April 04, 2023 Mascot-Num 2023, Le Croisic

Combining physics models and Gaussian processes for traffic prediction

Alexandra Würth¹ (Centre Inria d'Université Côte d'Azur) Joint work with Mickaël Binois¹ and Paola Goatin¹

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¹Université Côte d'Azur, Inria, CNRS, LJAD, 2004 route des Lucioles - BP 93, 06902 Sophia Antipolis Cedex, France. E-mail: {alexandra.vuerth, mickael.binois, paola.goatin}@inria.fr < □ > < ∂ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ > < ≥ >

Motivation



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

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Motivation



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Outline

1 Macroscopic traffic flow models

2 Calibration approaches

Synthetic traffic data

4 Traffic estimation and prediction

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Macroscopic traffic flow models

Calibration approaches

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Macroscopic traffic flow models

Consideration of averaged and aggregated traffic quantities such as:

- traffic **density** ρ (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-inmotion/inductive-loop/

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Generic Second Order Model (GSOM)

We consider a Generic Second Order traffic flow Model (GSOM)² consisting in a 2×2 hyperbolic system of conservation laws

$$\begin{cases} \partial_t \rho + \partial_x (\rho v) = 0, \\ \partial_t (\rho w) + \partial_x (\rho w v) = 0, \end{cases} \qquad x \in \mathbb{R}, \ t > 0, \tag{1}$$

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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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GSOM model

Initial Boundary Value Problem (IBVP)

We focus on the Initial Boundary Value Problem³ (IBVP) for (1):

$$\begin{cases} \partial_t \rho + \partial_x (\rho v) = 0, \\ \partial_t (\rho w) + \partial_x (\rho w v) = 0, \end{cases} & x \in]x_{in}, x_{out}[\subset \mathbb{R}, t > 0, \\ (\rho, w)(0, x) = (\rho_0, w_0)(x), \\ (\rho, w)(t, x_{in}) = (\rho_{in}, w_{in})(t), \\ (\rho, w)(t, x_{out}) = (\rho_{out}, w_{out})(t), \end{cases} & t > 0, \end{cases}$$

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with values in an invariant domain of the form

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

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

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Outline

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:

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

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 where $arepsilon\sim\mathcal{N}(0,\sigma_{arepsilon}^{2}).$

1. L^2 - approach:

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

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

with θ^* being the **optimal calibration parameter** computed by:

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

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2. Kennedy-O'Hagan⁴ (KOH) - approach:

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

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

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



where

$$\begin{split} \mathbf{b}_{\mathsf{n}} &= \tilde{b} + \varepsilon \sim \mathcal{N}\big(\mathbf{0}, \mathsf{K}_{\mathsf{n}}(\lambda)\big) \quad \text{with covariance} \quad \mathsf{K}_{\mathsf{n}}(\lambda) = \sigma^2\big(\mathsf{C}_{\mathsf{n}}(\mathit{l}_1, \mathit{l}_2) + g\mathsf{I}_{\mathsf{n}}\big), \\ \text{hyperparameters} \ \lambda &= (\sigma^2, \mathit{l}_1, \mathit{l}_2, g), \ \textit{n} \text{ number of observations and} \end{split}$$

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 θ^* the **optimal calibration parameter** computed by:

$$\theta^* = \operatorname*{argmax}_{\theta} \frac{1}{\sqrt{(2\pi)^n |\mathsf{K_n}(\lambda)|}} \exp{\left(-\frac{1}{2}\mathsf{b_n}(\theta)^\top \big(\mathsf{K_n}(\lambda)\big)^{-1} \mathsf{b_n}(\theta)\right)}.$$

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Gaussian process modeling

Given: *n* bias-observations $b_n = b(\mathcal{X}_n)$ at $\mathcal{X}_n = ((t_1, x_1), \dots, (t_n, x_n))$ \rightarrow at \hat{n} new locations $\hat{\mathcal{X}}_{\hat{n}} = ((\hat{t}_1, \hat{x}_1), \dots, (\hat{t}_{\hat{n}}, \hat{x}_{\hat{n}}))$ it holds:

