

Maps of Optimal Model Parameters by Efficient Fitting and Extrapolation Techniques

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Outline

- **Motivation**

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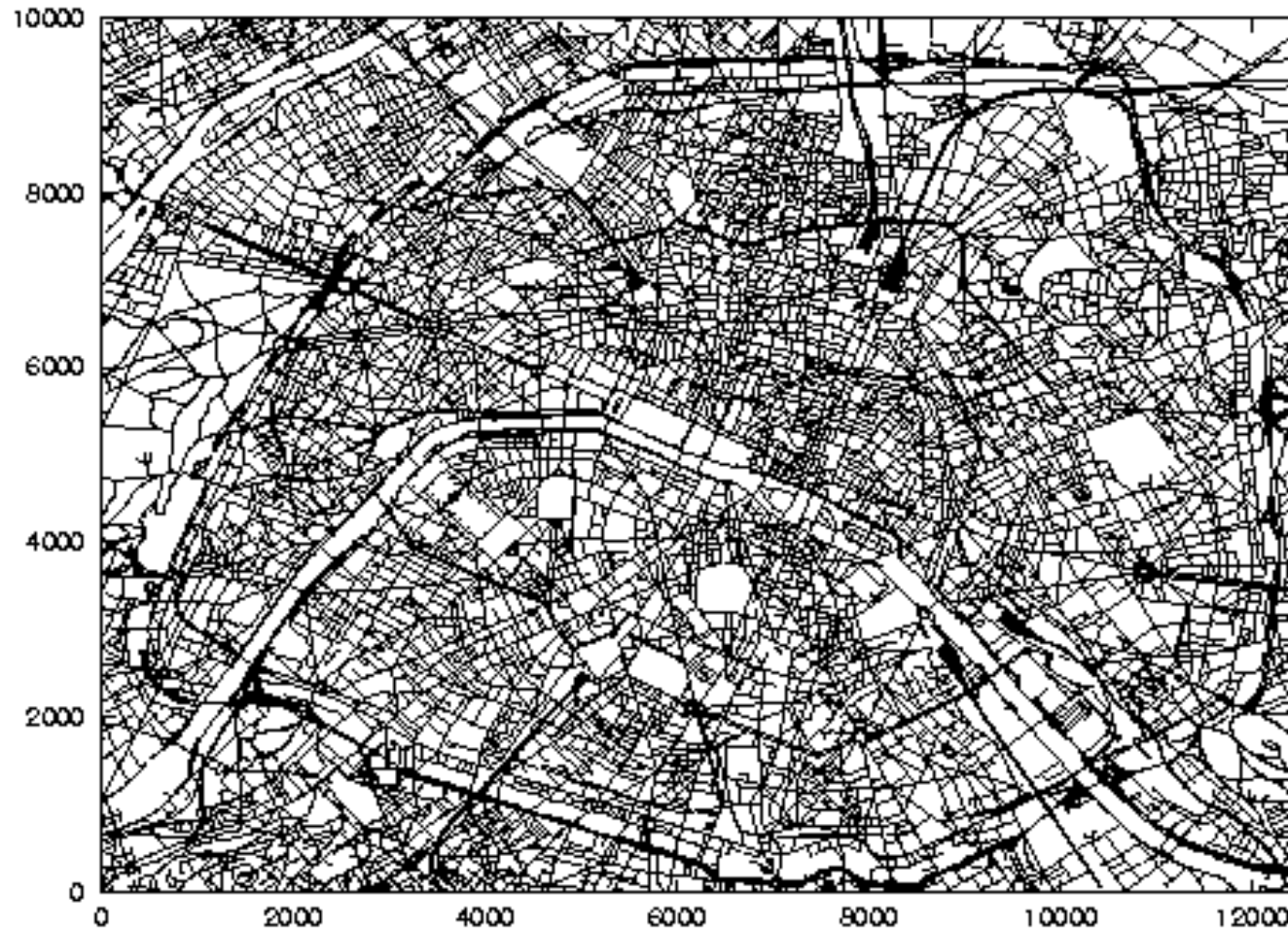
- **Motivation**
- **Modelfitting Procedure**
 - Minimization of Distance Measures
 - Minimization Methods
 - Numerical Examples

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- **Motivation**
- **Modelfitting Procedure**
 - Minimization of Distance Measures
 - Minimization Methods
 - Numerical Examples
- **Extrapolation Techniques**
 - Nonstatistical Extrapolation
 - Intensity Maps

