf{Z}} - \mathbf{A}_1 \mathbf{Z}) \Phi_{\sigma_\delta^2 \boldsymbol{I}}(\tilde{Z} - a\mathbf{1} - b\mathbf{A}_2\mathbf{Z}) \\
& \Phi_{\Sigma(\boldsymbol{\theta})}(\boldsymbol{Z} - \boldsymbol{X}\boldsymbol{\beta}) \pi(\sigma_e^2) \pi(\sigma_\delta^2) \pi(\boldsymbol{\beta}) \pi(\boldsymbol{\theta}).
\end{aligned}
$$

- Here
  - $X\beta$ = polynomial in (lat long) over fitted by reversible jump - not critical the app below
  - **Z** = truth vector for monitoring & cell sites

Hyperparameters: stationary case

- **sill** and **range** parameters σ & ρ have inverse prior distributions
- nevertheless, MH step within Gibbs needed for cope with **range**
- ν_s fixed at 1/2 (exponential spatial covariance) in soon-to-be published tech report-to speed up computation & enable more extensive assessment
- bias parameters (a, b) have joint normal

The MCMC algorithm

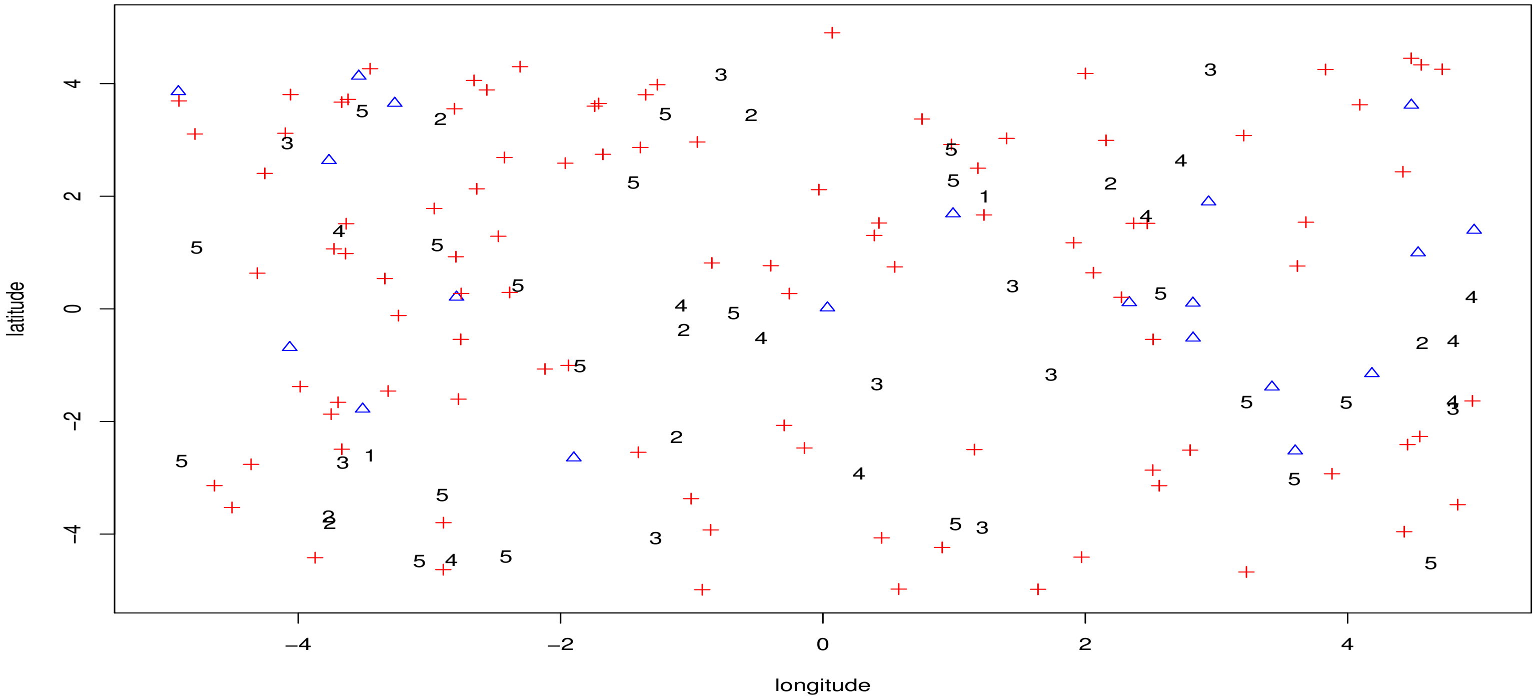
- Stage 1: Given all else, sample truth vector **Z**
- Stage 2: Given **Z** & β, sample $\theta = (\sigma, \rho)$. Then sample β given θ & **Z**
- Given all else, sample bias parameters and error variances.
- spatial prediction of truth at non-monitoring & non-cell sites output in Gibbs run

Simulation study

- 120 sites
  - 20 monitored
  - 100 unmonitored
  - 50 grid cells

.

