Estimating fugitive emissions of airborne particulate matter using a Gaussian plume model

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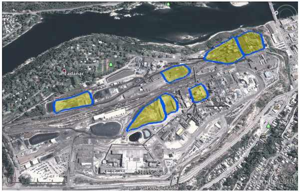
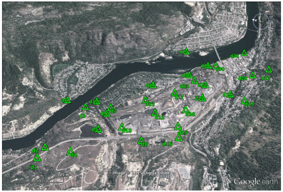
Fugitive emissions

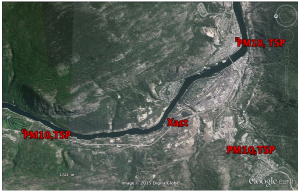
- Companies can place sensors on well-known sources.
- Unknown sources: piles of material, moving trucks, vents and windows, etc.
- Fugitive emissions are difficult to measure directly.
- Indirect measurements $\rightarrow$ source inversion

Fugitive emissions

- Teck Resources Ltd. at Trail, British Columbia.
- Integrated lead-zinc smelter.
- Different pollutants: zinc, lead, arsenic, SOx etc.
- During August 20 to September 19,2014.
- Multiple sensors: Dust-Fall jars, Xact, PM10 and TSP.
- Horizontal wind velocity and direction at a single post.

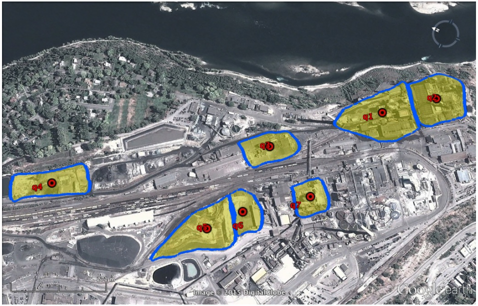






The forward problem

- Simplifying assumptions:
  - Ground is flat.
  - Horizontal wind velocity changes with altitude.
  - One type of contaminant with no chemical reactions.
  - Fixed deposition and settling velocities.
  - Only dry deposition (Ignore washout due to rain).
  - All sources in an area are approximated by a single point source.



The forward problem

- Gaussian plume (Ermak's[1]) solution for a point source at $(0, 0, H)$, x-axis pointing in the direction of wind:

$$c(\mathbf{x}) = \frac{q}{2\pi\sigma_y\sigma_z|u|}\exp\left(-\frac{y^2}{2\sigma_y^2} - \frac{W_{\text{set}}z}{2K_z} - \frac{W_{\text{set}}^2\sigma_z^2}{8K_z^2}\right)$$
$$\times\left[\exp\left(-\frac{H^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(H+2z)^2}{2\sigma_z^2}\right) - \exp\left(\frac{W_o(H+2z)}{K_z} + \frac{W_o^2\sigma_z^2}{2K_z^2}\right)\text{erf}\left(\frac{W_o\sigma_z}{\sqrt{2}K_z} + \frac{H+2z}{\sqrt{2}\sigma_z^2}\right)\right]. \tag{1}$$

- c concentration
- q rate of emissions
- u wind velocity
- W_{set} settling velocity
- W_{dep} deposition velocity
- $W_o = W_{\text{dep}} - \frac{1}{2}W_{\text{set}}$
- K_z vertical eddy diffusion coefficient
- σ_y, σ_z horizontal and vertical plume standard deviation

- Linear in the emission rates!
- Commonly used in industry standard software.

[1] Donald L. Ermak. "An analytical model for air pollutant transport and deposition from a point source". In: *Atmospheric Environment* 11.3 (1977), pp. 231–237.