$$\begin{split} \mathsf{b}(\hat{\mathcal{X}}_{\hat{n}}) \mid \mathsf{b}_{\mathsf{n}} &\sim \mathcal{N}(m_{n}(\hat{\mathcal{X}}_{\hat{n}}), \mathsf{s}_{n}^{2}(\hat{\mathcal{X}}_{\hat{n}}, \hat{\mathcal{X}}_{\hat{n}})), \\ m_{n}(\hat{\mathcal{X}}_{\hat{n}}) &:= \mathbb{E}[\mathsf{b}(\hat{\mathcal{X}}_{\hat{n}})|\mathsf{b}_{\mathsf{n}}] = \mathsf{k}_{\mathsf{n}}(\hat{\mathcal{X}}_{\hat{n}})^{\top}\mathsf{K}_{\mathsf{n}}^{-1}\mathsf{b}_{\mathsf{n}}, \\ \mathsf{s}_{n}^{2}(\hat{\mathcal{X}}_{\hat{n}}, \hat{\mathcal{X}}_{\hat{n}}) &:= \mathbb{C}ov[\mathsf{b}(\hat{\mathcal{X}}_{\hat{n}}), \mathsf{b}(\hat{\mathcal{X}}_{\hat{n}})|\mathsf{b}_{\mathsf{n}}] = k(\hat{\mathcal{X}}_{\hat{n}}, \hat{\mathcal{X}}_{\hat{n}}) - \mathsf{k}_{n}(\hat{\mathcal{X}}_{\hat{n}})^{\top}\mathsf{K}_{\mathsf{n}}^{-1}\mathsf{k}_{\mathsf{n}}(\hat{\mathcal{X}}_{\hat{n}}) \\ \end{split}$$
where $k(\cdot, \cdot) = \sigma^{2}\mathbb{C}orr(\mathsf{b}(\cdot), \mathsf{b}(\cdot)), \ \mathsf{k}_{n}(\hat{\mathcal{X}}_{\hat{n}}) := (k(\hat{\mathcal{X}}_{\hat{n}}^{(j)}, \mathcal{X}_{n}^{(j)}))_{1 \leq j \leq \hat{n}, 1 \leq i \leq n}. \end{split}$

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Standard formula:

$$\mathbb{C}orr(\mathbf{b}(t,x),\mathbf{b}(t',x')) = \exp\left(-\frac{(t-t')^2}{l_1^2}\right)\exp\left(-\frac{(x-x')^2}{l_2^2}\right)$$

⁵ Osborne M. A., Bayesian Gaussian processes for sequential prediction, optimisation and quadrature; 2010 🗇 🕨 < 🗄 🕨 🚊 🔊 🤉 🖓

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Integral extension⁵ (due to time data averages):

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Integral extension⁵ (due to time data averages):

$$\begin{split} &\mathbb{C}orr\Big(\frac{1}{\Delta t}\int\limits_{t}^{t+\Delta t}\mathbf{b}(s,x)\,\mathrm{d}s,\ \mathbf{b}(t',x')\Big) = \left(\frac{1}{\Delta t}\int\limits_{t}^{t+\Delta t}\exp\left(-\frac{(s-t')^2}{l_1^2}\right)\,\mathrm{d}s\right)\exp\left(-\frac{(x-x')^2}{l_2^2}\right)\\ &\mathbb{C}orr\Big(\frac{1}{\Delta t}\int\limits_{t}^{t+\Delta t}\mathbf{b}(s,x)\mathrm{d}s,\ \frac{1}{\Delta t'}\int\limits_{t'}^{t'+\Delta t'}\mathbf{b}(s',x)\mathrm{d}s'\Big)\\ &= \left(\frac{1}{\Delta t'}\frac{1}{\Delta t}\int\limits_{t'}^{t'+\Delta t'}\int\limits_{t}^{t+\Delta t'}\exp\left(-\frac{(s-s')^2}{l_1^2}\right)\,\mathrm{d}s\,\,\mathrm{d}s'\right)\exp\left(-\frac{(x-x')^2}{l_2^2}\right) \end{split}$$

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Integral extension⁵ (due to time data averages):

$$\mathbb{C}orr\left(\frac{1}{\Delta t}\int_{t}^{t+\Delta t} b(s,x) \,\mathrm{ds}, \ b(t',x')\right) = \left(\frac{1}{\Delta t}\int_{t}^{t+\Delta t} \exp\left(-\frac{(s-t')^2}{l_1^2}\right) \,\mathrm{ds}\right) \exp\left(-\frac{(x-x')^2}{l_2^2}\right)$$
$$\mathbb{C}orr\left(\frac{1}{\Delta t}\int_{t}^{t+\Delta t} b(s,x) \,\mathrm{ds}, \ \frac{1}{\Delta t'}\int_{t'}^{t'+\Delta t'} b(s',x) \,\mathrm{ds'}\right)$$
$$= \left(\frac{1}{\Delta t'}\frac{1}{\Delta t}\int_{t'}^{t'+\Delta t'} \int_{t}^{t+\Delta t'} \exp\left(-\frac{(s-s')^2}{l_1^2}\right) \,\mathrm{ds} \,\mathrm{ds'}\right) \exp\left(-\frac{(x-x')^2}{l_2^2}\right)$$