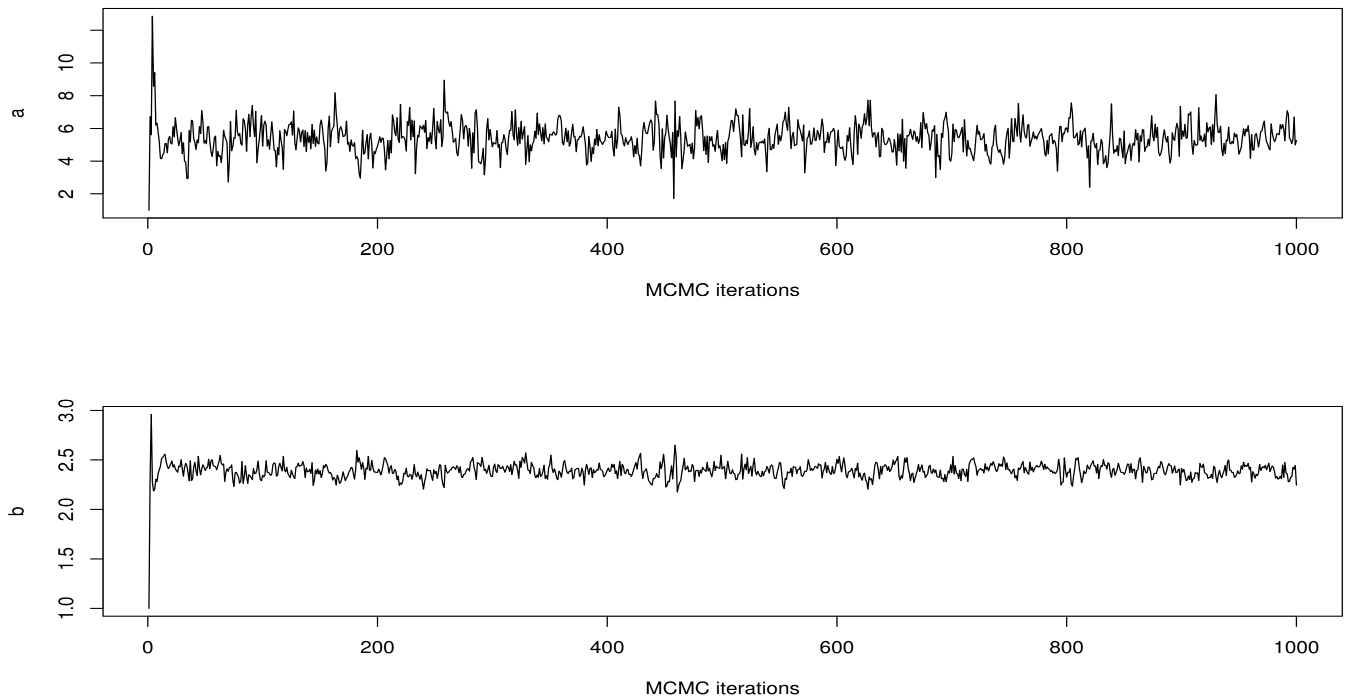
Simulation study



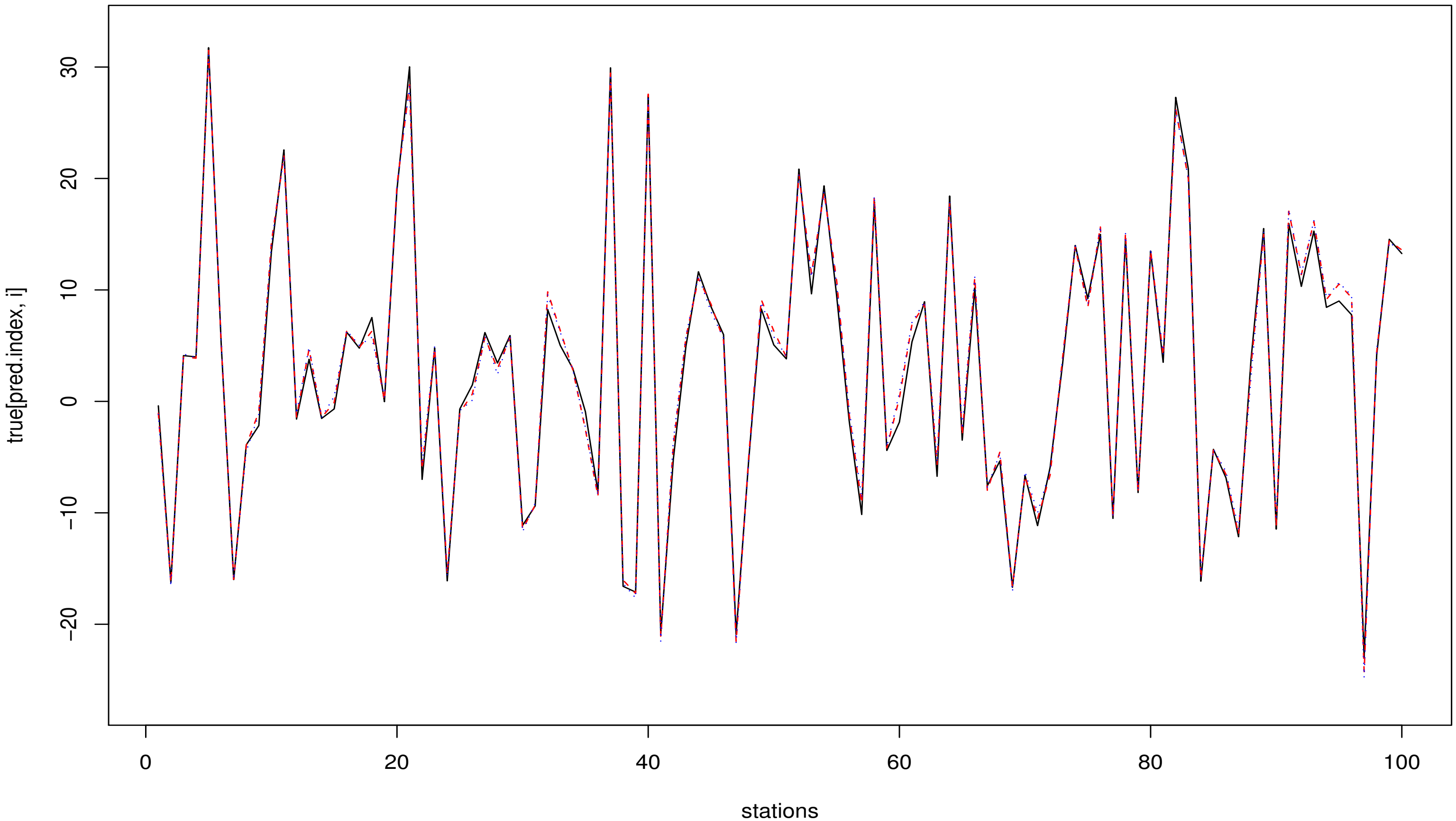
Site locations Monitoring sites:Δ; predictand sites: +; 1: 1st 2 gridpoints, 2: 3-10 gridpoints, 3: 11-20 grid points, 4: 21-30 gridpoints, 5: 31-50 gridpoints.

Simulation study

- **rapid MCMC convergence of bias parameters:** a (additive bias top panel) and b (multiplicative bias bottom panel) using just 10 grid cells.



Simulation study



Spatial prediction results for 100 unmeasured stations using Bayesian melding in the case of 50 grid cells. Solid line = truth.

Prediction interval calibration

Coverage probabilities Kriging and Melding varying number of grid cells.

		# grid cells used			
%	krige	0 cells	10 cells	. . .	50 cells
95	48	86	90	. . .	91
90	42	77	83	. . .	85
80	34	65	70	. . .	72
70	27	54	59	. . .	62
60	23	46	50	. . .	52
40	15	30	34	. . .	35