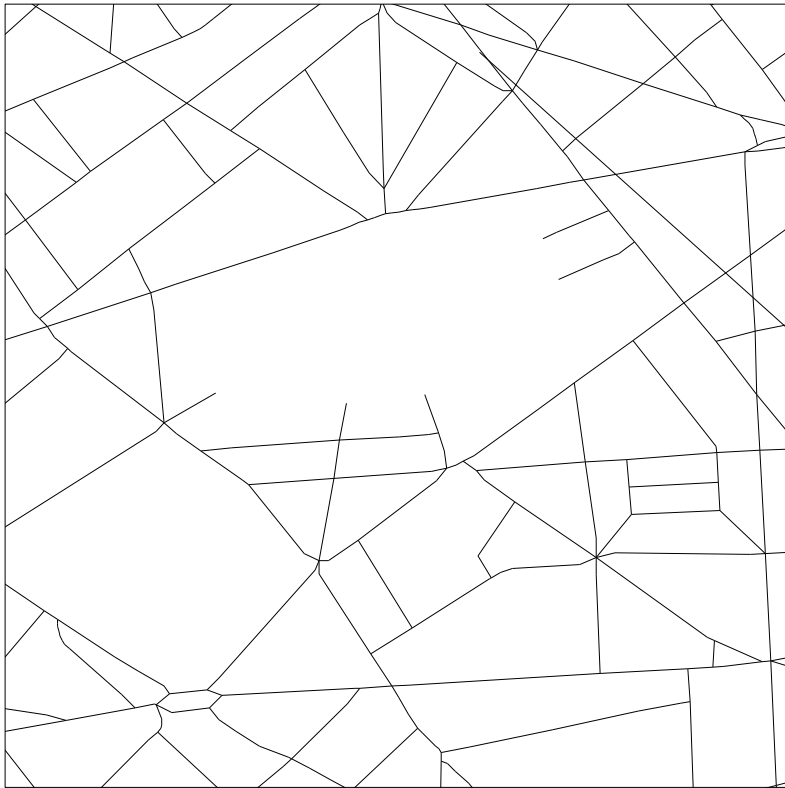
Motivation

Real Infrastructure Data of Paris

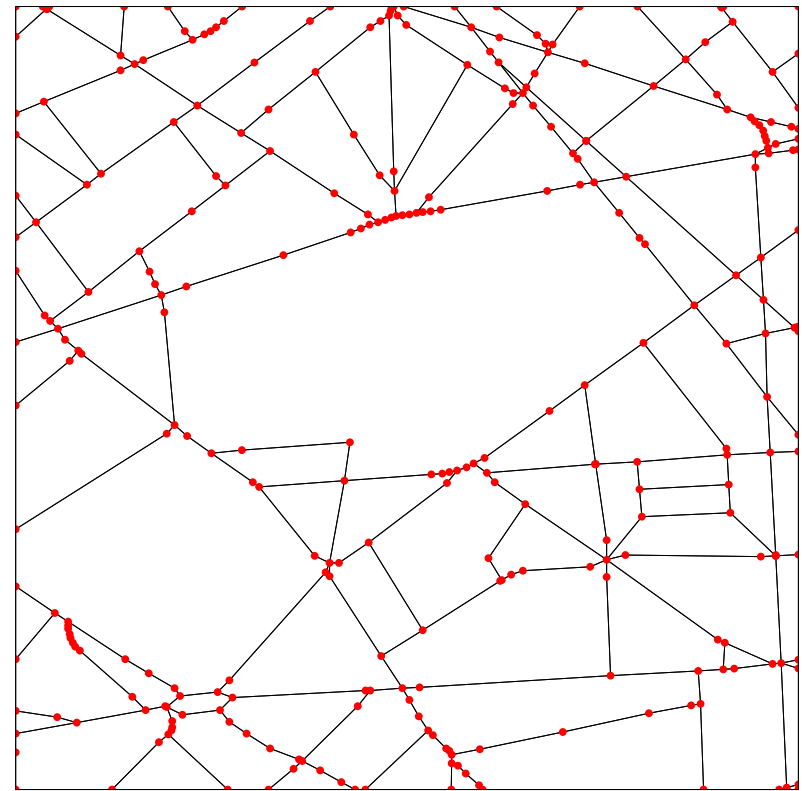


Motivation

Real Infrastructure Data of Paris



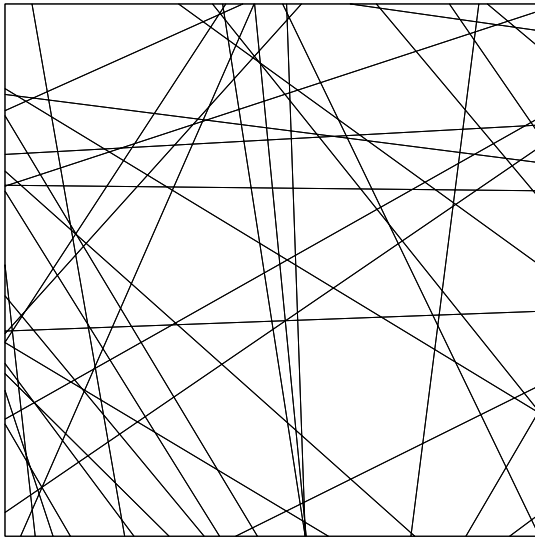
Raw data



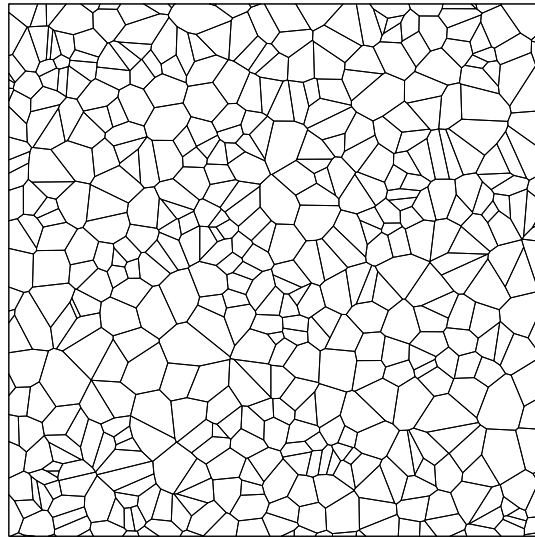
Preprocessed data

Motivation

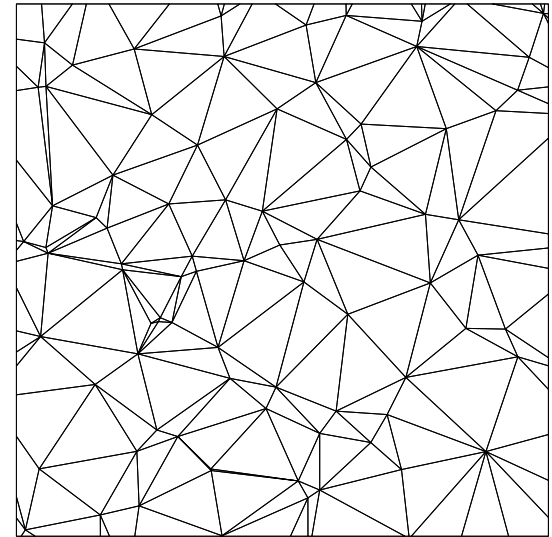
Simple Tessellation Models



PLT
(intensity 0.1)



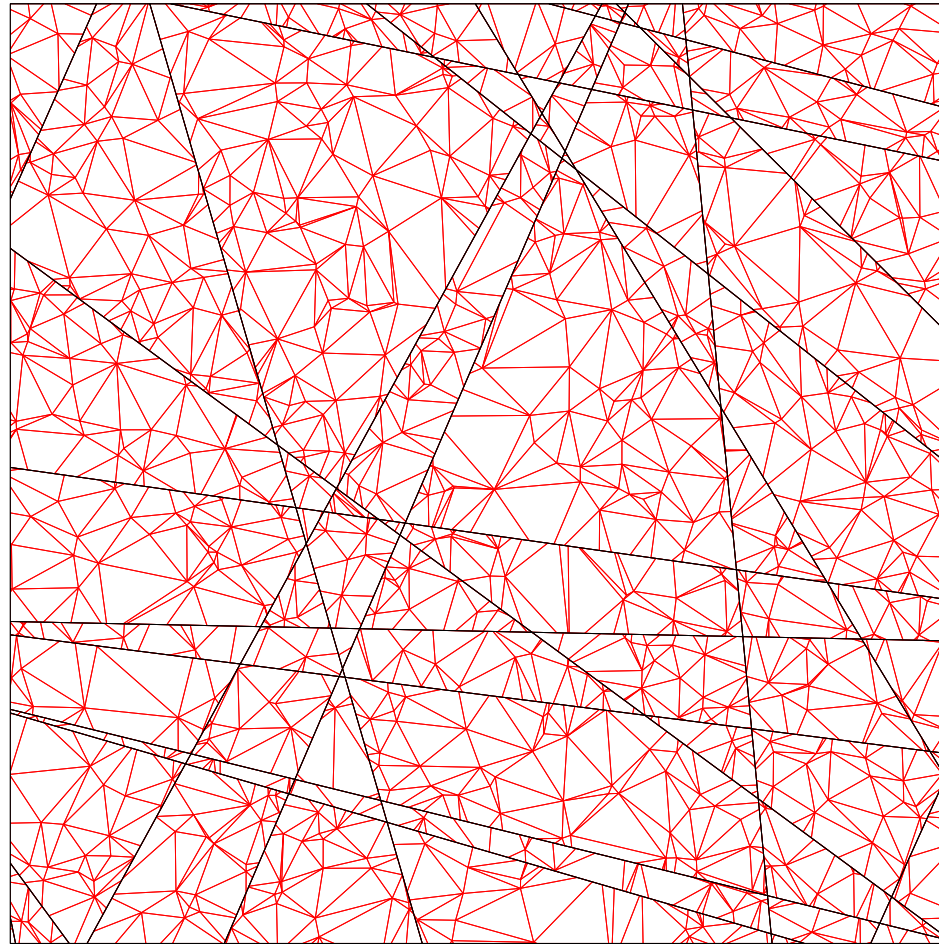
PVT
(intensity 0.005)



PDT
(intensity 0.001)

