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Industrial Atmospheric Pollution Estimation Using Gaussian Process Regression

Session ESSI1.1 - Strategies and Applications of AI and ML in a Spatiotemporal Context
Oral presentation: **PICO spot 2** on Wednesday, 26 April 2023, 14:23
PICO **Screen: PICO2.10**, Wednesday, 26 April 2023, 14:33-15:45

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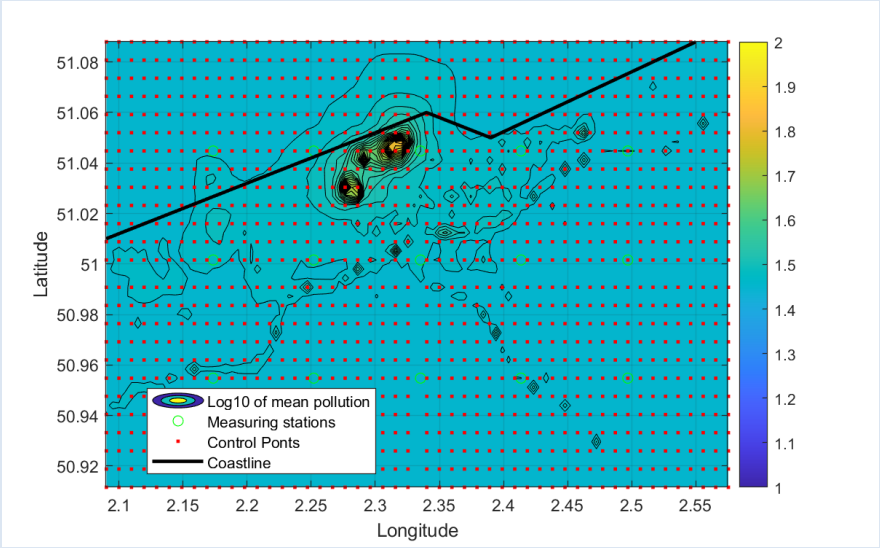
Problem: Spatial Interpolation of Air Pollution

Case of dispersed pollution:

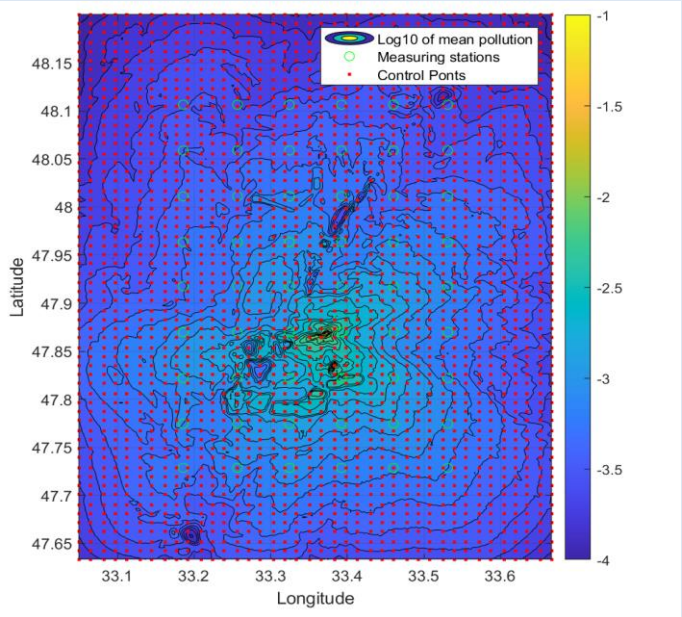
- **PM10** (µg/m^3) **simulated by (**coarse**) ADMS model**



- Industrialized Dunkerque region, North of France
- 15 measurement stations are simulated
- Interpolation based on Delaney triangulation
- **R2 = 0.85** ☺

Smoke-like narrow-directed industrial pollution:

- **SO2** (µg/m^3) **simulated by (**fine**) CALPUFF model**



- Industrialized Dnipropetrovsk Oblast, Ukraine
- 54 measurement stations are simulated
- Interpolation based on Delaney triangulation
- **R2 = 0.13** ☹

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- Interpolation with a **GPR based on temporal covariance**
- **R2 = 0.65** ☺

