# Combining physics models and Gaussian processes for traffic prediction 

Alexandra Würth ${ }^{1}$ (Centre Inria d'Université Côte d'Azur)<br>Joint work with Mickaël Binois ${ }^{1}$ and Paola Goatin ${ }^{1}$

[^0]
## Motivation



Source：https：／／www．larochellegc．com／realisations／analyse－congestion－routiere－avantagee－cloud／

## Motivation



Illustration of vehicle trajectory and travel time $\tau$ for sample scenario．

## Outline

(1) Macroscopic traffic flow models
(2) Calibration approaches
(3) Synthetic traffic data
(4) Traffic estimation and prediction

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4. Traffic estimation and prediction

## Macroscopic traffic flow models

Consideration of averaged and aggregated traffic quantities such as:

- traffic density $\rho$ (number of vehicles per space unit),
- vehicle velocity $v$ (distance covered by vehicles per time unit),
- traffic flow $q=\rho v$ (number of vehicles per time unit).


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Data can be measured by:

- magnetic loop detectors,
- video recordings,
- wireless sensor networks,
- etc.


Source: https://www.ecm-france.com/en/areas-of-activity/weigh-in-motion/inductive-loop/

## Generic Second Order Model (GSOM)

## We consider a Generic Second Order traffic flow Model (GSOM) ${ }^{2}$

 consisting in a $2 \times 2$ hyperbolic system of conservation laws$$
\left\{\begin{array}{l}
\partial_{t} \rho+\partial_{x}(\rho v)=0,  \tag{1}\\
\partial_{t}(\rho w)+\partial_{x}(\rho w v)=0,
\end{array} \quad x \in \mathbb{R}, t>0,\right.
$$

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where
$\rho=\rho(t, x)$ represents the density,
$w=w(t, x)$ the Lagrangian vehicle property,
$v=\mathcal{V}(\rho, w)$ the average speed of vehicles.

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## Initial Boundary Value Problem (IBVP)

We focus on the Initial Boundary Value Problem ${ }^{3}$ (IBVP) for (1):

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\partial_{t} \rho+\partial_{x}(\rho v)=0, \\
\partial_{t}(\rho w)+\partial_{x}(\rho w v)=0, & x \in] x_{\text {in }}, x_{\text {out }}[\subset \mathbb{R}, \\
t>0,
\end{array}\right. \\
(\rho, w)(0, x)=\left(\rho_{0}, w_{0}\right)(x), & x \in] x_{\text {in }}, x_{\text {out }}[, \\
(\rho, w)\left(t, x_{\text {in }}\right)=\left(\rho_{\text {in }}, w_{\text {in }}\right)(t), & t>0, \\
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\end{array}, \begin{array}{lr} 
\\
(\rho, w)\left(t, x_{\text {in }}\right)=\left(\rho_{\text {in }}, w_{\text {in }}\right)(t), & t>0,
\end{array}
$$

with values in an invariant domain of the form

$$
\Omega:=\left\{U=(\rho, w) \in \mathbb{R}^{2}: \rho \in\left[0, R\left(w_{\max }\right)\right], w \in\left[w_{\min }, w_{\max }\right]\right\}
$$

for some $0<w_{\min } \leq w_{\max }<+\infty$.

[^4]
## Outline

(1) Macroscopic traffic flow models
(2) Calibration approaches
(3) Synthetic traffic data
4. Traffic estimation and prediction

We denote by $F$ the so-called "field" where $P$, the real process under study, is physically observed.
It is generally assumed that $P$ and $F$ are related by:

$$
y^{F}(t, x)=y^{P}(t, x)+\varepsilon \text { where } \varepsilon \sim \mathcal{N}\left(0, \sigma_{\varepsilon}^{2}\right) \text {. }
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$$

1. $L^{2}$ - approach:

