MLPDES25 - Machine Learning and PDEs Workshop

Modern calibration strategies for macroscopic traffic flow models

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joint work with Alexandra Würth and Mickaël Binois







Macroscopic traffic flow models

Spatio-temporal evolution of aggregate quantities:

- the (mean) traffic density ρ : number of vehicles per unit space
- the (mean) velocity v: distance covered by vehicles per unit time
- the traffic flow $q = \rho v$: number of vehicles per unit time

Data sources:



magnetic loop detectors, video recordings, floating car data, etc



Loop detector data¹

Example:

355 # M3E;	2;	255;	Ma;	01/09/15;	00:00;	1240;	C;	109;	10;
355 # M3E;	2;	255;	Ma;	01/09/15;	00:00;	1407;	D;	96;	54;
305 # M3e;	2;	255;	Ma;	01/09/15;	00:00;	1449;	D;	100;	10;
709 # M7i;	264;	687;	Ma;	01/09/15;	00:00;	1874;	D;	104;	37;
709 # M7i;	264;	687;	Ma;	01/09/15;	00:00;	2248;	D;	83;	36;
709 # M7i;	264;	687;	Ma;	01/09/15;	00:00;	2368;	D;	78;	39;
577 # M6C;	16;	474;	Ma;	01/09/15;	00:00;	4237;	D;	120;	40;
:	:		:	:	:	:	:	:	:

where:

loop code

road milestone

distance from the milestone (m)

day of the week

date

time (hours:minutes)

seconds and hundredth

lane

vehicle speed (km/h)

vehicle length (dm)

¹courtesy of DirMED

Sensors types

- **single:** vehicle count at fixed position (flow rate) and *occupancy* measure (density and velocity inferred, assuming average vehicle length)
- double: direct speed measure

Lighthill-Whitham-Richards (LWR) model (mid 50s)



• Phenomenological speed-density relation:

 $\partial_t \rho + \partial_x q = 0$ $v = v(\rho)$

fundamental diagram



R maximal or *jam* density, ρ_c critical density:

- flux is increasing for $\rho \leq \rho_c$: free-flow phase
- flux is decreasing for $\rho \ge \rho_c$: congestion phase

$v = v(\rho)?$

Experimental observations of fundamental diagrams are more complex than postulated by first order traffic models



Data from A51 (Marseilles, France), September 2015, courtesy of DirMED

Improved models

• Additional equation for v: second order models

[Payne (1971); Helbing (1996); Aw-Rascle (2000); Zhang (2002); Colombo (2002); Lebacque-et-al (2005); ...]

• Phase transition

[Colombo (2002); Goatin (2006); Blandin-et-al (2011); ...]

• Stochastic and averaged models

[Boel-Mihaylova (2006); Wang-Ni-Chen-Li (2010); Chen-Wang (2011); Sumalee&al (2011); Jabari-Liu (2011); ...]

Multi-class

[Wong-Wong (2002); Benzoni-Colombo (2003); VanLint-Hoogendorn-Schreurer (2008); Nair-Mahmassani-Hooks (2011); Fan-Work (2015); Gashaw-Goatin-Harri (2016); ...]

• Multi-lane

[Michalopoulos-Beskos-Yamauchi (1984); Klar-Wagener (1999); Greenberg-Klar-Rascle (2003); Colombo-Corli (2006); HoldenRisebro (2019); ...]

• Non-local models

[Blandin-Goatin (2016); Friedrich-Kolb-Göttlich (2018); ...]

Generalized Second Order Model² (GSOM)

- Conservation of vehicles: $\partial_t \rho + \partial_x (\rho v) = 0$
- Variable fundamental diagram: $v = \mathcal{V}(\rho, w), w$ driver attribute
- Transport equation for w (follows vehicle trajectories):

 V_{i} $R \rho$ $R \rho$ ĥ • $w = const \longrightarrow$ LWR • $\mathcal{V}(\rho, w) = w - p(\rho) \longrightarrow \text{ARZ}$ • $\mathcal{V}(\rho, w) = w \left(1 - \exp\left(\frac{C}{V} \left(1 - \frac{R}{\rho} \right) \right) \right)$

²[Lebacque-Mammar-Salem, Transportation and Traffic Theory (2007)]

 $\partial_t w + v \partial_x w = 0$

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Initial-Boundary Value Problem for GSOM³

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

where

$$\begin{split} \mathcal{V}(\rho,w) &\geq 0, \quad \mathcal{V}(0,w) = w, \\ 2\mathcal{V}_{\rho}(\rho,w) + \rho\mathcal{V}_{\rho\rho}(\rho,w) < 0 \text{ for } w > 0, \\ \mathcal{V}_{w}(\rho,w) > 0, \\ \forall w > 0 \quad \exists \ R(w) > 0 : \quad \mathcal{V}(R(w),w) = 0, \end{split}$$

such that

$$\lambda_1(\rho,w) = \mathcal{V}(\rho,w) + \rho \mathcal{V}_{\rho}(\rho,w), \qquad \lambda_2(\rho,w) = \mathcal{V}(\rho,w) > 0$$