Plan of the talk

- Regions to be explored and simulated pollution data
- Pollution modelling: a few snapshots
- Simple Interpolation techniques in 2D
- Simple interpolation: results
- Gaussian Process Regression Interpolation
- GPR with explicitly estimated kernel: results
- GPR implementation: discussion
- Conclusions and perspectives

Regions to be explored and simulated pollution data

Dunkirk region, North of France

Sources of PM10 pollution:

- Local industry
- Sea port and English channel boat circulation
- Local transport
- Far away sources

Data on pollution: air quality agency ATMO-Nord (https://www.atmo-hdf.fr/)

Dunkirk with superposed population density

Pollution dispersion model **ADMS** (40 x 20 km) was used to simulate PM10 pollution
One year of modeling, pollution at surface level, resolution ~one hour, ~500 m

Dnipropetrovsk Oblast, Ukraine

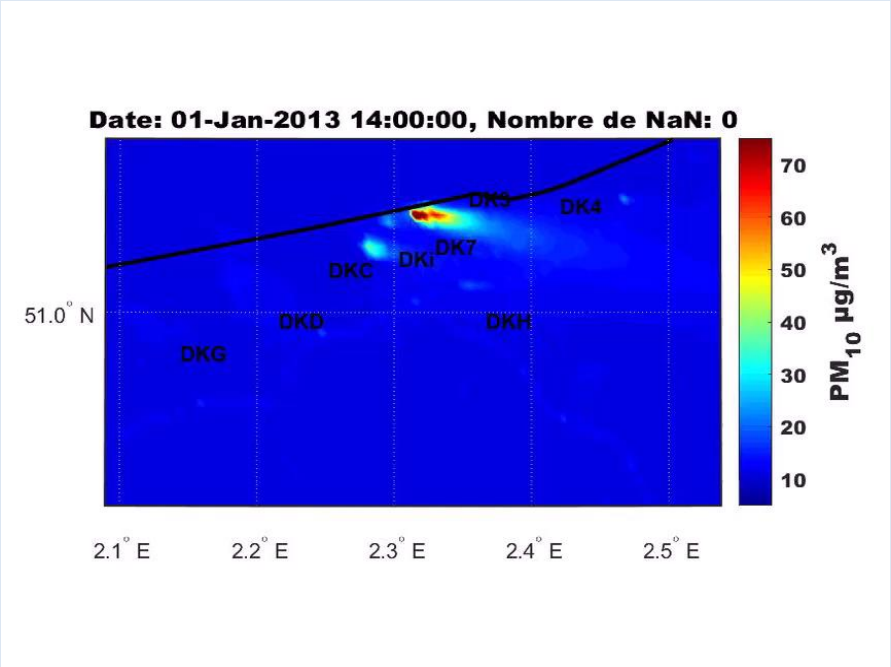
Sources of SO2 pollution:

- Local industry is a principal source of pollution
- Data on pollution: (https://partner.youairtest.com/)
- Transport and dispersion model **CALPUFF** was used to simulate **SO2** pollution,
- 40 x 60 km
- One year of modeling (2019), pollution at surface level, resolution ~one hour, ~100 m

Pollution modelling: a few snapshots

Dispersed pollution:

- **PM10** (µg/m^3) **simulated by ADMS model** (*)
- Industrialized Dunkerque region, North of France



(*) Sokolov et al. Optimization of environmental sensors placement in geophysical research. Proceedings of the 7th International Conference on Sensors Engineering and Electronics Instrumentation Advances (SEIA' 2021)

Smoke-like narrow-directed industrial pollution:

