Unclouding Pollution Maps

Ioannis Konstantinidis

February 21, 2014

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A philosopher, a mathematician, and an atmospheric scientist walk into a bar ...

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Special thanks to our major sponsors:

The Houston Endowment, the American Lung Association, and the University of Houston.

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The issue with ground-level ozone (O_3)

 Ground-level ozone is not emitted directly into the air, but forms through a reaction of nitrogen oxides (NO_x) and volatile organic compounds (VOC) in the presence of sunlight.

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- O_3 is a highly reactive gas, and the main component of smog. When inhaled, it damages the lung membrane, decreases lung capacity, and causes inflammation.

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• It is regulated by the EPA, which sets standards for acceptable exposure.

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- Following the current rule, the threshold for moderate to unhealthy for sensitive groups is 75ppb.

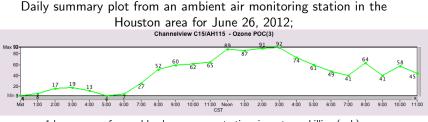
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- Following the current rule, the threshold for moderate to unhealthy for sensitive groups is 75ppb.
- Attaining compliance to the EPA standard requires that this threshold is exceeded no more than 4 days a year.
- There is a separate standard based on 1-hr averages that applies to areas which fail to comply with the 8-hr standard.

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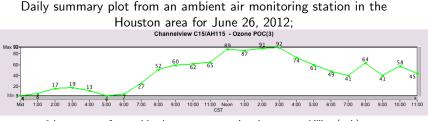
Houston, we have a problem



1-hr averages of ground-level ozone concentrations in parts per billion (ppb).

• The 8-hr averages exceeded 75 ppb for three time periods (those starting at 9am, 10am, and 11am).

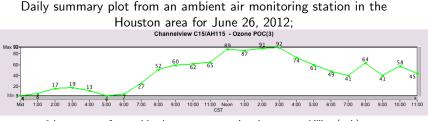
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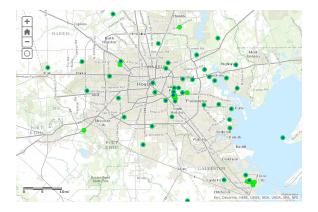


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- Until the standard is met, how can Houstonians stay informed about *current* ozone conditions in their daily lives?

Houston, we have a problem ... and it is not lack of data

On the monitoring side, the Texas Commission on Environmental Quality (TCEQ) maintains a network of 45 stations in the greater Houston area, collecting measurements every five minutes.



The problem is what we do with the data: clouding it

The TCEQ *retroactively* makes the data they collect available on the internet, reporting only the 1-hr average for the previous hour.

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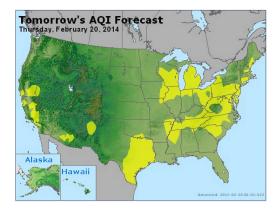
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but they do not produce forecasts or location-specific estimates.

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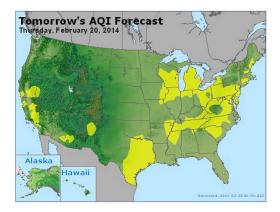
The problem is what we do with the data: mapping it

The EPA produces daily forecast maps for the AQI:



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The EPA produces daily forecast maps for the AQI:



but they do not capture the dynamics of ozone pollution, since they use coarse scales for time and location grids.

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Our task was to build mobile apps and a website that provide maps and individualized estimates of current ozone density, using the existing measurement framework.

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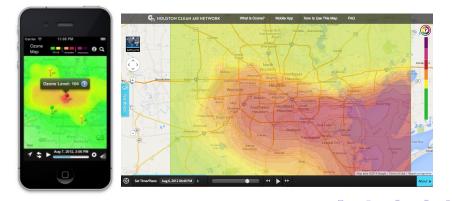
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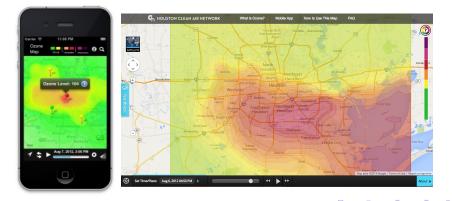
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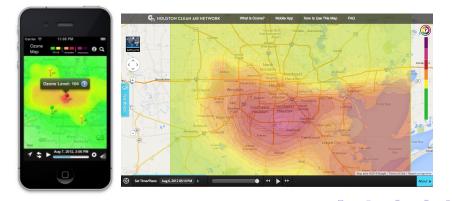
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Part II: the method

Assume an unknown

$$f: \mathbb{R}^D \to \mathbb{R}: \mathbf{x} \mapsto f(\mathbf{x})$$

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Assume an unknown

$$f: \mathbb{R}^D \to \mathbb{R}: \mathbf{x} \mapsto f(\mathbf{x})$$

and a set of N observations

$$\begin{bmatrix} \mathbf{X} \\ Y \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \dots & \mathbf{x}_N \\ y_1 & y_2 & \dots & y_N \end{bmatrix}$$

such that

$$y_n = f(\mathbf{x}_n), \ n = 1, \ldots, N$$

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Can we estimate f at a given $\mathbf{x}_{\star} \in \mathbb{R}^{D}$?

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Assume unknown

$$f: \mathbb{R}^D \to \mathbb{R}: \mathbf{x} \mapsto f(\mathbf{x})$$

AND

$$\phi: \mathbb{R}^D \to \mathbb{R}^P : \mathbf{x} \mapsto \phi(\mathbf{x})$$

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(ϕ stands for ϕ eature vector)

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Image: Image:

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(ϕ stands for ϕ eature vector) (\mathbb{R}^{P} stands for Pheature space)

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Key assumption: ϕ must be invertible and known.

