Calibration of complex system models for the construction of the digital twin of the autonomous vehicle

Soutenance de thèse de Doctorat en Mathématiques appliquées

Soutenue publiquement par Clara CARLIER
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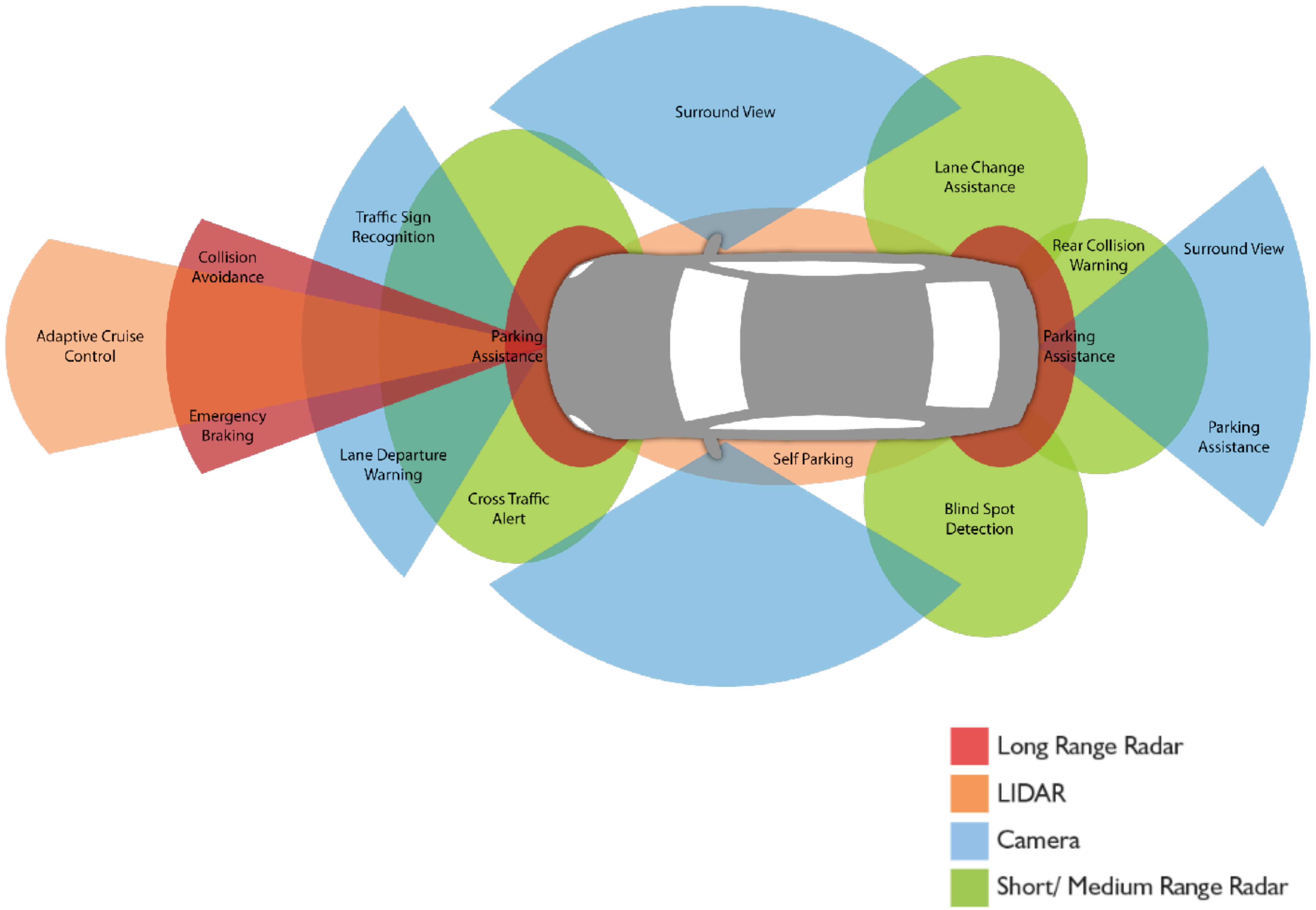
1. General introduction