- **SO2** (µg/m^3) **simulated by CALPUFF model**
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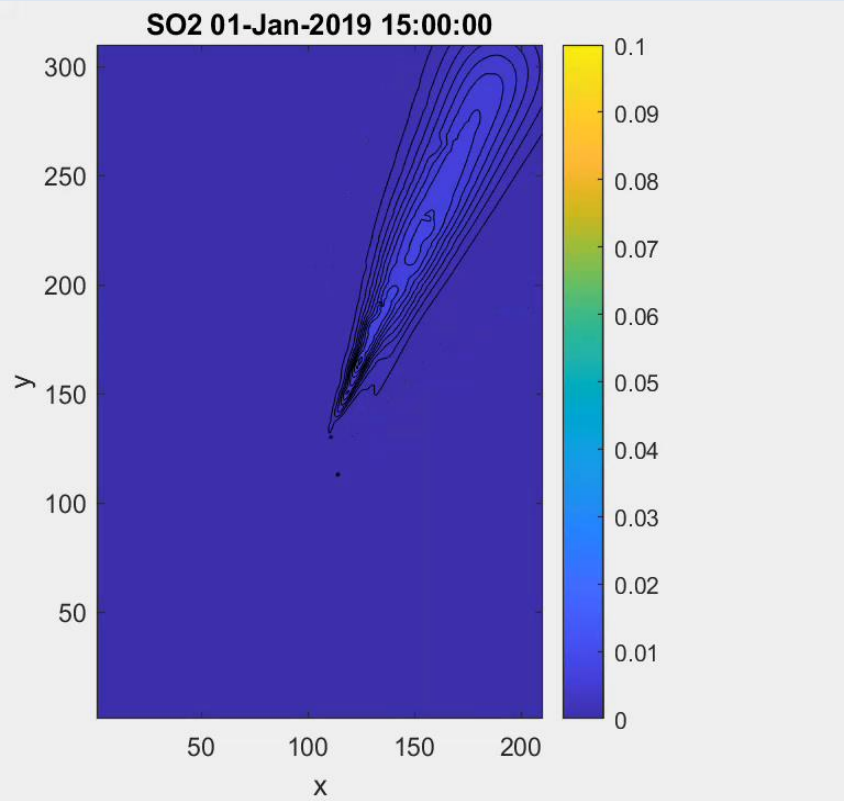


Simple Interpolation techniques in 2D

- ***These techniques do not take into account a time correlation between values of pollution at different points***

Inverse Distance Weighting

$$y(x) = \frac{\sum_{i=0}^{N} w_i(x) y_i}{\sum_{i=0}^{N} w_i(x)} \qquad w_i(x) = \frac{1}{\mathrm{d}(x, x_i)^p}$$