Simulation conclusions

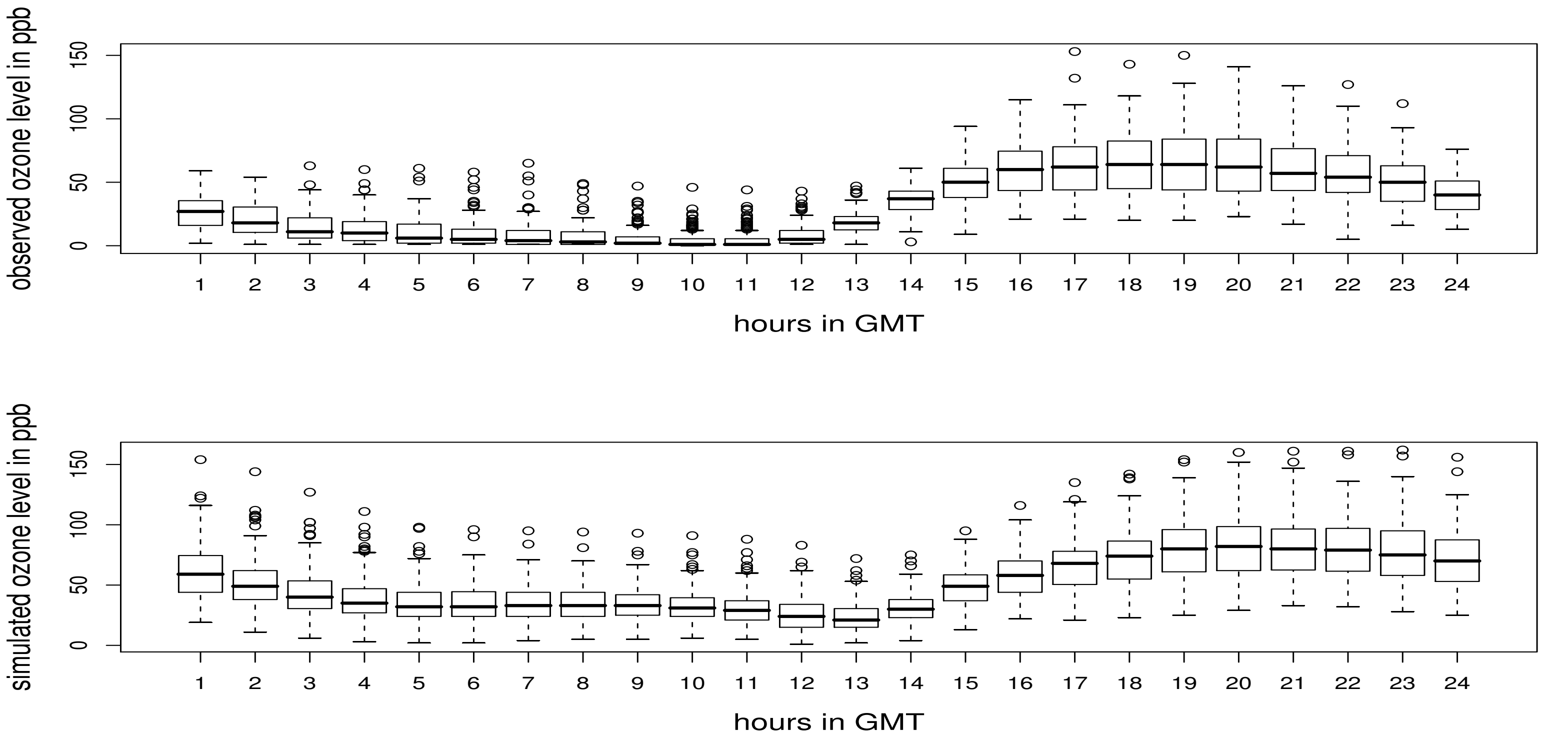
- estimates of bias parameters (a, b) and truth spatial mean parameters β are very good
- estimates of covariance parameters reasonably good - range is more difficult with heavy posterior tails
- increasing grid cell numbers-increasing accuracy
- melding beats kriging
- does not produce good estimates of covariance parameters unless sampling points close together
- computationally intensive

Ozone application

- data from > 200 monitoring sites EPA AIRS database
  - 120 days from May 15 - Sept 11 1995.
  - hourly concentrations O_3 (ozone)
- simulated data from **MULTISCALE AIR QUALITY SIMULATION PLATFORM (MAQSIP)** model
  - Resembles **GEOS-CHEM** the CTM used to set the **PRB** level for ozone
  - uncertainty about its bias and accuracy