Motivation

Nested Tessellation Models



PLT/PDT with intensities $\gamma_0 = 0.05$, $\gamma_1 = 0.007$

Minimization of Distance Measures

Simple Tessellations

- Considered tessellations : PLT, PVT, PDT
- Intensity parameter: γ
- Characteristics of simple tessellation per unit area
 - $\lambda_0(\gamma)$ = expected number of nodes
 - $\lambda_1(\gamma)$ = expected number of edge-midpoints
 - $\lambda_2(\gamma)$ = expected number of cell-centroids
 - $\lambda_3(\gamma)$ = expected length of edges

Minimization of Distance Measures

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 - $\lambda_3(\gamma)$ = expected length of edges
- Estimation of these characteristics : $\hat{\lambda}_0, \hat{\lambda}_1, \hat{\lambda}_2, \hat{\lambda}_3$

Minimization of Distance Measures

Simple Tessellations

	PLT	PVT	PDT
$\lambda_0(\gamma)$	$\frac{1}{\pi}\gamma^2$	2γ	γ
$\lambda_1(\gamma)$	$\frac{2}{\pi}\gamma^2$	3γ	3γ
$\lambda_2(\gamma)$	$\frac{1}{\pi}\gamma^2$	γ	2γ
$\lambda_3(\gamma)$	γ	$2\sqrt{\gamma}$	$\frac{32}{3\pi}\sqrt{\gamma}$

Mean Values for PLT, PVT, and PDT each with Intensity γ

Minimization of Distance Measures

The minimization problem

- Minimization of the relative Euclidean distance

$$F(\gamma) = \sqrt{\sum_{i=0}^3 \left(\frac{\lambda_i(\gamma) - \hat{\lambda}_i}{\hat{\lambda}_i} \right)^2}$$

- Side condition

$$\gamma > 0$$

Minimization of Distance Measures

The minimization problem

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- Other distances possible

Minimization of Distance Measures

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- Side condition

$$\gamma > 0$$

- Other distances possible
- Analytical solutions are known for
 - Euclidean distances (absolute and relative)
 - Absolute value distances (absolute and relative)

Minimization of Distance Measures

Nested Tessellations

- Nesting of the simple tessellations PLT, PVT and PDT
- Intensity parameter
 - Intensity of the initial tessellation : γ_0
 - Intensity of the component tessellation : γ_1
 - Bernoulli-thinning parameter : p
- Characteristics of iterated tessellations per unit area
 - $\lambda_0^{It}(\gamma_0, \gamma_1, p)$ = expected number of nodes
 - $\lambda_1^{It}(\gamma_0, \gamma_1, p)$ = expected number of edge-midpoints
 - $\lambda_2^{It}(\gamma_0, \gamma_1, p)$ = expected number of cell-centroids
 - $\lambda_3^{It}(\gamma_0, \gamma_1, p)$ = expected length of edges

Minimization of Distance Measures

Nested Tessellations

Mean value formulae for nested tessellation models

$$\lambda_0^{It}(\gamma_0, \gamma_1, p) = \lambda_0(\gamma_0) + p\lambda_0(\gamma_1) + \frac{4p}{\pi} \lambda_3(\gamma_0) \lambda_3(\gamma_1)$$

$$\lambda_1^{It}(\gamma_0, \gamma_1, p) = \lambda_1(\gamma_0) + p\lambda_1(\gamma_1) + \frac{6p}{\pi} \lambda_3(\gamma_0) \lambda_3(\gamma_1)$$

$$\lambda_2^{It}(\gamma_0, \gamma_1, p) = \lambda_2(\gamma_0) + p\lambda_2(\gamma_1) + \frac{2p}{\pi} \lambda_3(\gamma_0) \lambda_3(\gamma_1)$$

$$\lambda_3^{It}(\gamma_0, \gamma_1, p) = \lambda_3(\gamma_0) + p\lambda_3(\gamma_1)$$

Minimization of Distance Measures

The minimization problem

- Minimization of the relative Euclidean distance

$$F(\gamma_0, \gamma_1, p) = \sqrt{\sum_{i=0}^3 \left(\frac{\lambda_i(\gamma_0, \gamma_1, p) - \hat{\lambda}_i}{\hat{\lambda}_i} \right)^2}$$

- Side conditions

$$0 \leq p \leq 1$$

$$\gamma_0, \gamma_1 > 0$$

Minimization of Distance Measures

The minimization problem

- Minimization of the relative Euclidean distance

$$F(\gamma_0, \gamma_1, p) = \sqrt{\sum_{i=0}^3 \left(\frac{\lambda_i(\gamma_0, \gamma_1, p) - \hat{\lambda}_i}{\hat{\lambda}_i} \right)^2}$$

- Side conditions

$$0 \leq p \leq 1$$

$$\gamma_0, \gamma_1 > 0$$

- Other distances possible

Minimization of Distance Measures

Example PLT/PDT

$$\begin{aligned}
 \bullet F(\gamma_0, \gamma_1, p)^2 &= \left(\frac{\frac{\gamma_0^2}{\pi} + p\gamma_1 + \frac{128}{3\pi^2} p\gamma_0 \sqrt{\gamma_1} - \hat{\lambda}_0}{\hat{\lambda}_0} \right)^2 \\
 &+ \left(\frac{\frac{2\gamma_0^2}{\pi} + 3p\gamma_1 + \frac{64}{\pi^2} p\gamma_0 \sqrt{\gamma_1} - \hat{\lambda}_1}{\hat{\lambda}_1} \right)^2 \\
 &+ \left(\frac{\frac{\gamma_0^2}{\pi} + 2p\gamma_1 + \frac{64}{3\pi^2} p\gamma_0 \sqrt{\gamma_1} - \hat{\lambda}_2}{\hat{\lambda}_2} \right)^2 \\
 &+ \left(\frac{\gamma_0 + \frac{32}{3\pi} p\sqrt{\gamma_1} - \hat{\lambda}_3}{\hat{\lambda}_3} \right)^2
 \end{aligned}$$

Minimization of Distance Measures

Example PLT/PDT

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- Not convex in γ_0, γ_1

Minimization of Distance Measures

Example PLT/PDT

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 &+ \left(\frac{\gamma_0 + \frac{32}{3\pi} p\sqrt{\gamma_1} - \hat{\lambda}_3}{\hat{\lambda}_3} \right)^2
 \end{aligned}$$

- Not convex in γ_0, γ_1
- But convex in p (for all considered tessellations)

Minimization Methods

Sequential Optimization

- $F(\gamma_0, \gamma_1, p)$ is convex in p
- Global minimum of $F(\gamma_0, \gamma_1, p)$ w.r.t. p is root of derivative

$$p(\gamma_0, \gamma_1) = - \left(\frac{\frac{\lambda_0^0 - \hat{\lambda}_0}{\hat{\lambda}_0} g_0 + \frac{\lambda_1^0 - \hat{\lambda}_1}{\hat{\lambda}_1} g_1 + \frac{\lambda_2^0 - \hat{\lambda}_2}{\hat{\lambda}_2} g_2 + \frac{\lambda_3^0 - \hat{\lambda}_3}{\hat{\lambda}_3} g_3}{\frac{g_0^2}{\hat{\lambda}_0} + \frac{g_1^2}{\hat{\lambda}_1} + \frac{g_2^2}{\hat{\lambda}_2} + \frac{g_3^2}{\hat{\lambda}_3}} \right)$$

with

- $g_i = g_i(\gamma_0, \gamma_1) = \left(\frac{\partial \lambda_i^{It}(\gamma_0, \gamma_1, p)}{\partial p} \right) (\gamma_0, \gamma_1) \quad i = 0, \dots, 3$
- $\lambda_i^0 = i$ -th characteristic of initial tessellation