y : estimated PM_{10} pollution value at x position,

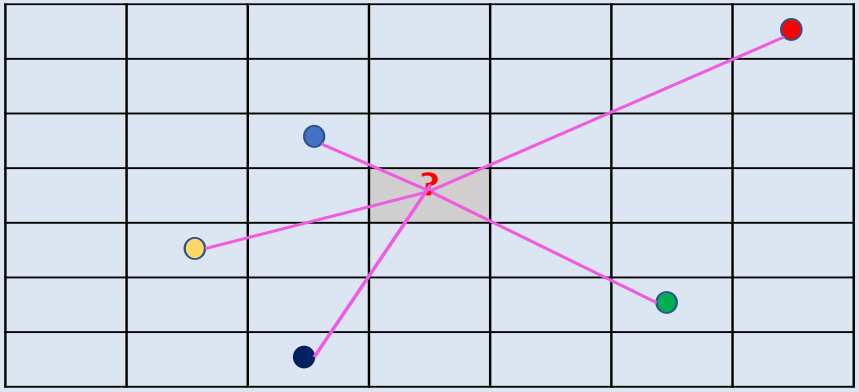
y_i: known values of the pollution

x_i: position of sensors,

$\mathrm{d}(x, x_i)$: the distance between x and x_i,

n : number of measurements,

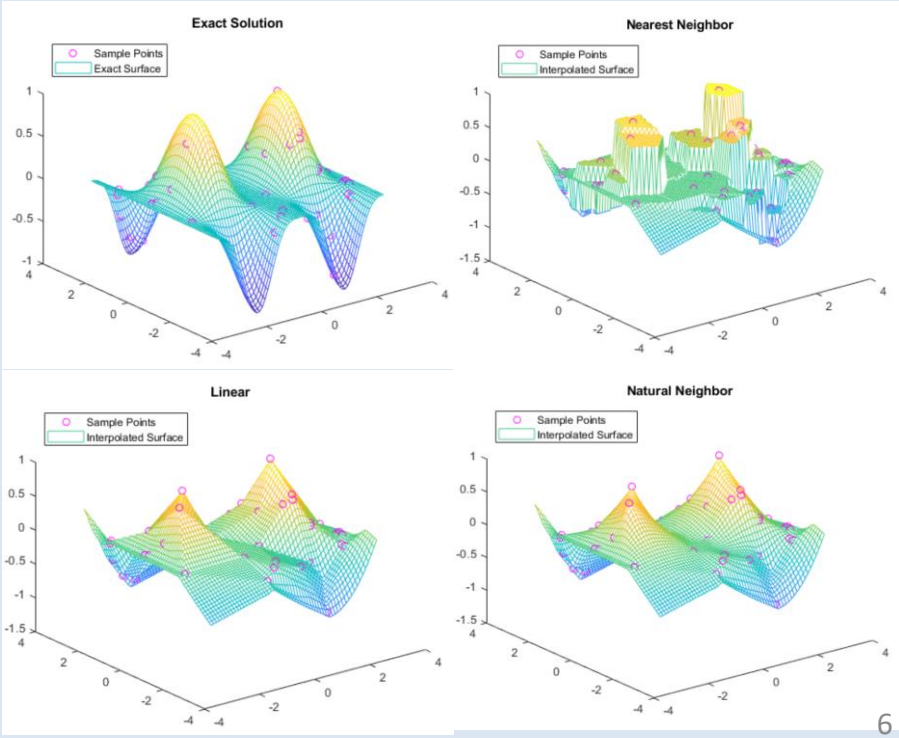
p : some hyperparameter



Delaunay Triangulation-based methods:

- Nearest neighbor (NN)
- Linier interpolation*
- Natural neighbor *

* NN method was used for extrapolation

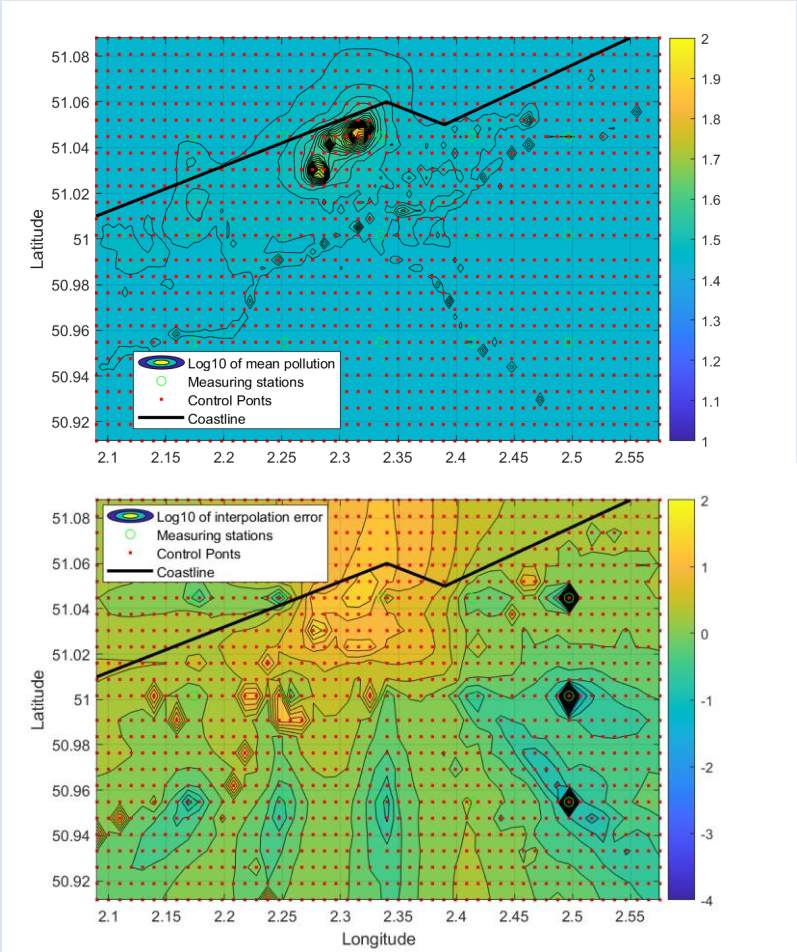


Examples are taken from Matlab software help for function $v(x,y)=\sin^4(x)\cdot\cos(y)$