 \implies existence of entropy weak solutions for BV data

³[Goatin-Würth, Nonlinear Analysis (2023)]

Numerical approximation⁴

Hilliges-Weidlich (HW) finite volume scheme: $\mathbf{u} = (\rho, y)^T = (\rho, \rho w)^T$

$$\mathbf{u}_{j}^{n+1} = \mathbf{u}_{j}^{n} - \frac{\Delta t}{\Delta x} \left(\mathbf{F}_{j+1/2}^{n} - \mathbf{F}_{j-1/2}^{n} \right), \qquad \mathbf{F}_{j+1/2}^{n} = \left(F_{j+1/2}^{\rho, n}, F_{j+1/2}^{y, n} \right)^{T}$$

where

$$F_{j+1/2}^{\rho,n} = \rho_j^n \mathcal{V}^+(\rho_{j+1}^n, w_{j+1}^n)$$
 and $F_{j+1/2}^{y,n} = w_j^n F_{j+1/2}^{\rho,n}$

and

$$(CFL) \quad \Delta t \left\{ \left\| \mathcal{V} \right\|_{\infty} + R(w_{max}) \left\| \mathcal{V}_{\rho} \right\|_{\infty} \right\} \le \Delta x,$$

Maximum principle

- If $\Delta t \|\mathcal{V}\|_{\infty} \leq \Delta x$, scheme (HW) is positivity preserving.
- Under (CFL), if $R(w) = \mathbf{R}_{\max} \quad \forall w$, the approximate solution constructed by (HW) scheme satisfies $\rho_j^n \leq \mathbf{R}_{\max} \text{ (and } \mathcal{V}(\rho_j^n, w_j^n) \geq 0) \text{ for all } j \in \mathbb{Z} \text{ and } n \in \mathbb{N}.$

 $\sim 40\%$ computational time reduction

⁴[Würth-Goatin-Villada, HYP2022 Proceedings]

Bayesian calibration with $bias^5$

Combining field data and computer simulations for calibration and prediction

[Kennedy-O'Hagan, J. Royal Statistical Society B, 2001; Higdon&al, SISC, 2004]

Look for θ^* , b and ϵ s.t.

observation simulation discrepancy obs. error assuming $b \sim \mathcal{MVN}(0, \sigma^2 Corr)$ and $\epsilon \sim \mathcal{N}(0, \sigma_{\epsilon}^2) \longrightarrow$ Gaussian Process

 $\underbrace{y^F(t,x)}_{}=\underbrace{y^M(t,x,\theta^*)}_{}+\underbrace{b(t,x,\theta^*)}_{}+\underbrace{\epsilon(t,x)}_{}$

Correct the simulation output as

$$y_c^M(t, x, \theta^*) = y^M(t, x, \theta^*) + m_N(t, x).$$



⁵[Würth-Binois-Goatin-Göttlich, Adv. Comput. Math., 2022]

Gaussian process modeling⁶

- Set of N observation points: $\mathcal{X}_N = ((t_1, x_1), \dots, (t_N, x_N))$
- Set of observed (noisy) biases: $\mathbf{b}_N(\theta) = y^F(\mathcal{X}_N) y^M(\mathcal{X}_N, \theta)$

⁶[Rasmussen-Williams, Gaussian processes for machine learning, 2006]

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- \mathbf{b}_N is modeled by a **realization** of a **MVN distribution**:

$$\mathbf{b}_N \sim \mathcal{N}(\mathbf{0}_N, \mathbf{K}_N) ext{ with } \mathbf{K}_N = \sigma^2(\mathbf{C}_N + g\mathbf{I}_N), g = rac{\sigma_arepsilon^2}{\sigma^2}$$

and (stationary) Gaussian kernel correlation matrix:

$$\mathbf{C}_{N} := \mathbb{C}orr(b(t, x), b(t', x')) = \exp\left(-\frac{(t - t')^{2}}{l_{1}^{2}}\right) \exp\left(-\frac{(x - x')^{2}}{l_{2}^{2}}\right)$$

0

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• (Hyper)parameter estimation by maximization of the concentrated log-likelihood:

$$\log \tilde{\mathcal{L}}(l_1, l_2, g, \mathbf{b}_N) = -\frac{N}{2} \log 2\pi - \frac{N}{2} \log \hat{\sigma}^2(l_1, l_2, g, \mathbf{b}_N) - \frac{1}{2} \log |\mathbf{C}_N + g\mathbf{I}_N| - \frac{N}{2}$$