Mathematical model, $M$, represents perfectly the real system:

$$
y^{F}(t, x)=y^{M}\left(t, x, \theta^{*}\right)+\varepsilon
$$

with $\theta^{*}$ being the optimal calibration parameter computed by:

$$
\theta^{*}=\underset{\theta}{\operatorname{argmin}} \sum_{(t, x) \in(T, x)}\left|y^{F}(t, x)-y^{M}(t, x, \theta)\right|^{2} .
$$

2. Kennedy-O'Hagan ${ }^{4}$ (KOH) - approach:

Model the inadequacy between the mathematical model and the reality by a discrepancy (bias) term:

$$
\underbrace{y^{F}(t, x)}_{\text {observation }}=\underbrace{y^{M}\left(t, x, \theta^{*}\right)}_{\text {simulation }}+\underbrace{\tilde{b}\left(t, x, \theta^{*}\right)}_{\text {discrepancy }}+\underbrace{\varepsilon}_{\text {obs. error }}
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$$

where
$\mathrm{b}_{\mathrm{n}}=\tilde{b}+\varepsilon \sim \mathcal{N}\left(0, \mathrm{~K}_{\mathrm{n}}(\lambda)\right)$ with covariance $\mathrm{K}_{\mathrm{n}}(\lambda)=\sigma^{2}\left(\mathrm{C}_{\mathrm{n}}\left(I_{1}, I_{2}\right)+g \mathrm{I}_{\mathrm{n}}\right)$, hyperparameters $\lambda=\left(\sigma^{2}, I_{1}, l_{2}, g\right)$, $n$ number of observations and

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$\theta^{*}$ the optimal calibration parameter computed by:

$$
\theta^{*}=\underset{\theta}{\operatorname{argmax}} \frac{1}{\sqrt{(2 \pi)^{n}\left|\mathrm{~K}_{\mathrm{n}}(\lambda)\right|}} \exp \left(-\frac{1}{2} \mathrm{~b}_{\mathrm{n}}(\theta)^{\top}\left(\mathrm{K}_{\mathrm{n}}(\lambda)\right)^{-1} \mathrm{~b}_{\mathrm{n}}(\theta)\right) .
$$

[^7]
## Gaussian process modeling

Given: $n$ bias-observations $\mathrm{b}_{\mathrm{n}}=b\left(\mathcal{X}_{n}\right)$ at $\mathcal{X}_{n}=\left(\left(t_{1}, x_{1}\right), \ldots,\left(t_{n}, x_{n}\right)\right)$ $\rightarrow$ at $\hat{n}$ new locations $\hat{\mathcal{X}}_{\hat{n}}=\left(\left(\hat{t}_{1}, \hat{x}_{1}\right), \ldots,\left(\hat{t}_{\hat{n}}, \hat{x}_{\hat{n}}\right)\right)$ it holds:

$$
\begin{aligned}
& \mathrm{b}\left(\hat{\mathcal{X}}_{\hat{n}}\right) \mid \mathrm{b}_{\mathrm{n}} \sim \mathcal{N}\left(m_{n}\left(\hat{\mathcal{X}}_{\hat{n}}\right), s_{n}^{2}\left(\hat{\mathcal{X}}_{\hat{n}}, \hat{\mathcal{X}}_{\hat{n}}\right)\right), \\
& m_{n}\left(\hat{\mathcal{X}}_{\hat{n}}\right):=\mathbb{E}\left[\mathrm{b}\left(\hat{\mathcal{X}}_{\hat{n}}\right) \mid \mathrm{b}_{n}\right]=\mathrm{k}_{\mathrm{n}}\left(\hat{\mathcal{X}}_{\hat{n}}\right)^{\top} \mathrm{K}_{\mathrm{n}}^{-1} \mathrm{~b}_{\mathrm{n}}, \\
& s_{n}^{2}\left(\hat{\mathcal{X}}_{\hat{n}}, \hat{\mathcal{X}}_{\hat{n}}\right):=\mathbb{C o v}\left[\mathrm{b}\left(\hat{\mathcal{X}}_{\hat{n}}\right), \mathrm{b}\left(\hat{\mathcal{X}}_{\hat{n}}\right) \mid \mathrm{b}_{\mathrm{n}}\right]=k\left(\hat{\mathcal{X}}_{\hat{n}}, \hat{\mathcal{X}}_{\hat{n}}\right)-\mathrm{k}_{n}\left(\hat{\mathcal{X}}_{\hat{n}}\right)^{\top} \mathrm{K}_{\mathrm{n}}^{-1} \mathrm{k}_{\mathrm{n}}\left(\hat{\mathcal{X}}_{\hat{n}}\right)
\end{aligned}
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where $k(\cdot, \cdot)=\sigma^{2} \operatorname{Corr}(\mathrm{~b}(\cdot), \mathrm{b}(\cdot)), \mathrm{k}_{n}\left(\hat{\mathcal{X}}_{\hat{n}}\right):=\left(k\left(\hat{\mathcal{X}}_{\hat{n}}^{(j)}, \mathcal{X}_{n}^{(i)}\right)\right)_{1 \leq j \leq \hat{n}, 1 \leq i \leq n}$.