Simple interpolation: Results

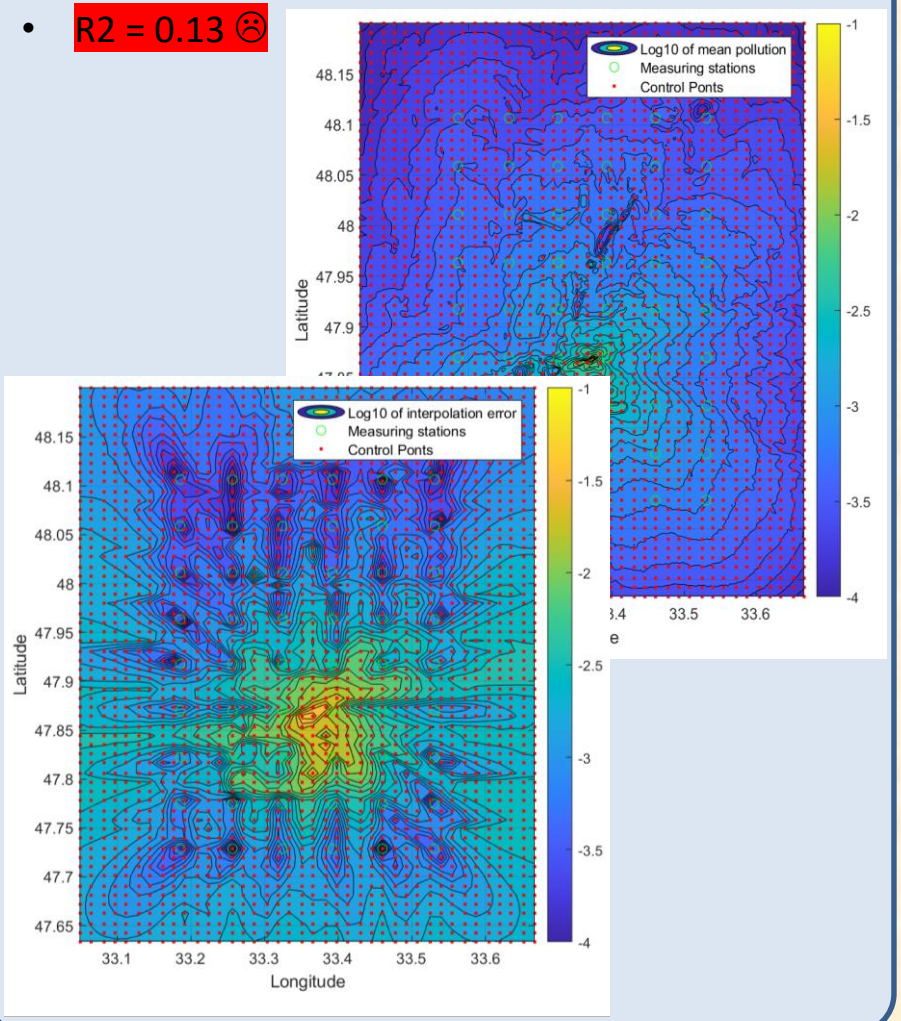
Case of dispersed pollution:

- **PM10** (μg/m^3) **simulated by ADMS model**
- 15 measurement stations, 1250 control points
- R2 = 0.85 ☺



Smoke-like narrow-directed industrial pollution:

- **SO2** (μg/m^3) **simulated by CALPUFF model**
- 54 measurement stations, 2400 control points
- R2 = 0.13 ☹



Gaussian Process Regression Interpolation

Gaussian process (GP) is a collection of random variables, any finite number of which follows a multivariate normal distribution (MVN):

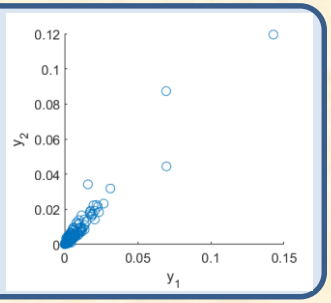
$$y = f(\boldsymbol{x}) \sim \mathcal{GP}\big(m(\boldsymbol{x}), k(\boldsymbol{x}, \boldsymbol{x}')\big),$$