40

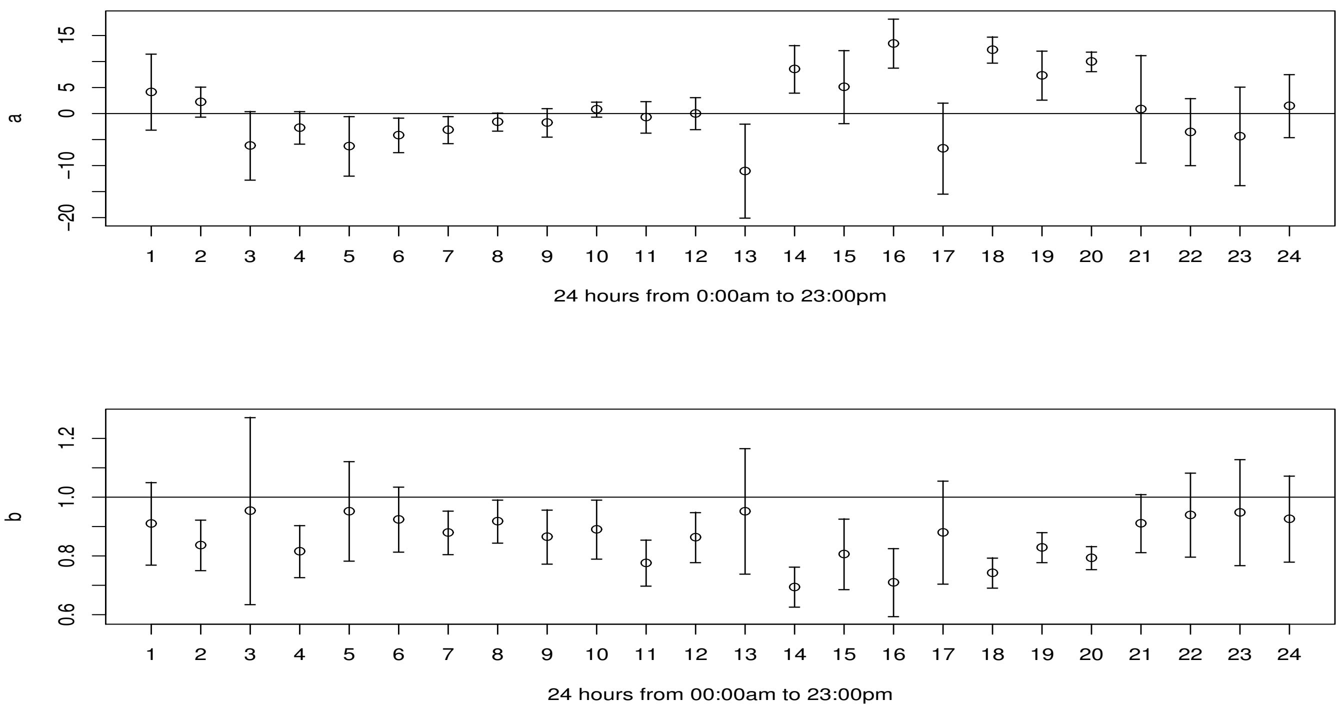
Sample model outputs vs measurements



Top panel: monitoring site measurements (ppb). **Bottom:** MAQSIP outputs for cell containing that monitoring site.