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Sequential Optimization

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- Global minimum of $F(\gamma_0, \gamma_1, p)$ w.r.t. p is root of derivative

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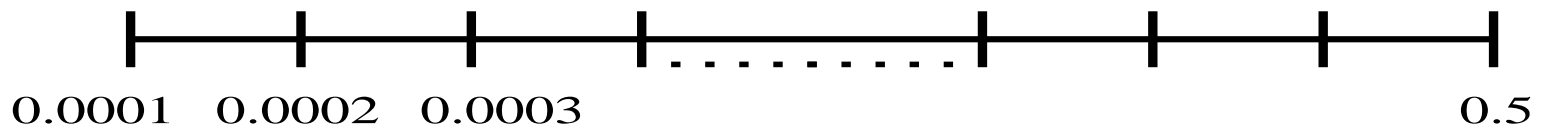
with

- $g_i = g_i(\gamma_0, \gamma_1) = \left(\frac{\partial \lambda_i^{It}(\gamma_0, \gamma_1, p)}{\partial p} \right) (\gamma_0, \gamma_1) \quad i = 0, \dots, 3$
- $\lambda_i^0 = i$ -th characteristic of initial tessellation
- Insertion into $F(\gamma_0, \gamma_1, p)$
 $\Rightarrow F(\gamma_0, \gamma_1, p(\gamma_0, \gamma_1)) = \tilde{F}(\gamma_0, \gamma_1)$

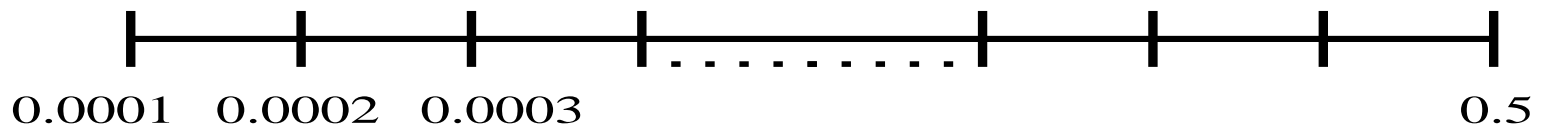
Minimization Methods

Traversing method

- $\tilde{F}(\gamma_0, \gamma_1) \rightarrow \min$
- Intensities $\gamma_0 \in (0, \gamma_0^{max}), \gamma_1 \in (0, \gamma_1^{max})$
- Evaluate \tilde{F}
 - for all γ_0 between 0 and γ_0^{max} (i.e.= 0.5) with distance, i.e. 0.0001



- for all γ_1 between 0 and γ_0^{max} (i.e.= 0.5) with distance, i.e. 0.0001



- Take minimal value of \tilde{F}

Minimization Methods

Traversing Method

- Advantage : Minimum is always found
- Problem : Critical Runtime
 - i.e 5000^2 computation cases
 - More precise results for smaller steps but much more runtime

Minimization Methods

Nelder Mead (1965)

- Numerical iteration method
- Direct search method without side conditions
- Side conditions are represented by a penalty value
- $F : \mathbb{R}^2 \rightarrow \mathbb{R}$
- Method based on evaluating F at the vertices of a triangle
- After evaluating F : decision to reflect, expand, contract or shrink the triangle
- Algorithm stops if difference between function values at the vertices is small

Minimization Methods

Nelder Mead - Algorithm

- The vertices $x_1, x_2, x_3 \in \mathbb{R}$ ordered w.l.o.g.
 $F(x_1) \leq F(x_2) \leq F(x_3)$

- Calculate the middle of the best vertices

$$x^c = \frac{1}{2}(x_1 + x_2)$$

- Calculate the **reflection** on x^c

$$x^r = x^c + \rho(x^c - x_3) \quad \rho > 0$$

Minimization Methods

Nelder Mead - Algorithm

- If $F(x_1) \leq F(x^r) < F(x_2)$

- $x_3 = x^r$

- If $F(x^r) < F(x_1)$ try **expansion**

$$x^e = x^c + \beta(x^r - x^c) \quad \beta > 1$$

- If $F(x^e) < F(x^r) : x_3 = x^e$

- Else : $x_3 = x^r$

- If $F(x^r) \geq F(x_2)$ try **contraction**

Minimization Methods

Nelder Mead - Algorithm

• If $F(x^r) \geq F(x_2)$ try **contraction**

• If $F(x^r) \geq F(x_3)$

$$x^k = x^c + \delta(x_3 - x^c) \quad 0 < \delta < 1$$

• If $F(x^k) < F(x_3) : x_3 = x^k$

• Else **shrinking**

$$x_j = \frac{1}{2}(x_j + x_1) \quad j = 2, 3$$

• Else

$$x^k = x^c + \delta(x^r - x^c) \quad 0 < \delta < 1$$

• If $F(x^k) < F(x^r) : x_3 = x^k$

• Else **shrinking**

$$x_j = \frac{1}{2}(x_j + x_1) \quad j = 2, 3$$

Minimization Methods

Nelder Mead - Algorithm

- Stopping condition

$$\sqrt{\frac{1}{3} \sum_{j=1}^3 |F(x_j) - F(x^c)|^2} < \varepsilon$$

with given $\varepsilon > 0$

Minimization Methods

Nelder Mead (1965)

- Problem : Global minimum may depend on initial values
 - Start with different initial values (randomly chosen)

Minimization Methods

Nelder Mead (1965)

- Problem : Global minimum may depend on initial values
 - Start with different initial values (randomly chosen)
- Advantage :
 - Faster than Traversing-method
 - Most times it delivers more precise results than Traversing-method

Minimization Methods

Projected Gradient Algorithm

- Numerical iteration method
- Usage of the gradient
- Side conditions are included by a projection
 $Pr_D : \mathbb{R}^n \rightarrow D$, where

$$Pr_D(x) = \arg \min_{y \in D} \|y - x\|.$$

Minimization Methods

Projected Gradient Algorithm

Choose parameters $0 < \beta, \mu < 1$, and $\gamma > 0$

Find $x_0 \in D$

For $k = 0, 1, 2, \dots$ do:

 Compute $\nabla f(x_k)$

 IF x_k is stationary point THEN

 stop

 ELSE

$x_k(\alpha) = Pr_D(x_k - \alpha \nabla f(x_k))$ with $\alpha > 0$

$x_{k+1} = x_k(\alpha_k)$, with $\alpha_k = \beta^{m_k} \gamma$ where m_k the

 lowest natural number for which

$f(x_{k+1}) \leq f(x_k) + \mu \nabla f(x_k)^T (x_{k+1} - x_k)$

 holds.