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## Gaussian kernel correlation matrix

## Standard formula:

$$
\operatorname{Corr}\left(\mathrm{b}(t, x), \mathrm{b}\left(t^{\prime}, x^{\prime}\right)\right)=\exp \left(-\frac{\left(t-t^{\prime}\right)^{2}}{l_{1}^{2}}\right) \exp \left(-\frac{\left(x-x^{\prime}\right)^{2}}{l_{2}^{2}}\right)
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Integral extension ${ }^{5}$ (due to time data averages):

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Integral extension ${ }^{5}$ (due to time data averages):

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\begin{aligned}
& \operatorname{Corr}\left(\frac{1}{\Delta t} \int_{t}^{t+\Delta t} \mathrm{~b}(s, x) \mathrm{ds}, \mathrm{~b}\left(t^{\prime}, x^{\prime}\right)\right)=\left(\frac{1}{\Delta t} \int_{t}^{t+\Delta t} \exp \left(-\frac{\left(s-t^{\prime}\right)^{2}}{l_{1}^{2}}\right) \mathrm{ds}\right) \exp \left(-\frac{\left(x-x^{\prime}\right)^{2}}{l_{2}^{2}}\right) \\
& \operatorname{Corr}\left(\frac{1}{\Delta t} \int_{t}^{t+\Delta t} \mathrm{~b}(s, x) \mathrm{ds}, \frac{1}{\Delta t^{\prime}} \int_{t^{\prime}}^{t^{\prime}+\Delta t^{\prime}} \mathrm{b}\left(s^{\prime}, x\right) \mathrm{ds}^{\prime}\right) \\
& \quad=\left(\frac{1}{\Delta t^{\prime}} \frac{1}{\Delta t} \int_{t^{\prime}}^{t^{\prime}+\Delta t^{\prime} t+\Delta t} \int_{t} \exp \left(-\frac{\left(s-s^{\prime}\right)^{2}}{l_{1}^{2}}\right) \mathrm{ds} \mathrm{ds} s^{\prime}\right) \exp \left(-\frac{\left(x-x^{\prime}\right)^{2}}{l_{2}^{2}}\right)
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$\operatorname{Corr}\left(\frac{1}{\Delta t} \int_{t}^{t+\Delta t} \mathrm{~b}(s, x) \mathrm{ds}, \frac{1}{\Delta t^{\prime}} \int_{t^{\prime}}^{t^{\prime}+\Delta t^{\prime}} \mathrm{b}\left(s^{\prime}, x\right) \mathrm{ds}^{\prime}\right)$

$$
=\left(\frac{1}{\Delta t^{\prime}} \frac{1}{\Delta t} \int_{t^{\prime}}^{t^{\prime}} \int_{t} \exp \left(-\frac{\left(s-s^{\prime}\right)^{2}}{l_{1}^{2}}\right) \mathrm{ds} d s^{\prime}\right) \exp \left(-\frac{\left(x-x^{\prime}\right)^{2}}{I_{2}^{2}}\right)
$$