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Assume unknown

$$f: \mathbb{R}^D \to \mathbb{R}: \mathbf{x} \mapsto f(\mathbf{x})$$

AND

$$\phi: \mathbb{R}^D \to \mathbb{R}^P : \mathbf{x} \mapsto \phi(\mathbf{x})$$

Key assumption: ϕ must be invertible and known. Now replace **X** by $\mathbf{\Phi} = \phi(\mathbf{X})$ and consider the observations

$$\begin{bmatrix} \mathbf{\Phi} \\ \mathbf{Y} \end{bmatrix} = \begin{bmatrix} \phi_1 & \phi_2 & \dots & \phi_N \\ y_1 & y_2 & \dots & y_N \end{bmatrix}$$

such that

$$y_n=f\circ\phi^{-1}(\phi_n),\;n=1,\ldots,N$$
 Can we estimate $ilde{f}=f\circ\phi^{-1}$ at a given $\phi_\star\in\mathbb{R}^P?$

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 Φ is a (finite) frame for its span in \mathbb{R}^{P} . Let $\mathcal{H} = \text{span}\Phi$ Obligatory definitions follow:

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- Analysis/Bessel

$$L: \mathcal{H} \to \mathbb{R}^N : \boldsymbol{\phi} \mapsto \boldsymbol{\Phi}^T \boldsymbol{\phi} = \{ \langle \boldsymbol{\phi}, \boldsymbol{\phi}_n \rangle \}_{n=1}^N$$

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- Frame operator

$$S: \mathcal{H} \to \mathcal{H}: \boldsymbol{\phi} \mapsto \boldsymbol{\Phi} \boldsymbol{\Phi}^{\mathsf{T}} \boldsymbol{\phi} = \sum_{n=1}^{N} \langle \phi, \phi_n \rangle \phi_n$$

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- Gram matrix

$$G = \mathbf{\Phi}^T \mathbf{\Phi}$$

- Gram operator

$$\mathbb{R}^{N} \to \mathbb{R}^{N} : Y \mapsto \mathbf{\Phi}^{T} \mathbf{\Phi} Y$$

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More frames

Lemma

If
$$\tilde{f}$$
 is a linear functional, i.e., $\tilde{f}(\phi_{\star}) = \phi_{\star}^{T} \alpha$, and $y_{n} = \tilde{f}(\phi_{n})$, then

$$\alpha = (\mathbf{\Phi}\mathbf{\Phi}^{\mathsf{T}})^{-1}\mathbf{\Phi}Y = \mathbf{\Phi}(\mathbf{\Phi}^{\mathsf{T}}\mathbf{\Phi})^{-1}Y$$

More frames

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Proof.

Since $y_n = \tilde{f}(\phi_n)$, we have $Y = \Phi^T \alpha$, so $L^*(Y) = \Phi Y = \Phi \Phi^T \alpha = S(\alpha)$ Hence,

$$\alpha = S^{-1}L^{\star}(Y) = (\mathbf{\Phi}\mathbf{\Phi}^{T})^{-1}\mathbf{\Phi}Y$$

Note that,

$$L^*G = L^*(LL^*) = (L^*L)L^* = SL^*$$
$$S^{-1}(L^*G)G^{-1} = S^{-1}(SL^*)G^{-1}$$
$$S^{-1}L^* = L^*G^{-1}$$

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Corollary

If \tilde{f} is a linear functional, i.e., $\tilde{f}(\phi_{\star}) = \phi_{\star}^{\mathsf{T}} \alpha$, and

$$\phi_{\star} \in \mathcal{H} = span \mathbf{\Phi} \subset \mathbb{R}^{P},$$

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(1)

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• What if $\phi_{\star} = \phi(x_{\star}) \notin \mathcal{H}$?

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(1)

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- What if $\phi_{\star} = \phi(x_{\star}) \notin \mathcal{H}$?
- Replace Φ^TΦ by Φ^TΦ + σ²I in Eq (1) to find the expected value of the Bayesian estimation of *f̃*, given a zero-mean Gaussian prior for α ~ N(0, I) and assuming additive errors in measurement that follow N(0, σ²):

$$\tilde{f}(\boldsymbol{\phi}_{\star}) = \boldsymbol{\phi}_{\star}^{T} \boldsymbol{\Phi} (\boldsymbol{\Phi}^{T} \boldsymbol{\Phi} + \sigma^{2} \mathbb{I})^{-1} \boldsymbol{Y}$$

Remark: If we can extend the mapping

$$G: \{\mathbf{x}_n\}_{n=1}^N \times \{\mathbf{x}_n\}_{n=1}^N \to \mathbb{C}$$
$$(\mathbf{x}_n, \mathbf{x}_m) \mapsto \langle \phi_n, \phi_m \rangle$$

to a kernel

$$G:\mathbb{R}^D\times\mathbb{R}^D\to\mathbb{C}$$

then we can drop our key assumption; we don't need an explicit formula for the feature map ϕ , since we only need to compute $\langle \phi(\mathbf{x}_{\star}), \phi(\mathbf{x}_{n}) \rangle$ for Eq (1).

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A common assumption is homogeneity, i.e., that there exists h such that

$$G(\mathbf{x}_n,\mathbf{x}_m)=h(\|\mathbf{x}_n-\mathbf{x}_m\|)$$

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A common choice for h is a Gaussian, leading to Gaussian Process Regression

Part III

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The Golden Jubilee

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