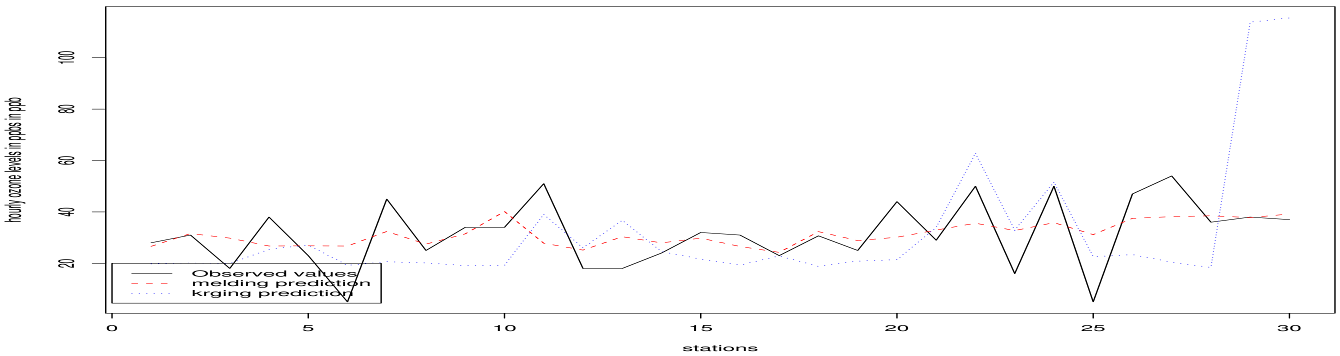
Sample results

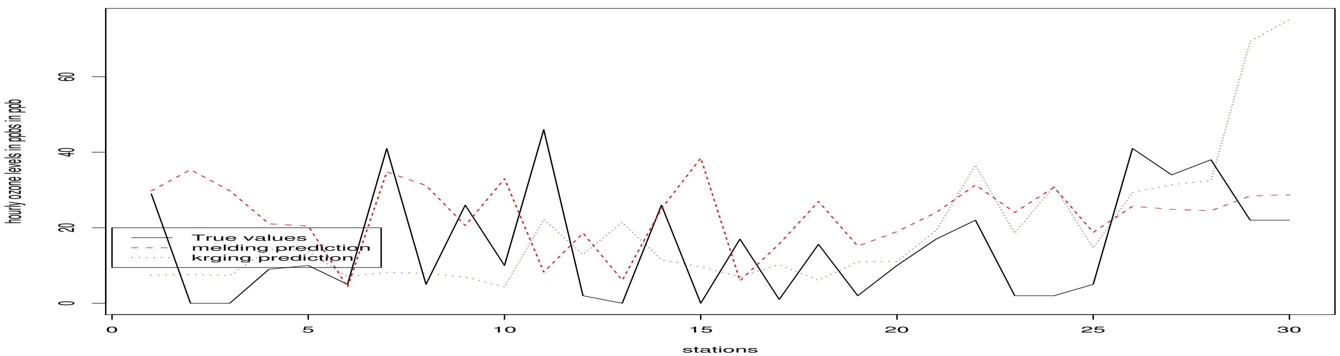
Substantial model bias at certain hours a (additive bias - upper panel) b (multiplicative bias - lower panel)



Sample results

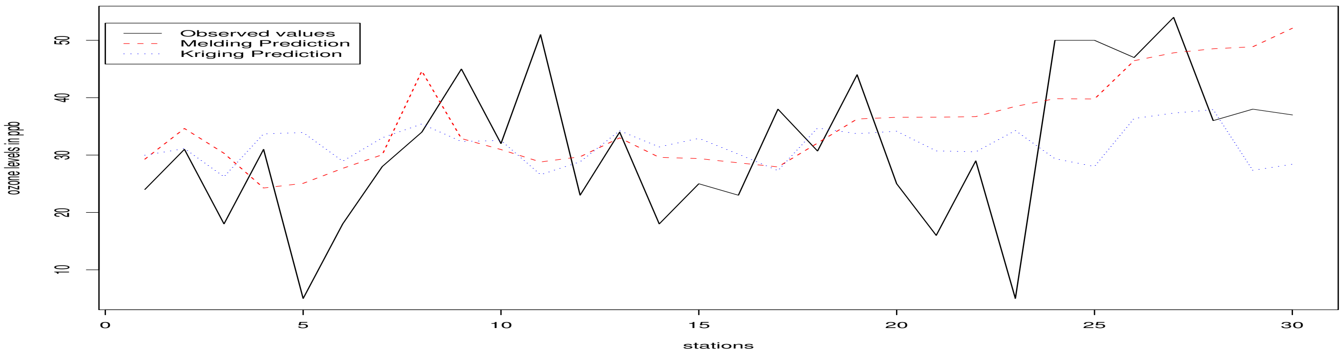
Comparison: melding (Red)and kriging (**Blue**) - 2 hours
30 target sites