Minimization Methods

Projected Gradient Algorithm

- Advantage :
 - Very fast convergence
 - High precision of the found (local) minimum

Minimization Methods

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- Problem : Global minimum is not found for the considered fitting problem even if there are different initial values (randomly chosen)

Minimization Methods

Projected Gradient Algorithm

- Advantage :
 - Very fast convergence
 - High precision of the found (local) minimum
- Problem : Global minimum is not found for the considered fitting problem even if there are different initial values (randomly chosen)
- Application : Improvement of the minimum found by the Nelder-Mead algorithm

Numerical Examples

Comparison of Minimization Methods - Simulated Data

Simulation of a PLT/PLT with intensities $\gamma_0 = 0.1$, $\gamma_1 = 0.06$, $p = 1.0$

Numerical Examples

Comparison of Minimization Methods - Simulated Data

Simulation of a PLT/PLT with intensities $\gamma_0 = 0.1$, $\gamma_1 = 0.06$, $p = 1.0$

Method	Results					
	Best fitting model	Rel. Eucl. distance	γ_0	γ_1	p	Times of NMA time
Traversing-Method	PLT/PLT	0.008977	0.061400	0.100600	1.0	620
Nelder Mead Algorithm (NMA)	PLT/PLT	0.008964	0.061663	0.100305	1.0	1
Projected Gradients (PG)	PLT/PLT	0.017023	0.080599	0.080599	1.0	2
NMA & PG	PLT/PLT	0.008964	0.061663	0.100305	1.0	1

Fixed Bernoulli thinning parameter $p = 1.0$

Numerical Examples

Comparison of Minimization Methods - Simulated Data

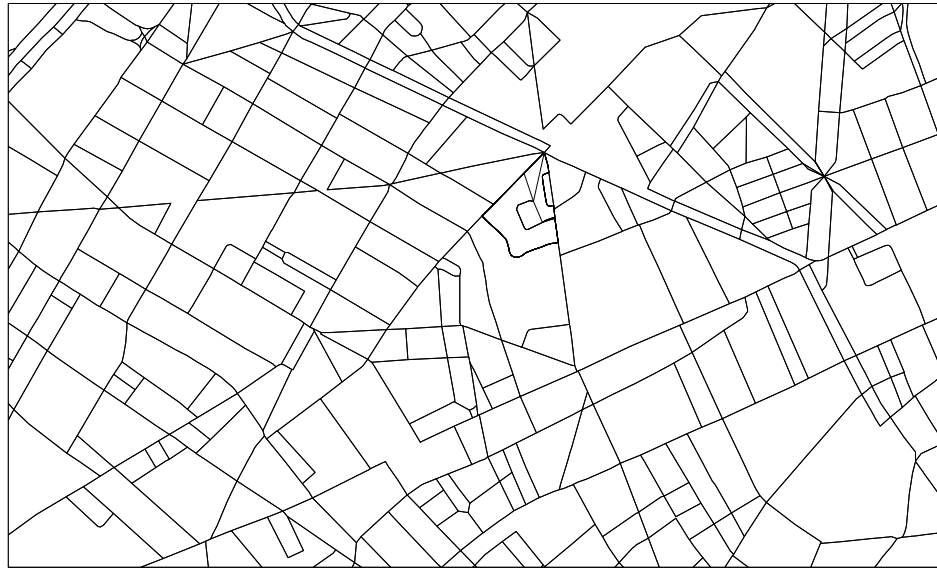
Simulation of a PDT/PVT with intensities $\gamma_0 = 0.001$, $\gamma_1 = 0.005$, $p = 0.9$

Method	Results					
	Best fitting model	Rel. Eucl. distance	γ_0	γ_1	p	Times of NMA time
Traversing-Method	PDT/PVT	0.008605	0.000867	0.007534	0.700000	2400
Nelder Mead Algorithm (NMA)	PDT/PVT	0.008598	0.000868	0.007535	0.700000	1
Projected Gradients (PG)	PVT/PLT	0.046419	0.007372	0.057193	0.940029	1
NMA & PG	PDT/PVT	0.008598	0.000868	0.007535	0.700000	1

Bernoulli thinning parameter p in $[0.7, 1.0]$

Numerical Examples

Comparison of Minimization Methods - Real Data



Part of Paris

Estimated characteristic values:

$$\hat{\lambda}_0 = 0.000106, \hat{\lambda}_1 = 0.000177, \hat{\lambda}_2 = 0.000072, \hat{\lambda}_0 = 0.017659.$$

Numerical Examples

Comparison of Minimization Methods - Real Data

Method	Results					
	Best fitting model	Rel. Eucl. distance	γ_0	γ_1	p	Times of NMA time
Traversing-Method	PVT/PDT	0.019028	$6.250 \cdot 10^{-6}$	$1.334 \cdot 10^{-5}$	1.0	230
Nelder Mead Algorithm (NMA)	PVT/PDT	0.018760	$6.307 \cdot 10^{-6}$	$1.329 \cdot 10^{-5}$	1.0	1
Projected Gradients (PG)	PDT/PDT	0.031667	$6.357 \cdot 10^{-6}$	$6.357 \cdot 10^{-6}$	1.0	0.1
NMA & PG	PVT/PDT	0.018760	$6.307 \cdot 10^{-6}$	$1.329 \cdot 10^{-5}$	1.0	1

Fixed Bernoulli thinning parameter $p = 1$

Numerical Examples

Experimental Verification of Nelder-Mead

- Simulation of a PLT/PLT with intensities $\gamma_0 = 0.05$, $\gamma_1 = 0.04$, and $p = 1.0$.
- 1 time fitting with traversing method
- 1000 times fitting with Nelder-Mead algorithm

This is repeated 50 times.

Numerical Examples

Experimental Verification of Nelder-Mead

- Simulation of a PLT/PLT with intensities $\gamma_0 = 0.05$, $\gamma_1 = 0.04$, and $p = 1.0$.
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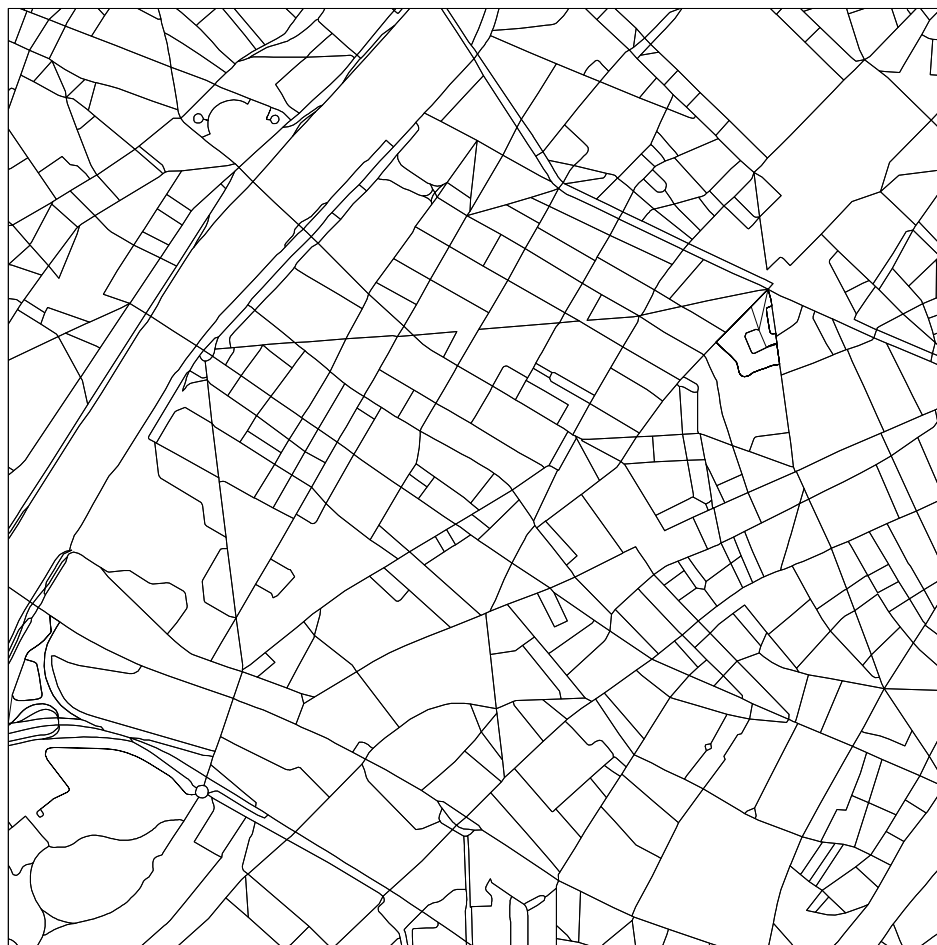
This is repeated 50 times.