The forward problem

- Wind data measured at times $\{\tau_1, \tau_2, \cdots, \tau_{N_w}\}$.
- Piece-wise constant wind data for $t \in (\tau_i, \tau_{i+1}]$.
- Piece-wise constant Ermak's solution for each sensor.
- $q_i(t)$, rate of emission of source $i \in \{1, 2, \cdots, N_q\}$.
- Sensor j is actively measuring on intervals $\{I_{j,1}, I_{j,2}, \cdots, I_{j,N_j}\}$, $I_{j,k} := \{t \in (a_{j,k}, b_{j,k}]\}$.
- Model sensor measurements as $d_{j,k} = B_j \int_{I_{j,k}} \sum_{i=1}^{N_q} c_{i,j}(t)dt$.
- Discretize on a grid $\{t_1, t_2, \cdots, t_{N_T}\}$, over the interval $(0, T]$.
- Concatenate and regroup to get

$$\mathbf{d} = \mathbf{F}\mathbf{q}$$

.

The inverse problem

- Additive, uncorrelated Gaussian noise

$$\mathbf{d} = \mathbf{F}\mathbf{q} + \boldsymbol{\epsilon}, \quad \epsilon \sim N(0, \boldsymbol{\Sigma}).$$

- Bayes' rule[2]

$$\pi_{\text{post}}(\mathbf{q}|\mathbf{d}) \propto \underbrace{\exp\left(-\frac{1}{2}\left\|\boldsymbol{\Sigma}^{-1/2}(\mathbf{F}\mathbf{q}-\mathbf{d})\right\|_2^2\right)}_{\text{likelihood}} \pi_{\text{prior}}(\mathbf{q})$$

- Three choices for the prior: constant+positivity, smoothness and smoothness+positivity

[2] Jari P. Kaipio and Erkki Somersalo. *Statistical and computational inverse problems*. Springer, 2005.

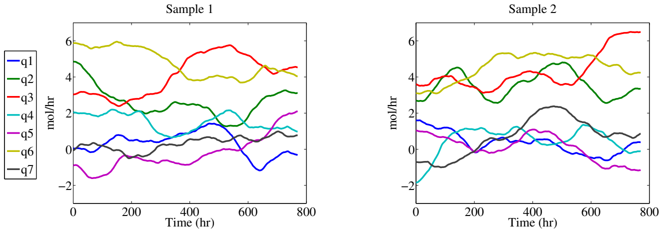
The inverse problem

- **Constant+positivity:**
  - Take $\mathbf{p} = (p_1, \cdots, p_{N_q})$ and $\mathbf{q} = \mathbf{B}\mathbf{p}$
  - Reduces to N_q dimensional problem.
  - Maximum likelihood estimator (MLE) will suffice

$$\mathbf{q}_{\mathsf{c}} = \mathbf{B}\mathbf{p}_{\mathsf{mle}}, \quad \mathbf{p}_{\mathsf{mle}} := \arg\min_{\mathbf{p}\succeq 0} \left\| \boldsymbol{\Sigma}^{-1/2}(\mathbf{F}\mathbf{B}\mathbf{p} - \mathbf{d}) \right\|_2^2 .$$

The inverse problem

- **Smoothness:**
  - Use constant emissions as prior mean.
  - Gaussian smoothness prior, $\pi_{\text{prior}}(\mathbf{q}) = N(\mathbf{q}_{\text{c}}, \mathbf{C})$.
  - $\mathbf{C} = \mathbf{I}_{N_q} \otimes \mathbf{L}^{-2}$, where $\mathbf{I}_{N_q}$ is the $N_q \times N_q$ identity matrix.
  - $\mathbf{L}$ is a discretization of $\alpha(I - \gamma\partial_{tt})$ with homogeneous Neumann bc.



  - Linear forward map $\rightarrow \pi_{\text{post}} = N(\mathbf{q}_{\text{s}}, \mathbf{C}_{\text{s}})$,

$$\mathbf{q}_{\text{s}} := \mathbf{q}_{\text{c}} + \mathbf{C}\mathbf{F}^*(\boldsymbol{\Sigma} + \mathbf{F}\mathbf{C}\mathbf{F}^*)^{-1}(\mathbf{d} - \mathbf{F}\mathbf{q}_{\text{c}}),$$
$$\mathbf{C}_{\text{s}} := \mathbf{C} - \mathbf{C}\mathbf{F}^*(\boldsymbol{\Sigma} + \mathbf{F}\mathbf{C}\mathbf{F}^*)^{-1}\mathbf{F}\mathbf{C}.$$