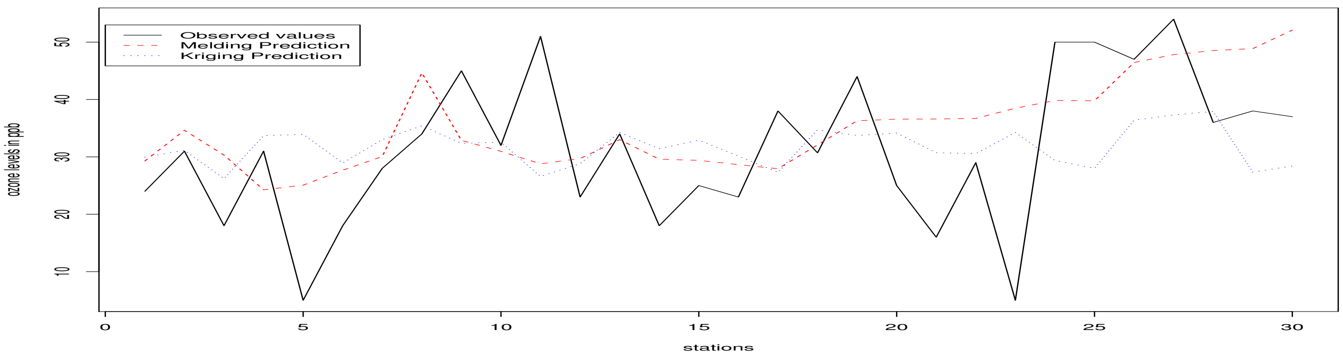




Sample results

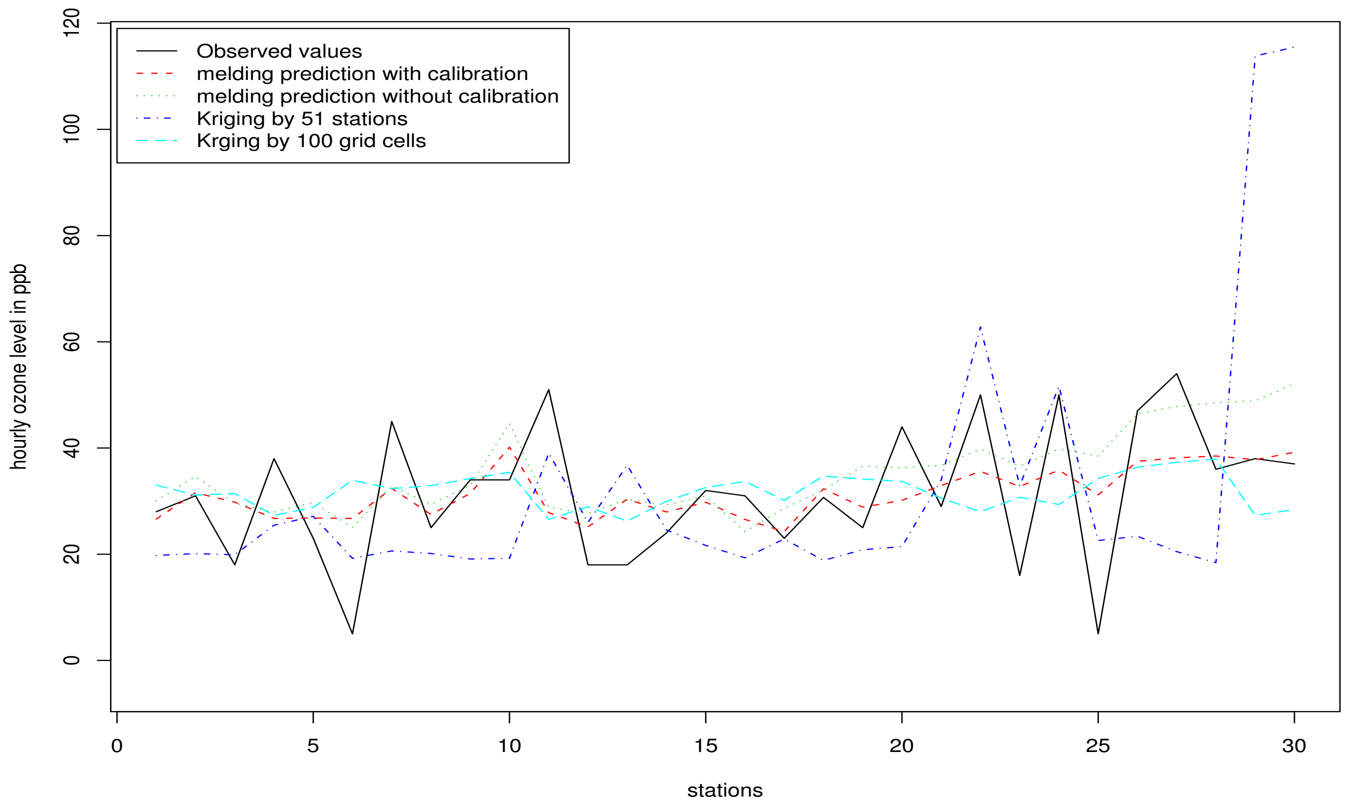
Comparison: melding (Red) simulated data only & kriging (Blue) - 2 hours, 30 target sites