Result:

In all 50.000 cases the minimum found by Nelder-Mead is lower or equal than the minimum found by the Traversing method.

Extrapolation Techniques

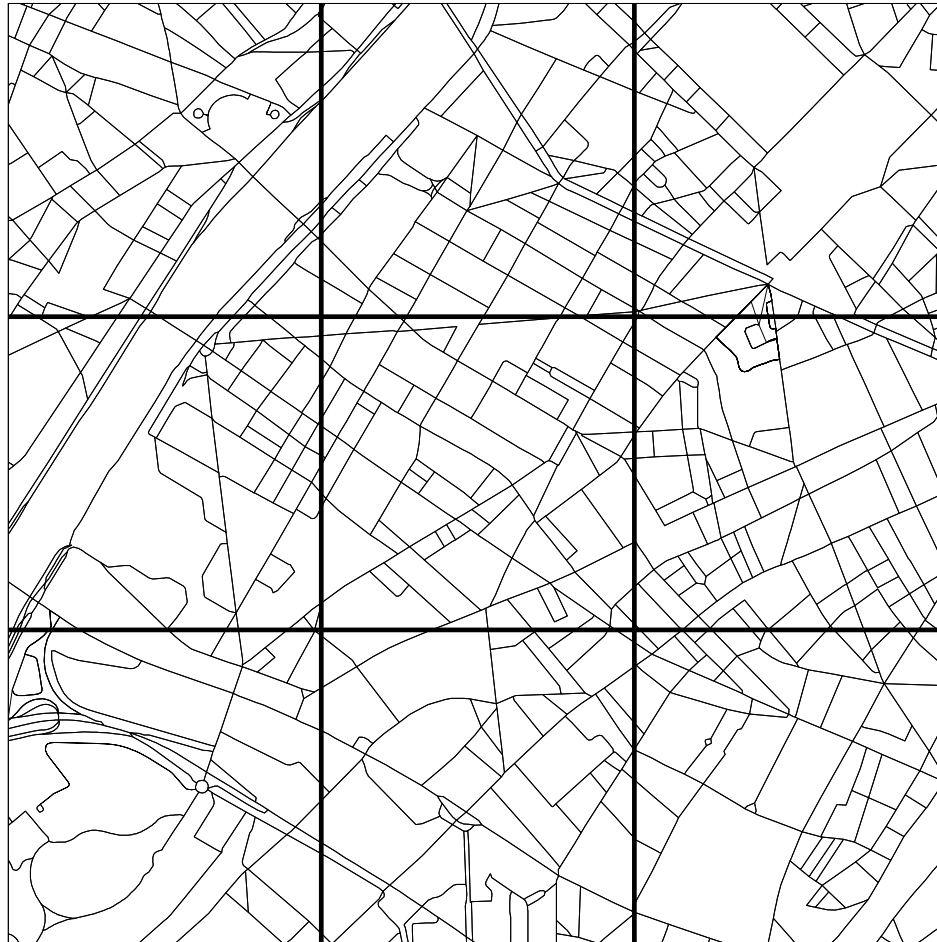
Motivation



Data of Paris

Extrapolation Techniques

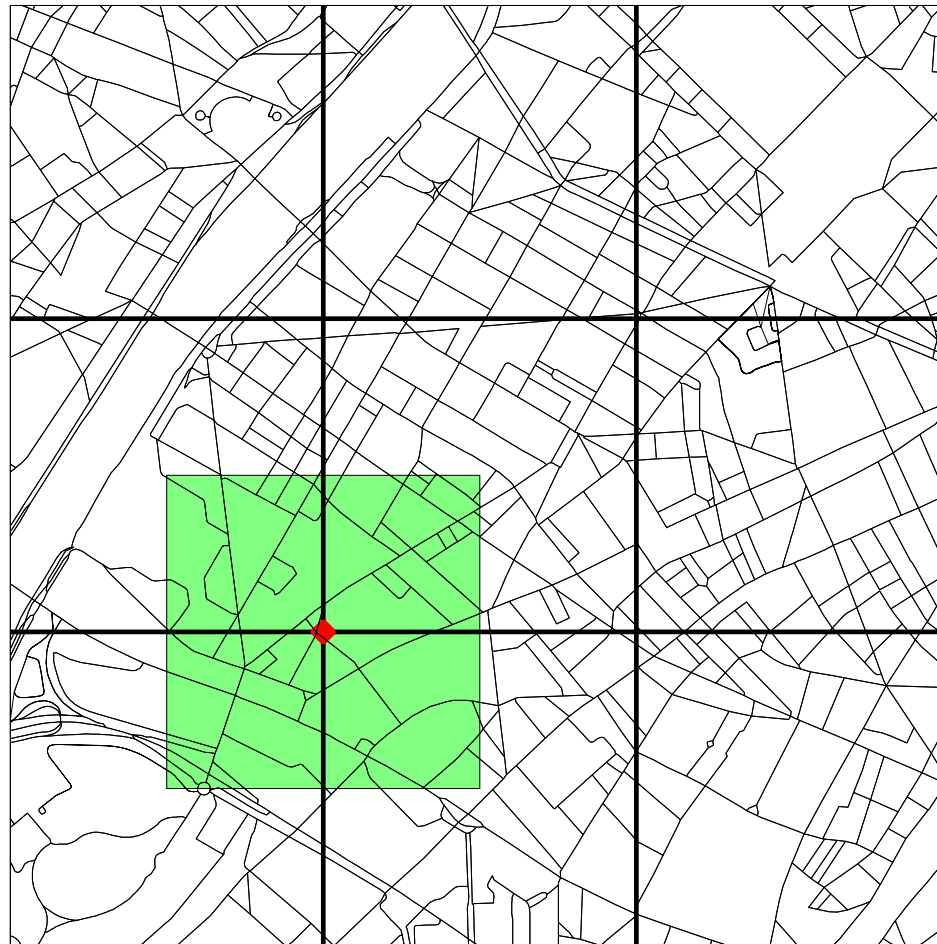
Motivation



Data of Paris

Extrapolation Techniques

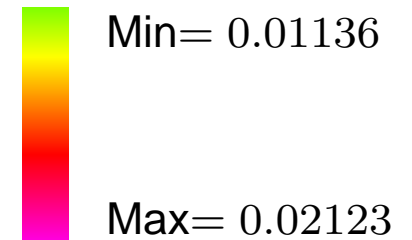
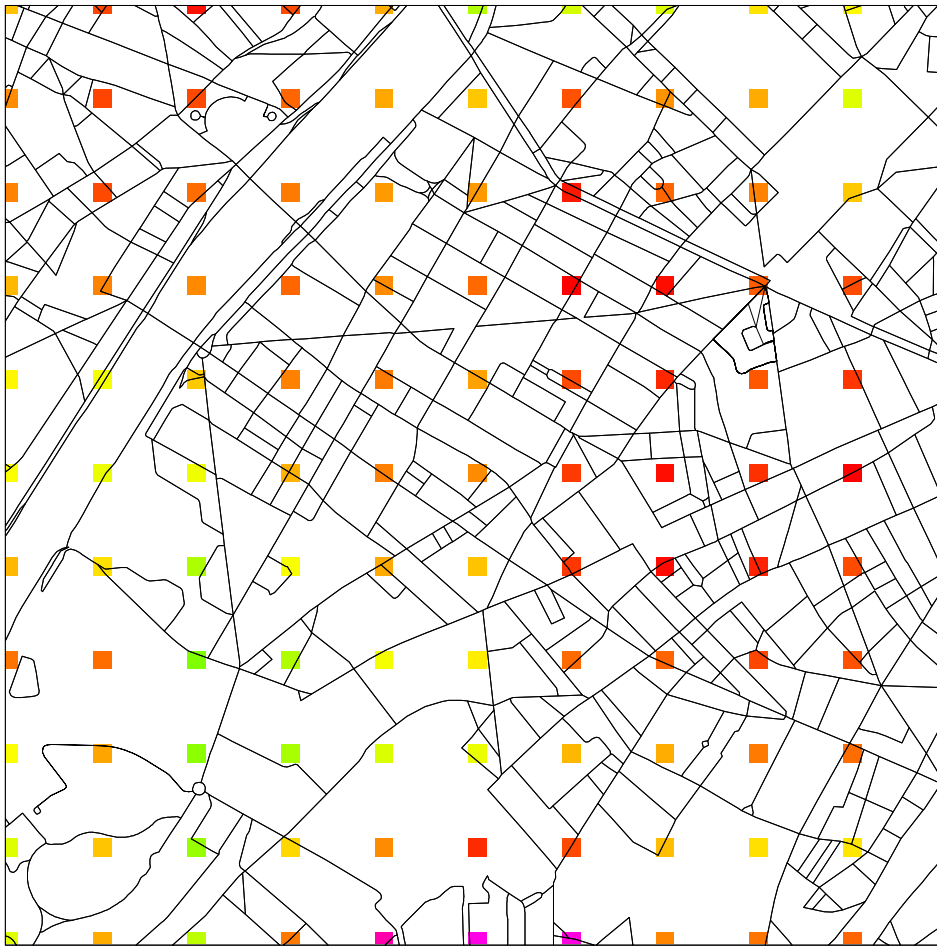
Motivation



Data of Paris