$$m(\boldsymbol{x}) = E[f(\boldsymbol{x})],$$

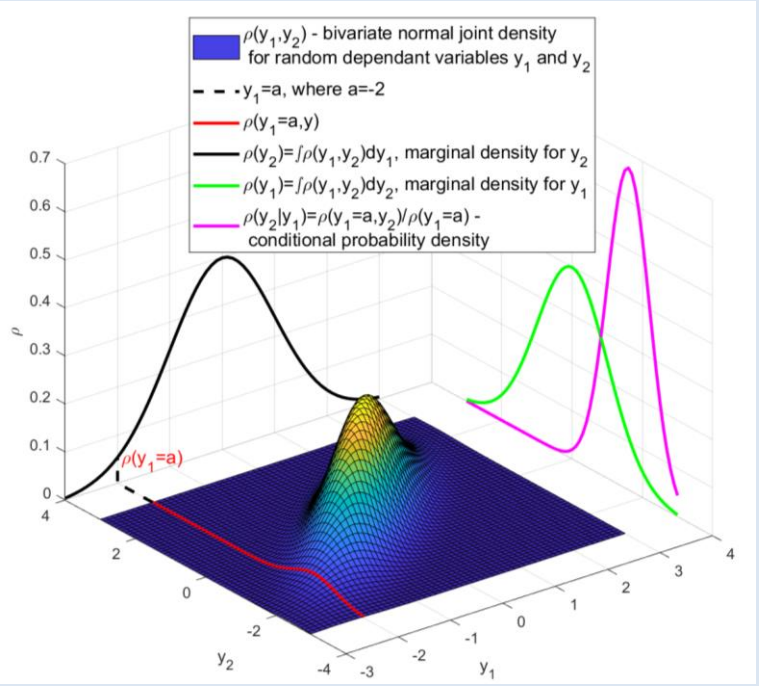
$$k(\boldsymbol{x}, \boldsymbol{x}') = E\big[\big(f(\boldsymbol{x}) - m(\boldsymbol{x})\big)\big(f(\boldsymbol{x}') - m(\boldsymbol{x}')\big)\big]$$

- $\boldsymbol{x}$ corresponds to position (latitude, longitude),
- $y = f(\boldsymbol{x})$ corresponds to a pollution value at $\boldsymbol{x}$
- mean $m(\boldsymbol{x})$ and kernel $k(\boldsymbol{x}, \boldsymbol{x}')$ should be somehow estimated from the available data
  - often a family of kernels $k(\boldsymbol{x}, \boldsymbol{x}'|\theta)$ depending on an optimized hyperparameter θ are used
  - here, the data of the temporal dimension allows estimating mean and kernel explicitly

- Suppose that we have a measurement of pollution at some point y_1
- The pollution value at a neighboring point y_2 will be highly correlated with y_1



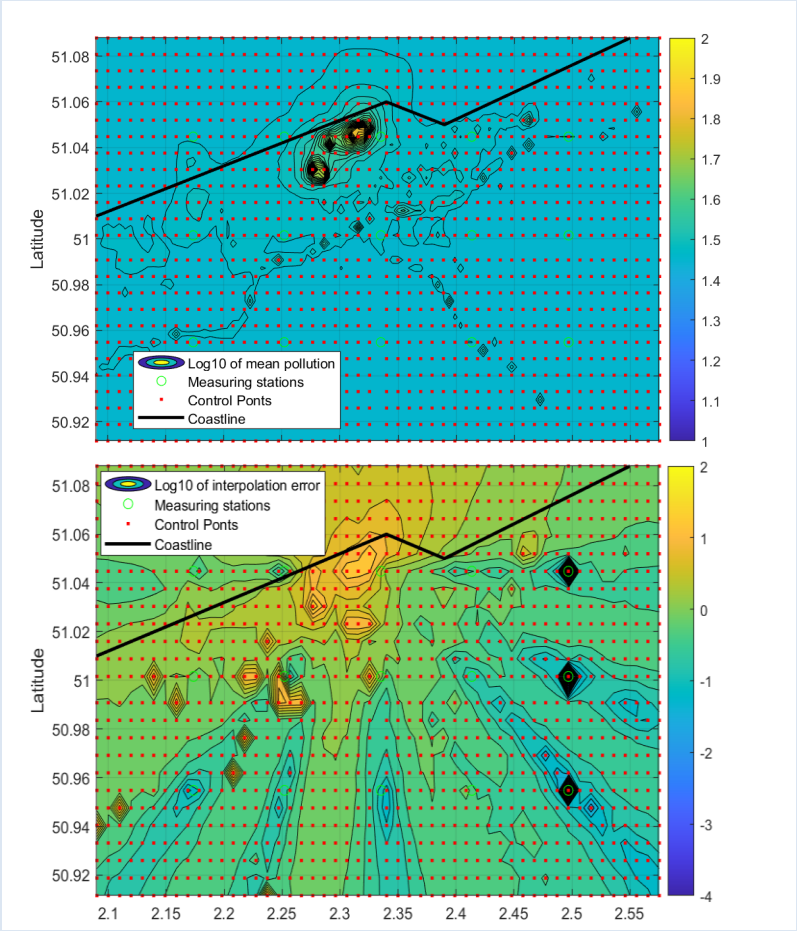
- If the joint probability density function (PDF) $\rho(y_1, y_2)$ is known, we can determine the posterior probability for y_2
- In particular, If y_1 and y_2 follows MVN, a posterior (conditional) $y_2|y_1$ will follow a normal low with known parameters
- Note below, that magenta curve (posterior) is narrow compared to green (marginal)
- Thus, the information on y_1 allows to specify y_2