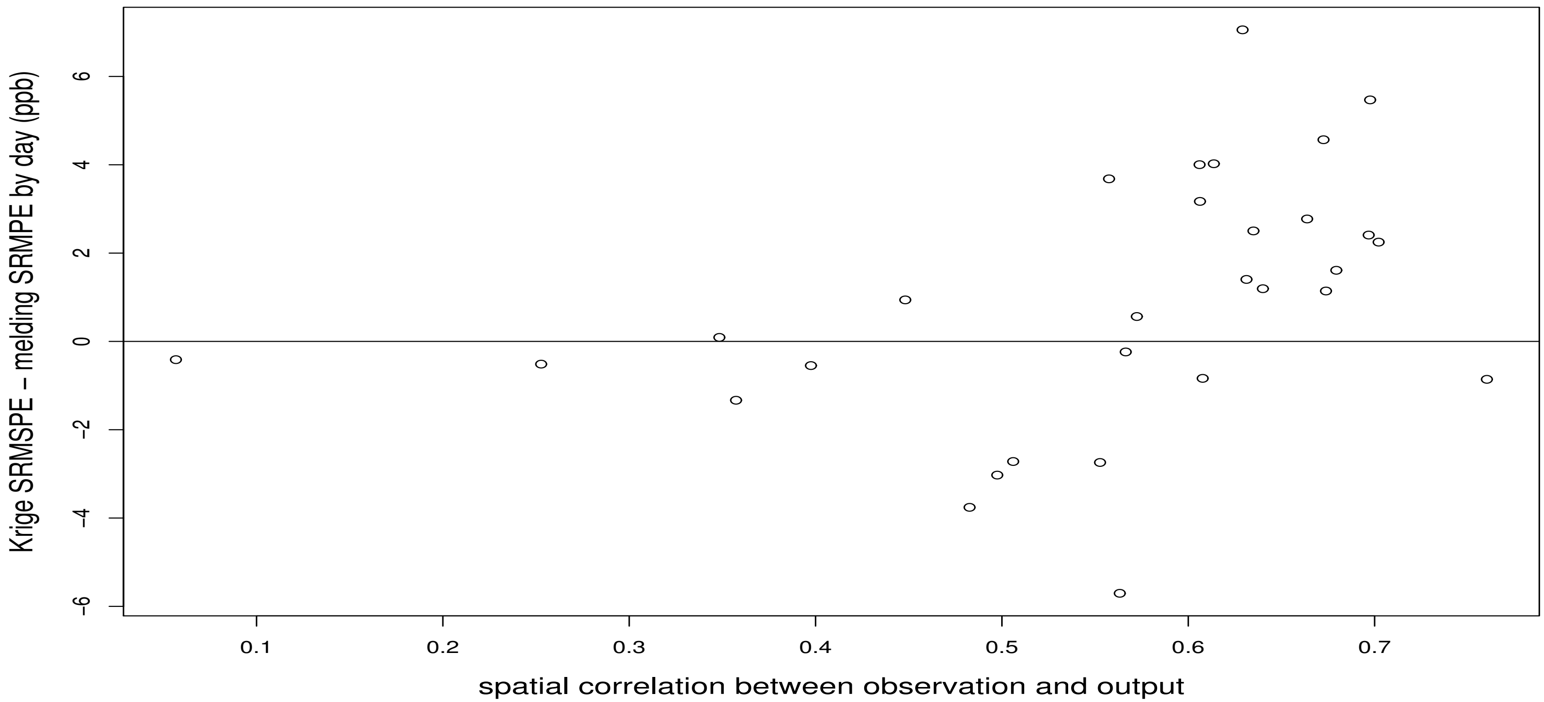


Sample results

Comparison: melding & kriging single hour, 30 target sites.**Red plot** - bias adjusted melding improves prediction. **dotted green plot** - no model bias adjustment. **dashed turquoise plot**-kriging the grid cell data



Sample results



Root mean square prediction error difference between Kriging & melding plotted against spatial correlation between **daily** average measuaaaaaaaaaarements and modeling outputs

Observations based on application

- increasing spatial correlation increases melding's performance over kriging for spatial prediction
- for daily average concentrations melding's 90% nominal predictive credibility interval has 87% actual coverage - pretty good
- melding predictive credibility intervals likely to be better calibrated than kriging

50

Overall conclusions

- melding provides a natural way of dealing with change of support problem and avoids naive comparisons of things on different scales
- only somewhat better at spatial prediction than kriging
- computationally expensive making less complicated alternatives worth exploring
- space-time methods will likely beat melding because they borrow strength across time and space
- **unlike kriging it can be used to estimate bias for hunting the elusive PRB level**

Concluding Remarks

- Setting air quality standards a complex process
  - combines uncertain science & public policy making
  - increasingly involves sophisticated statistical methods
  - part of a larger trend from “normal science” to “post - normal science”

Concluding Remarks

Funtowicz, Ispra Ravetz (2004?) Nusap.net:

> "...key properties of complex systems, radical uncertainty and plurality of legitimate perspectives....When facts are uncertain, values in dispute, stakes high, and decisions urgent the ...guiding principle of research science, the goal of achievement of truth,...must be modified. In post-normal conditions, such products may be ...an irrelevance."

REFERENCES

- **Spatial interpolation/melding software:** http://enviro.stat.ubc.ca/
- http://www.stat.ubc.ca/Research/TechReports/