Nonstatistical Extrapolation

Measurement Points



Measurement Points (PLT)

Nonstatistical Extrapolation

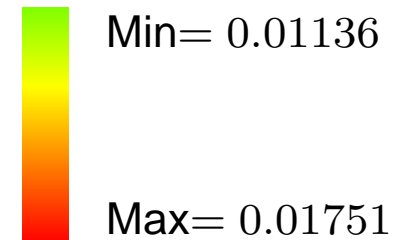
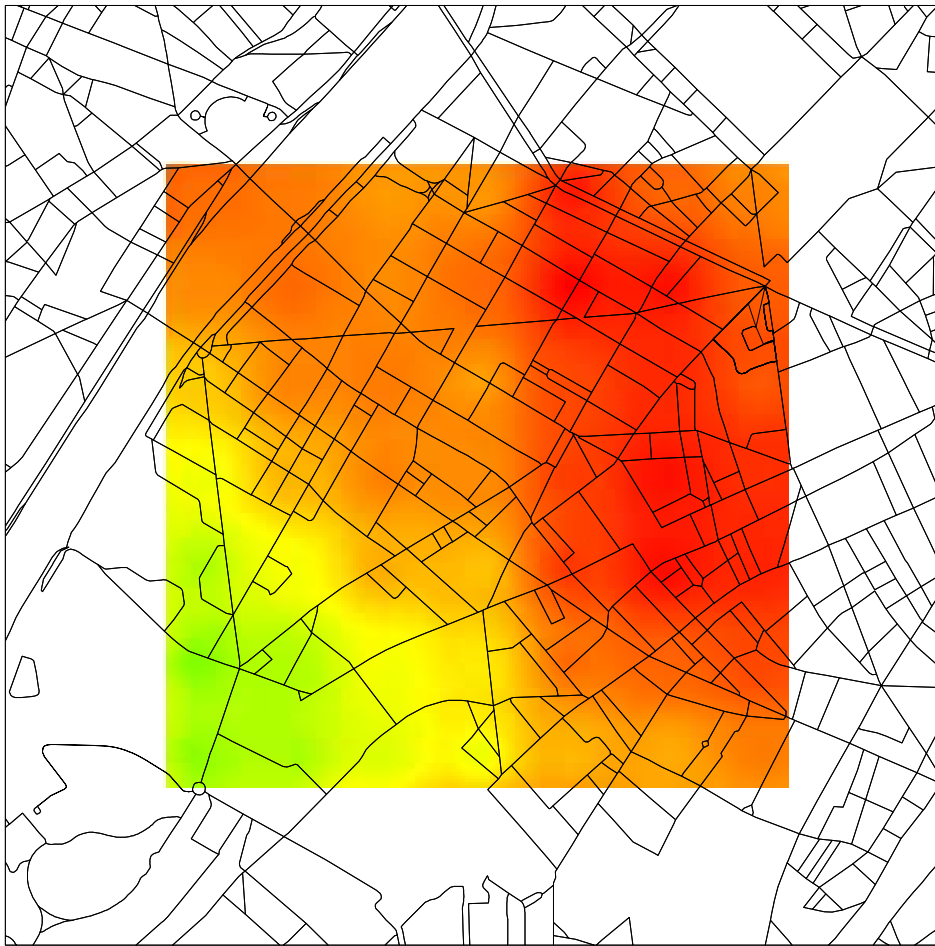
Inverse distance extrapolation

$$\hat{Z}(x_0) = \sum_{i=1}^n w_i(x_0) Z(x_i) \quad x_i \text{ Sampling Points}$$

where $w_i(x_0) = \frac{1}{h_i^p} \left(\sum_{j=1}^n \frac{1}{h_j^p} \right)^{-1}$ with
 $h_i = \|x_i - x_0\| \quad i = 1, \dots, n, p \in \mathbb{N}$