(with
$$\hat{\sigma}^{2}(l_{1}, l_{2}, g, \mathbf{b}_{N}) = \frac{\mathbf{b}_{N}^{\top}(\mathbf{C}_{N} + g\mathbf{I}_{N})^{-1}\mathbf{b}_{N}}{n}$$
)
 $\theta^{*} \leftarrow \operatorname*{argmax}_{\theta} \left[\max_{l_{1}, l_{2}, g} \log \tilde{\mathcal{L}}(l_{1}, l_{2}, g, \mathbf{b}_{N}(\theta)) \right]$

⁶[Rasmussen-Williams, Gaussian processes for machine learning, 2006]

Model comparison

Comparing LWR and GSOM



Optimal parameters - fundamental diagram (DirMED data)

		LWR		GSOM			
	V^*	C^*	R^*	V^*	C^*	R^*	
DirMed	83.51	23.84	390.00	94.74	17.02	348.22	
RTMC	87.37	29.15	422.51	91.56	18.39	478.23	

Model comparison

Comparing LWR and GSOM



Optimal parameters - speed profile validation (DirMED data)

			LWR		GSOM				
	Eflow	E^{speed}	Edensity	Е	Eflow	E^{speed}	E^{density}	E	
DirMed	1.245	1.370	3.695	6.311 (+85%)	0.917	0.879	1.619	3.414	
RTMC	0.883	1.929	2.548	5.360 (+93%)	1.184	0.863	0.730	2.777	

Parameters uncertainty

Bayesian formulation (MCMC method, Metropolis algorithm):

• prior multivariate normal distribution

$$\pi(\theta_{\rm VCR}) \propto \frac{1}{\sqrt{|\Sigma_{\theta_{\rm VCR}}|}} \exp\left\{-0.5 \left(\theta_{\rm VCR} - \mu_{\theta_{\rm VCR}}\right)^{\top} \Sigma_{\theta_{\rm VCR}}^{-1} \left(\theta_{\rm VCR} - \mu_{\theta_{\rm VCR}}\right)\right\}$$

with mean $\mu_{\theta_{\text{VCR}}}$ and covariance matrix $\Sigma_{\theta_{\text{VCR}}}$.

• proposal multivariate normal distribution

$$\hat{\theta}_{\text{VCR}} \sim \mathcal{N}((\theta_{\text{VCR}})_{i-1}, \Sigma_{\text{VCR}}^p)$$

with covariance matrix Σ_{VCR}^p .

• sampling model for y^F

$$\mathcal{L}(y^F \mid \theta^*) \propto \left| \hat{\sigma}^2(\theta^*) \left(\mathbf{C}_n \left(l_1, l_2 \right) + g \mathbf{I}_n \right) \right|^{-1/2}$$

• posterior distribution (Bayes theorem)

$$\pi(heta^* \mid y^F) = \; rac{\mathcal{L}\left(y^F \mid heta^*
ight) imes \pi(heta_{ ext{VCR}})}{\pi(y^F)}$$

Parameters uncertainty

Metropolis algorithm: 10^5 iterations, 10% burn-in phase effective sample sizes: 720 (LWR), 11250 (GSOM)



GSOM model - parameters distribution (DirMED data)

	LWR				GSOM			
	E_{MCMC}^{flow}	E_{MCMC}^{speed}	$E_{MCMC}^{density}$	$\mathbf{E}_{\mathrm{MCMC}}$	E_{MCMC}^{flow}	E_{MCMC}^{speed}	$E_{MCMC}^{density}$	$\mathbf{E}_{\mathrm{MCMC}}$
DirMed	1.056	1.272	4.336	6.664 (+101%)	0.929	0.827	1.567	3.322
RTMC	0.896	2.507	2.218	5.621 (+111%)	1.166	0.687	0.813	2.667

Comparison of calibration approaches⁷

On synthetic data with discrepancy and noise:

- Run a simulation y_{sim} with given $\theta^0 = (V^0, C^0, R^0) = (100, 20, 350)$
- Add bias to y_{sim} ($\tau \in \{0, 0.02, 0.1\}$): read data: $y^P(t, x) := y_{\text{sim}}(t, x) + \tau \max(y_{\text{sim}}(t, x)) \cdot \sin(t + x)$
- Generate 6 min noisy average loop detector data (s = 0.15): field data: $y^F = \bar{y}^P + s\bar{y}^P \mathcal{N}(0, 1)$



 $\tau = 0.1.$

⁷[Würth-Binois-Goatin, MT-ITS 2023]

Comparison of calibration approaches

Speed profiles (GSOM - KOH) and RSME between \bar{y}^P and corrected simulation:



Conclusion and perspectives

Summary

- Existence of entropy weak solutions for IBVP with vacuum
- Cheap finite volume scheme
- Statistical framework for traffic state reconstruction
- Introduction of a **bias term** to compensate model limitations
- Extension to **traffic state** and **travel time prediction** [Würth-Binois-Goatin, Traffic prediction by combining macroscopic models and Gaussian processes, submitted.]

Perspectives

- Consideration of more complex traffic scenarios.
- Local variations of the bias on the road.

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