$\rightarrow$ Slight improvement observed

[^11]
## Alternative calibration approach

M. Plumlee,

Bayesian calibration of inexact computer models Journal of the American Statistical Association, 2017

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- Orthogonality condition on bias function and mathematical model
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- Correlation matrix:

$$
C_{n}{ }^{\text {plum }}=C_{n}-C_{n} \delta y^{M}\left(\left(\delta y^{M}\right)^{\top} C_{n} \delta y^{M}\right)^{-1}\left(\delta y^{M}\right)^{\top} C_{n}
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$$

$\rightarrow$ No improvement observed (only approximation for derivative available)

## Outline

(1) Macroscopic traffic flow models
(2) Calibration approaches
(3) Synthetic traffic data

## Generation of traffic data by a microscopic simulator $\mathrm{SUMO}^{6}$ :

${ }^{6}$ Lopez et al. Microscopic Traffic Simulation using SUMO, 2018

## Generation of traffic data by a microscopic simulator $\mathrm{SUMO}^{6}$ :

- 10 km long road stretch,
- 3 lanes, no ramps,
- speed limit: $100 \mathrm{~km} / \mathrm{h}$,
- different classes of vehicle types (normal, fast and slow cars).

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Artificial traffic scenario

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Artificial traffic scenario

[^14]
with $\theta_{\mathrm{L}^{2}}^{*}=(83,48,328)$.

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## Traffic estimation.



Traffic estimation.


Traffic estimation.


Traffic prediction.



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Traffic prediction.

## GP prediction

Standard approach: predictive mean formula

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Rong et al,
AutoIP: A United Framework to Integrate Physics into Gaussian Processes International Conference on Machine Learning, 2022
$\rightarrow$ Variational posterior distribution with large set of hyperparameters

## GP prediction

Standard approach: predictive mean formula Extension: integrate PDE into GP modeling

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APIK: Active Physics-Informed Kriging Model with Partial Differential Equations
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Solving and Learning Nonlinear PDEs with Gaussian Processes
Journal of Computational Physics, 2021
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On going work: consideration of PDE constraint in hyperparameter optimization

## Travel time error

Consideration of $N=875$ vehicle trajectories starting every 10 seconds.

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The travel time error is given by:

$$
\mathrm{E}^{\top}=\sqrt{\frac{1}{N} \sum_{i=1}^{N}\left(\tau_{i}-\hat{\tau}_{i}\right)^{2}}
$$

where $\hat{\tau}_{i}$ denotes the estimated (or predicted) travel time.


Traffic estimation.


Traffic estimation.


Traffic prediction.

## Conclusion

- Proposition of a statistical framework for traffic state reconstruction
- Introduction of a discrepancy term to compensate model limitations
A. Würth, M. Binois, P. Goatin and S. Göttlich,

Data driven uncertainty quantification in macroscopic traffic flow models Advances in Computational Mathematics, 2022

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A. Würth, M. Binois, P. Goatin and S. Göttlich, Data driven uncertainty quantification in macroscopic traffic flow models Advances in Computational Mathematics, 2022
- Extension of framework for traffic state prediction
- Better performance when combining physics and GP in traffic prediction


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國 A. Würth, M. Binois, P. Goatin and S. Göttlich, Data driven uncertainty quantification in macroscopic traffic flow models Advances in Computational Mathematics, 2022

- Extension of framework for traffic state prediction
- Better performance when combining physics and GP in traffic prediction


## Outlook

- Consideration of real traffic data
- Improvement of boundary loop detector predictions


## Thank you

## Any questions?

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## Travel time error



Traffic estimation.


Traffic prediction.