GPR with explicitly estimated kernel: Results

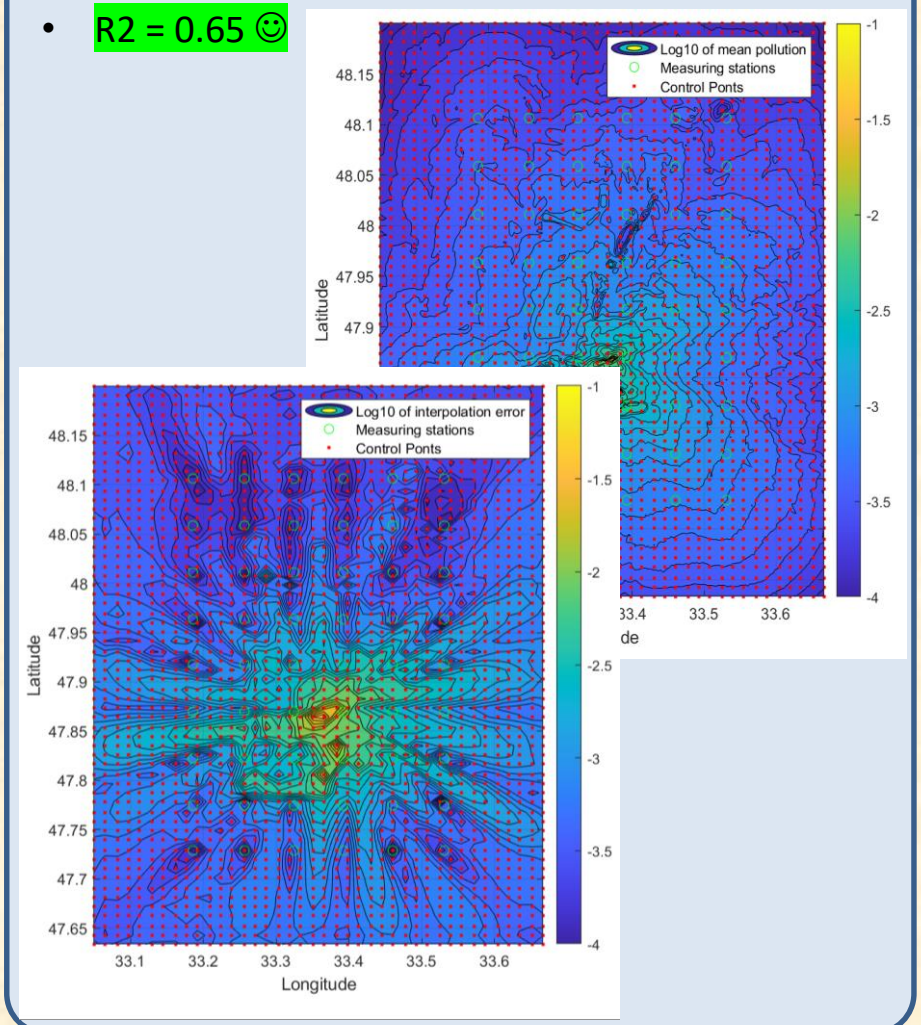
Case of dispersed pollution:

- **PM10** ($\mu g/m^3$) **simulated by ADMS model**
- 15 measurement stations, 1250 control points
- R2 = 0.96 ☺