Nonstatistical Extrapolation

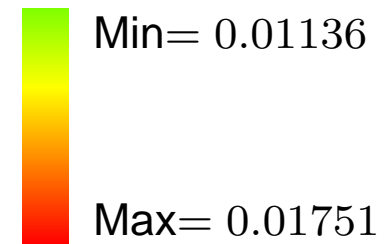
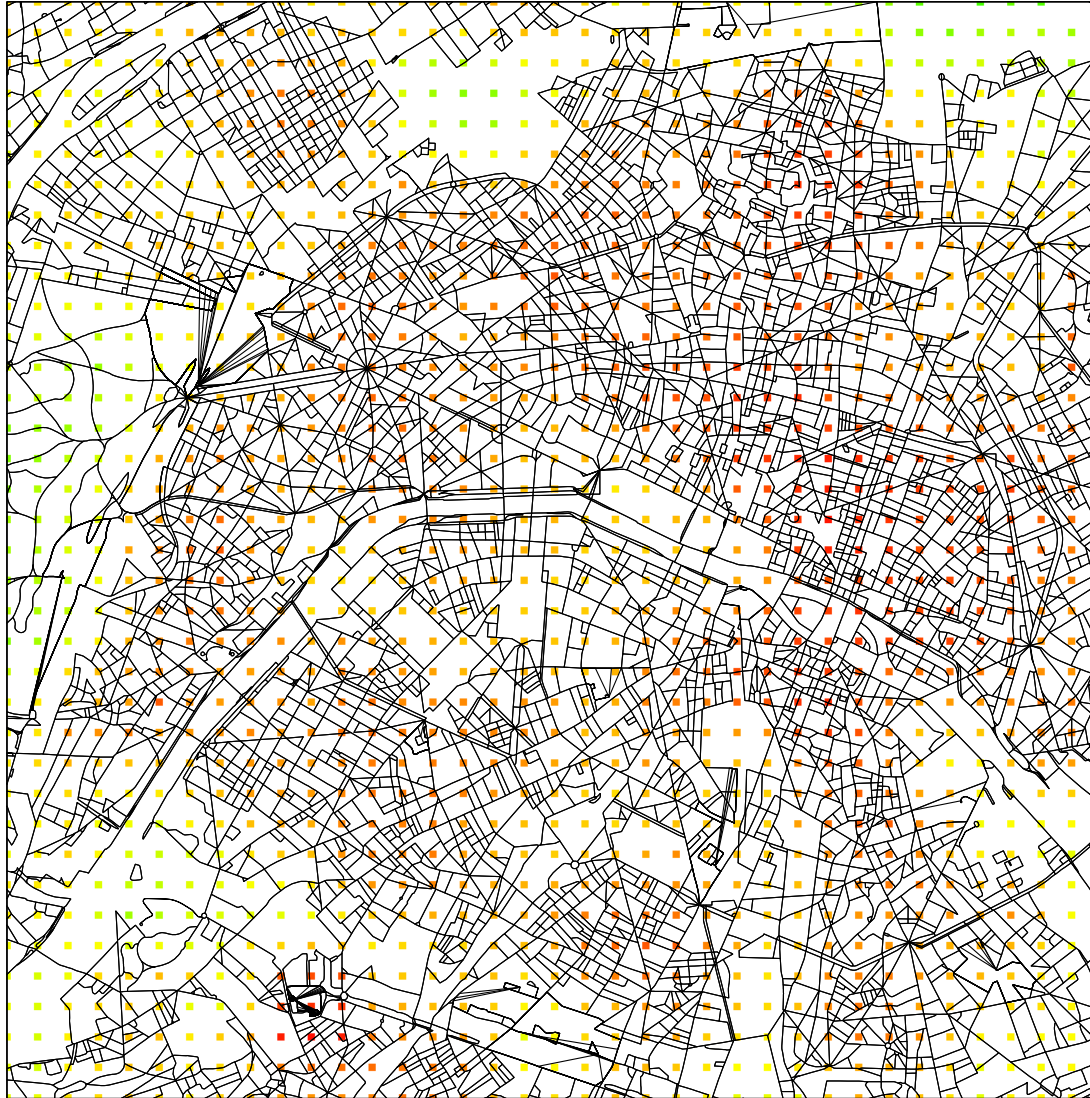
Intensity Map



Real data of Paris and Intensity Map (PLT)

Statistical Extrapolation - Kriging

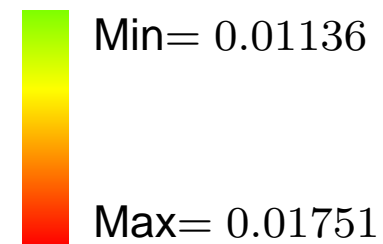
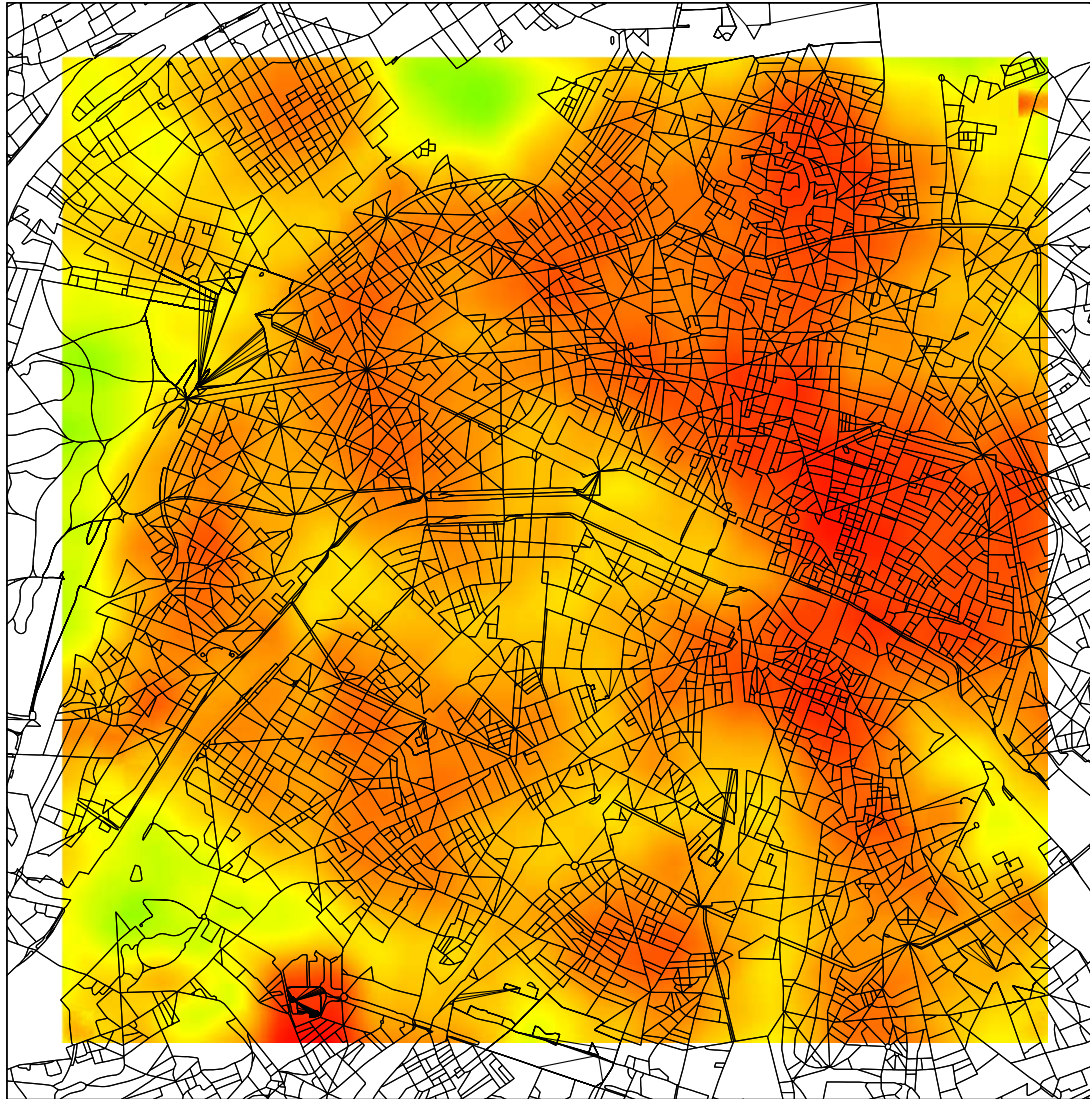
Intensity Map



Measurement Points (PLT)

Statistical Extrapolation - Kriging

Intensity Map



Real data of Paris and
Intensity Map (PLT)

References

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Thank you for your attention!

Questions?