## Two methods of GP prediction




## Definition (Weak entropy solution)

A function $W \in \mathrm{~L}^{\infty}\left((] 0, T[\times] x_{\text {in }}, x_{\text {out }}[) ; \mathcal{W}\right)$ is a weak entropy solution to the IBVP if

- for any entropy-flux pair $(\mathcal{E}, \mathcal{Q})$ and any test function $\phi \in \mathrm{C}_{\mathrm{c}}^{\infty}\left((]-\infty, T[\times] x_{\text {in }}, x_{\text {out }}[) ; \mathbb{R} \geq 0\right)$, it holds

$$
\int_{0}^{T} \int_{x_{\text {in }}}^{x_{\text {out }}}\left\{\mathcal{E}(u(W)) \partial_{t} \phi+\mathcal{Q}(u(W)) \partial_{x} \phi\right\} \mathrm{dxdt}+\int_{x_{\text {in }}}^{x_{\text {out }}} \mathcal{E}\left(u\left(W_{0}(x)\right)\right) \phi(0, x) \mathrm{dx} \geq 0 ;
$$

- for any boundary entropy pair $(\alpha, \beta)$ and any $\gamma(t) \in \mathrm{L}^{1}(] 0, T\left[; \mathbb{R}_{\geq 0}\right)$ it holds

$$
\begin{aligned}
& \underset{x \rightarrow x_{\text {in }}+}{\operatorname{ess}} \lim _{0}^{T} \beta\left(u(W(t, x)), u\left(W_{\text {in }}(t)\right)\right) \gamma(t) \mathrm{dt} \leq 0, \\
& \underset{x \rightarrow x_{\text {out }}-}{\operatorname{ess} \lim } \int_{0}^{T} \beta\left(u(W(t, x)), u\left(W_{\text {out }}(t)\right)\right) \gamma(t) \mathrm{dt} \geq 0
\end{aligned}
$$

## Definition (Boundary entropy pair)

An entropy pair $\left(\alpha\left(u_{1}, u_{2}\right), \beta\left(u_{1}, u_{2}\right)\right), u_{1}, u_{2} \in \mathbb{R}^{2}$ is called a boundary entropy pair ${ }^{7}$ if for every fixed $u_{2} \in \mathbb{R}^{2}$

$$
\alpha\left(u_{2}, u_{2}\right)=\beta\left(u_{2}, u_{2}\right)=\nabla_{1} \alpha\left(u_{2}, u_{2}\right)=(0,0)^{\top} .
$$

The entropy boundary conditions with respect to the left (resp. right) boundary state $W_{B}=\left(v_{B}, W_{B}\right)$ and for $j \in\{1,2\}$ reads as follows:

$$
\beta^{j}\left(W, W_{B}\right):=\mathcal{Q}^{j}(W)-\mathcal{Q}^{j}\left(W_{B}\right)-\nabla_{\mu} \mathcal{E}^{j}\left(W_{B}\right) \cdot\left(f(W)-f\left(W_{B}\right)\right) \leq(\geq) 0 .
$$

We consider the following families of entropy-flux pairs ${ }^{8}$ :

$$
\begin{aligned}
& \mathcal{E}^{1}(u(W))= \begin{cases}0 & \text { if } v \leq \bar{v}, \\
1-\frac{\mathcal{R}(v, w)}{\mathcal{R}(\bar{v}, w)} & \text { if } v>\bar{v},\end{cases} \\
& \mathcal{Q}^{1}(u(W))= \begin{cases}0 & \text { if } v \leq \bar{v}, \\
\bar{v}-\frac{v \mathcal{R}(v, w)}{\mathcal{R}(\bar{r}, w)} & \text { if } v>\bar{v}\end{cases}
\end{aligned}
$$

for any $\bar{v} \in\left[0, w_{\text {max }}\right]$ and $^{9}$

$$
\begin{aligned}
& \mathcal{E}^{2}(u(W))=\mathcal{R}(v, w)|\bar{w}-w| \\
& \mathcal{Q}^{2}(u(W))=\mathcal{R}(v, w) v|\bar{w}-w|
\end{aligned}
$$

for any $\bar{w} \in\left[w_{\min }, w_{\max }\right]$.

[^15]
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