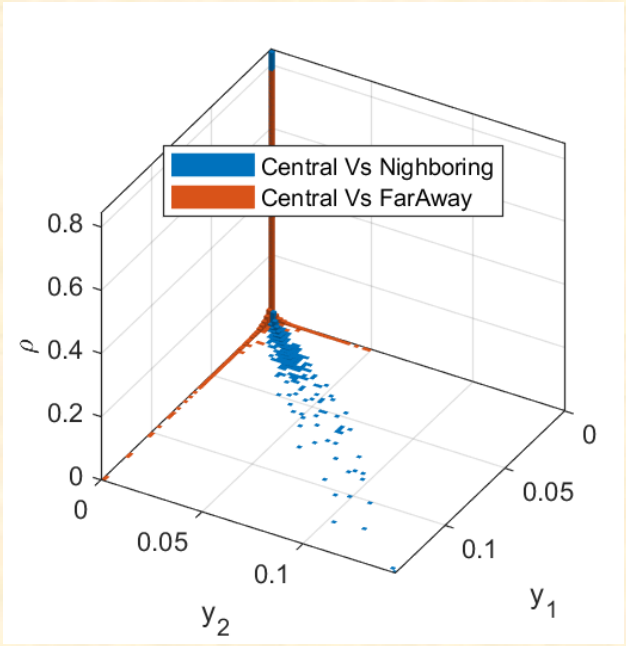
Smoke-like narrow-directed industrial pollution:

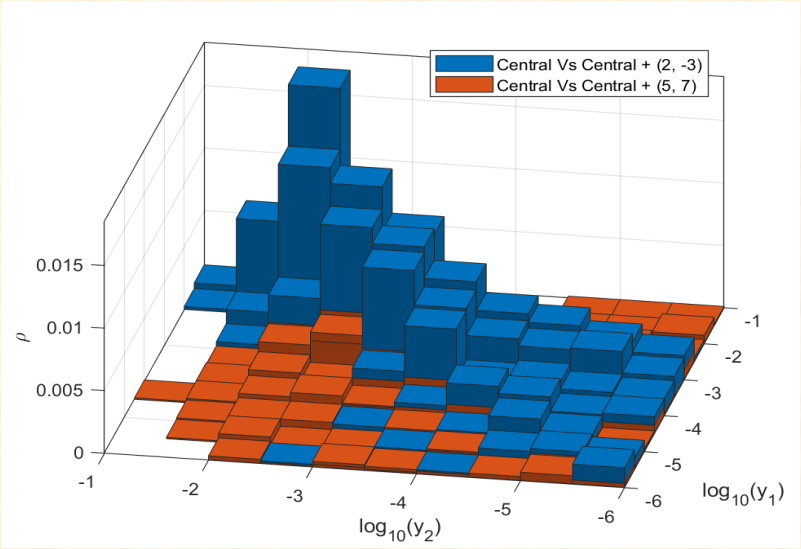
- **SO2** ($\mu g/m^3$) **simulated by CALPUFF model**
- 54 measurement stations, 2400 control points
- R2 = 0.65 ☺



GPR implementation : Discussion

- For kernel calculation pollution data has been smoothed and coarsened
- **Problem**: 5% of negative pollution values ☹
- **Problem**: in GPR variables should follow MVN distribution
- Is it the case?
  - The answer is no… ☹
- And if we use log transformation of the pollution?
  - What should we do with **zero values**?
  - Still not an MVN... ☹





- Two possible solutions could further be explored:

1) Find some other one to one transformation that allow getting an MVN distribution: Wrapping function. Unfortunately standard BoxCox transformation does not work…
2) Approximate the joint PDF by a (multivariate) gaussian mixture

Conclusions

- Simple 2D techniques are not suitable for efficient interpolation of smoke-like industrial pollution at scales of a few kilometers.
- This kind of problem can be tackled with GPR with the kernel explicitly estimated on the basis of time-depended pollution data.
- The proposed approaches was verified on two test-cases:
  - Dispersed PM10 pollution simulated by ADMS model for Dunkirk region
  - Smoke-like SO2 pollution simulated by CALPUFF model for Dnipropetrovsk Oblast
- A sufficient precision of interpolation was achieved for these test cases.

Perspectives

- Optimization of smoothing of the kernel function.
- Rigorous statistical validation
- Wrapping of pollution data to obtain MVN distribution in GPR
- Optimization of the observation network

Thank you for your attention…