The inverse problem

- **Smoothness+positivity**
  - Introduce an auxiliary variable: $\mathbf{q} = \max\{\mathbf{v}, \mathbf{0}\}$.
  - Pose nonlinear problem for $\mathbf{v}$

$$\pi(\mathbf{v}|\mathbf{d}) \propto \exp\left(-\frac{1}{2}\left\|\boldsymbol{\Sigma}^{-1/2}(\mathbf{F}(\max\{\mathbf{v},\mathbf{0}\}) - \mathbf{d})\right\|_2^2\right) \pi_{\mathsf{prior}}(\mathbf{v}).$$

  - Use smoothness prior on $\mathbf{v}$

$$\pi_{\mathsf{prior}}(\mathbf{v}) = N(\mathbf{q}_{\mathsf{c}}, \mathbf{C})$$

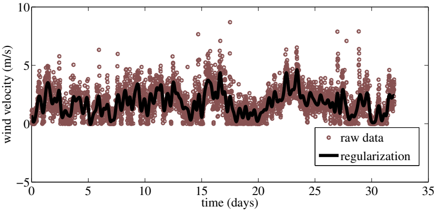
  - Use Markov Chain Monte Carlo to compute $\mathbf{v}_{\mathsf{CM}}$ (posterior mean), $\mathbf{q}_{\mathsf{sp}} := \max\{\mathbf{v}_{\mathsf{CM}}, \mathbf{0}\}$, standard deviations, etc.

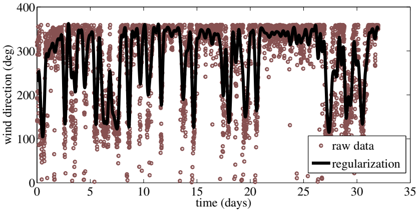
Application: setup

- During August 20 to September 19, 2014.
- PbO particulates.

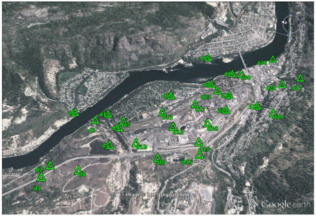
Density $[kgm^{-3}]$	Diameter $[m]$	Deposition vel. $[ms^{-1}]$	Settling vel. $[ms^{-1}]$
ρ	d	W_{dep}	W_{set}
9530	5×10^{-6}	0.005	0.0026

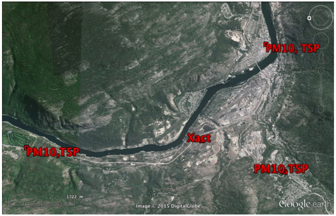
- Wind data at 10 minute intervals.





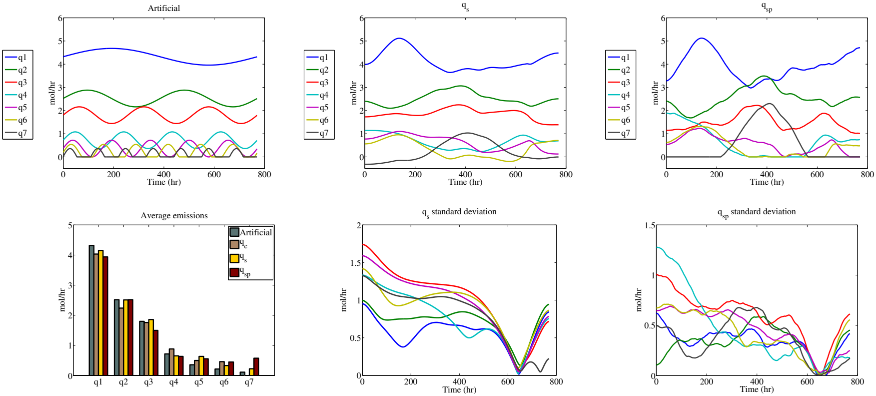
Application: setup





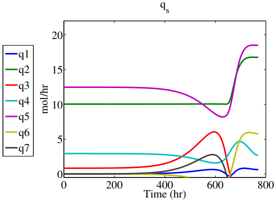
Type	Dust-fall jar	TSP	PM10	Xact
Sched.	entire month	every two days	every week	every hour
SNR	11	100	100	100
# meas.	1	16	6	761