 \rightarrow Slight improvement observed

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⁵Osborne M. A., Bayesian Gaussian processes for sequential prediction, optimisation and quadrature 2010 🗇 🕨 < 🖹 🕨 🚊 🔊 🤉 🔇

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
- Requires derivative of simulator: δy^M

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• Orthogonality condition on bias function and mathematical model

- Requires derivative of simulator: δy^M
- Correlation matrix:

$$\mathsf{C}_{\mathsf{n}}^{\mathrm{plum}} = \mathsf{C}_{\mathsf{n}} - \mathsf{C}_{\mathsf{n}} \,\, \delta y^{\mathcal{M}} \Big((\delta y^{\mathcal{M}})^{\top} \,\, \mathsf{C}_{\mathsf{n}} \,\, \delta y^{\mathcal{M}} \Big)^{-1} (\delta y^{\mathcal{M}})^{\top} \mathsf{C}_{\mathsf{n}}$$

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

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^{6&}lt;sub>Lopez et al.</sub> Microscopic Traffic Simulation using SUMO, 2018

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

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Traffic estimation.

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Traffic estimation and prediction



Traffic estimation and prediction





Traffic prediction.

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Traffic estimation and prediction





Standard approach: predictive mean formula

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

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

Long 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

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Long et al,

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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.

Travel time error

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

The travel time error is given by:

$$\mathsf{E}^{\mathsf{T}} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(\tau_i - \hat{\tau}_i)^2}$$

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

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Traffic estimation.



Traffic estimation.

Traffic prediction.

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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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Outlook

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

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Thank you Any questions?

Alexandra Würth Centre Inria d'Université Côte d'Azur, France alexandra.wuerth@inria.fr

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Travel time error



Traffic estimation.

Traffic prediction.

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Two methods of GP prediction



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Definition (Weak entropy solution)

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

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

$$\int_0^T \int_{x_{in}}^{x_{out}} \left\{ \mathcal{E}(u(W)) \partial_t \phi + \mathcal{Q}(u(W)) \partial_x \phi \right\} dx dt + \int_{x_{in}}^{x_{out}} \mathcal{E}(u(W_0(x))) \phi(0, x) dx \ge 0;$$

• for any boundary entropy pair (α, β) and any $\gamma(t) \in L^1(]0, T[; \mathbb{R}_{\geq 0})$ it holds

$$\begin{split} & \underset{x \to x_{in}+}{\mathrm{ess}\lim} \int_{0}^{T} \beta(u(W(t,x)), u(W_{in}(t)))\gamma(t) \mathrm{dt} \leq 0, \\ & \underset{x \to x_{out}-}{\mathrm{ess}\lim} \int_{0}^{T} \beta(u(W(t,x)), u(W_{out}(t)))\gamma(t) \mathrm{dt} \geq 0. \end{split}$$

Definition (Boundary entropy pair)

An entropy pair $(\alpha(u_1, u_2), \beta(u_1, u_2))$, $u_1, u_2 \in \mathbb{R}^2$ is called a boundary entropy pair⁷ if for every fixed $u_2 \in \mathbb{R}^2$

$$\alpha(\boldsymbol{u}_2,\boldsymbol{u}_2) = \beta(\boldsymbol{u}_2,\boldsymbol{u}_2) = \nabla_1 \alpha(\boldsymbol{u}_2,\boldsymbol{u}_2) = (0,0)^\top.$$

7 Chen, G. and Frid, H., Divergence Measure Fields and Hyperbolic Conservation Laws, 1999 🛛 🗧 ト 🛛 🗧 ト 🤞 📑

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

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

We consider the following families of **entropy-flux pairs**⁸:

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

for any $\bar{v} \in [0, w_{max}]$ and⁹

$$\mathcal{E}^2(u(W)) = \mathcal{R}(v, w)|ar{w} - w|$$
 $\mathcal{Q}^2(u(W)) = \mathcal{R}(v, w)v|ar{w} - w|$
y $ar{w} \in [w_{min}, w_{max}].$

for an

⁸Andreianov, B., Donadello, C. and Rosini, M. D., A second-order model for vehicular traffics with local point constraints on the flow, 2016 ⁹Serre, D., Systemes de Lois de Conservation, 1996