General introduction

Context

- Advanced driver assistance systems (ADAS) are becoming increasingly important and complex around the world



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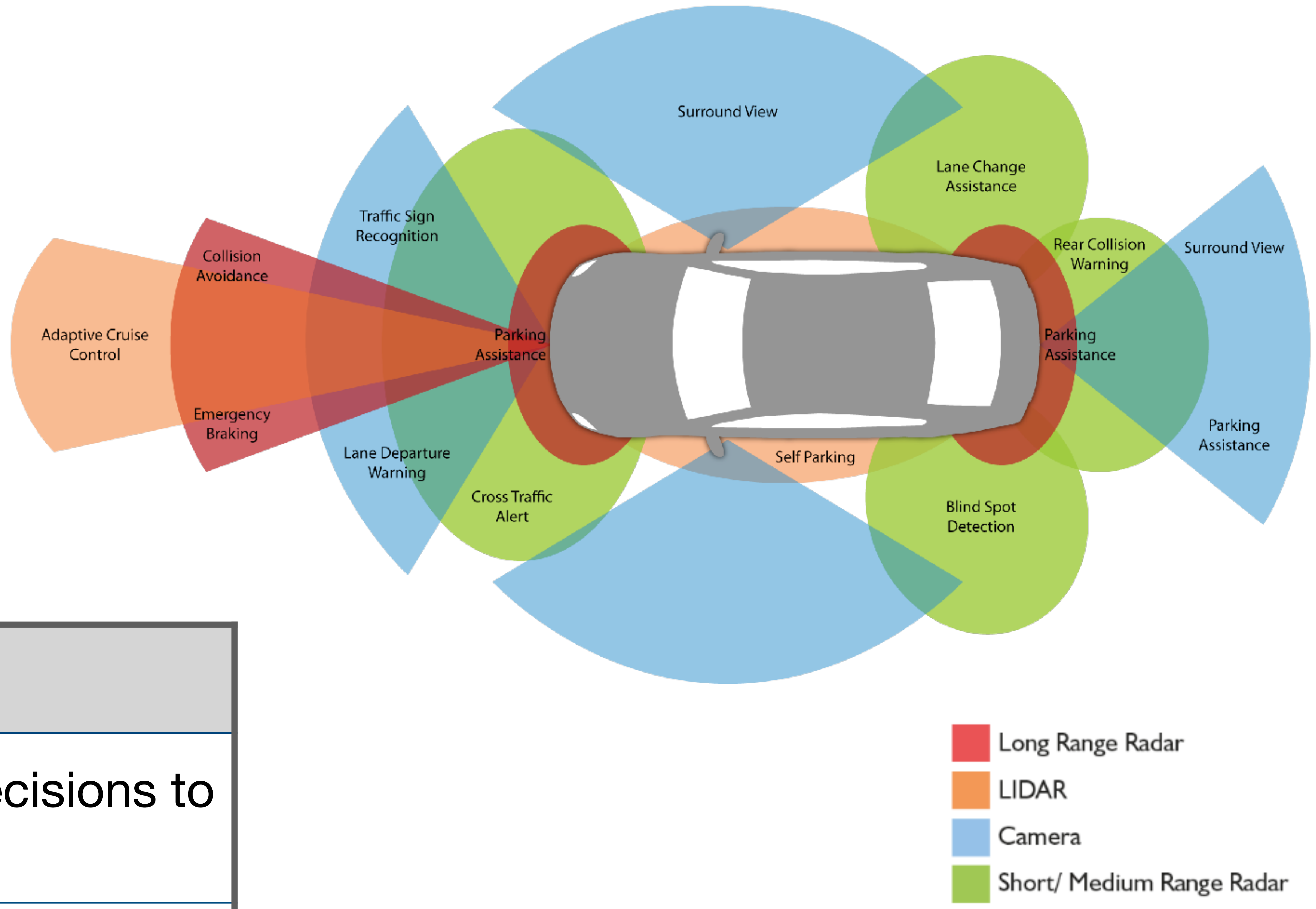

Passive ADAS	**Active ADAS**
Provide drivers with information to help them make safer decisions	Autonomously making decisions to prevent accidents
• forward collision warning • lane change assist	• **automatic emergency braking** • adaptive cruise control