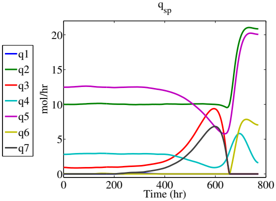
Application: synthetic data set

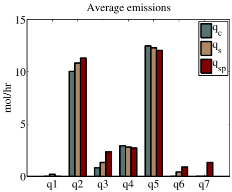


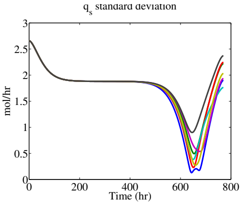
Application: actual data

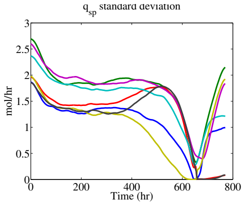
	$[tn/yr]$
q_c	54.0
q_s	57.5 ± 5
q_{sp}	63.0 ± 5
Prev. study	$25 - 40$
Indep.	$15 - 50$



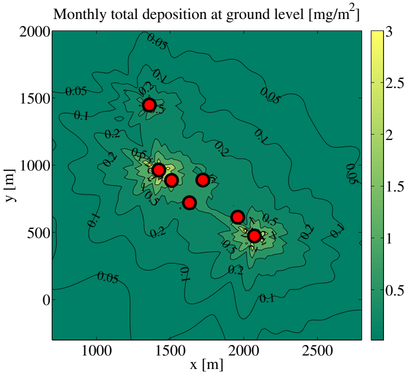


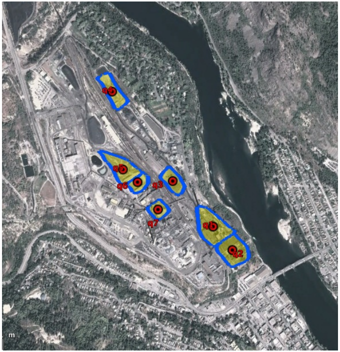






Application: impact assessment

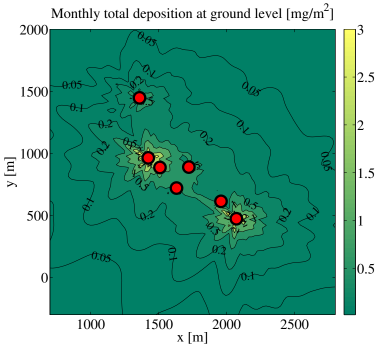


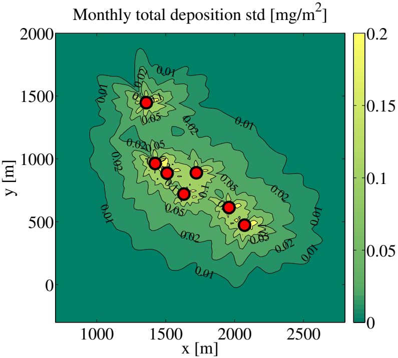


Application: uncertainty propagation

- Approximate posterior by $N(\mathbf{q}_{\mathsf{sp}}, \tilde{\mathbf{C}}_{\mathsf{sp}})$.
- Forward problem is linear

$$\pi_{\mathsf{deposition}} = N(\tilde{\mathbf{F}}\mathbf{q}_{\mathsf{sp}}, \tilde{\mathbf{F}}\tilde{\mathbf{C}}_{\mathsf{sp}}\tilde{\mathbf{F}}^*).$$





Closing remarks

- Estimating fugitive emissions is difficult.
- We solve three inverse problems.
  - Constant and positive emissions.
  - Smoothness.
  - Smoothness and positivitiy.
- Insufficient data.
- Room for improvement:
  - Better prior.
  - Faster algorithms.
  - Improve uncertainty propagation.
  - Include wind uncertainty.
  - Design of experiments.

Thank you!

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