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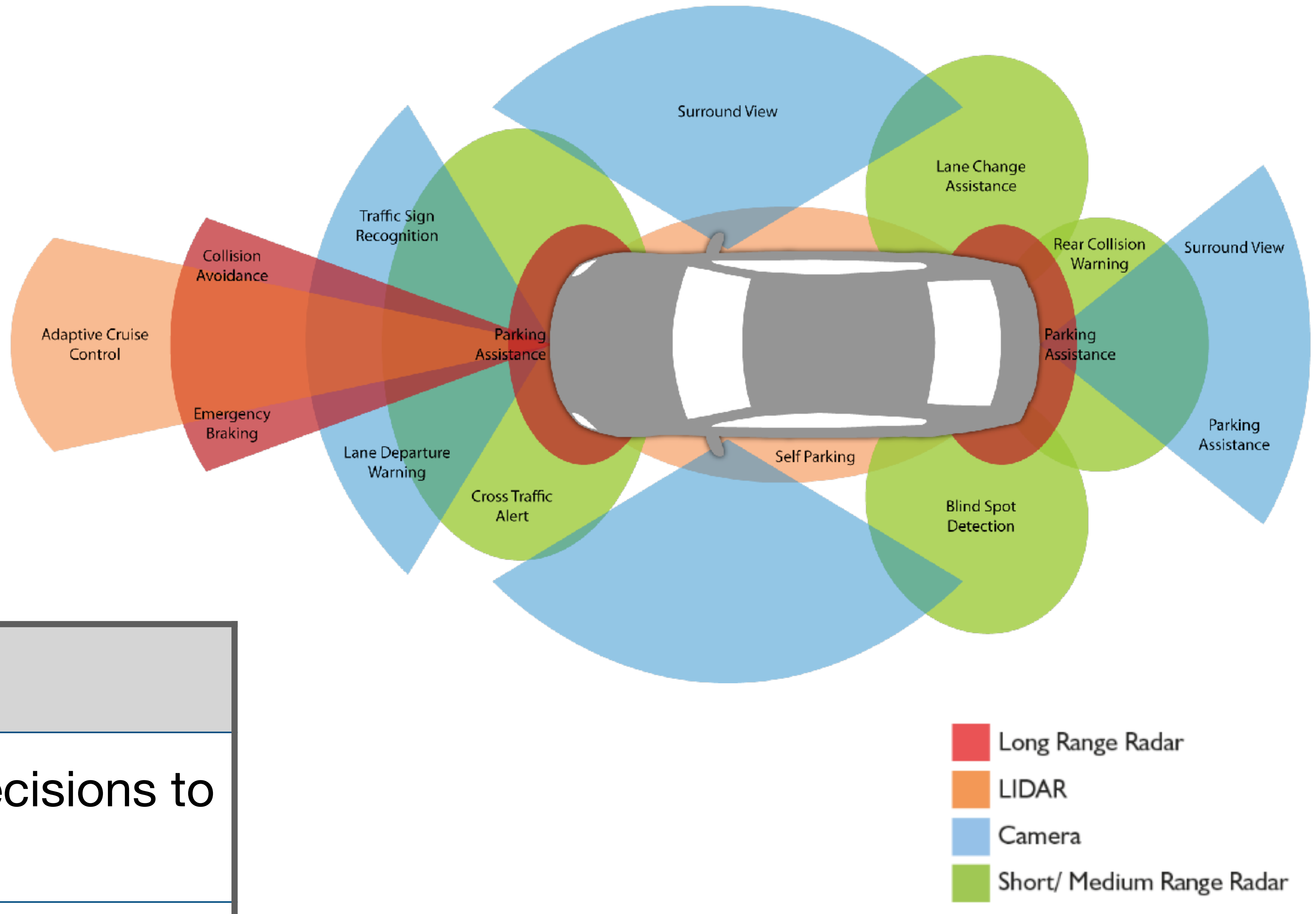

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- Some statistics
  - 96% of new vehicles are equipped with at least one ADAS function
  - 86% of people surveyed express doubts about their reliability

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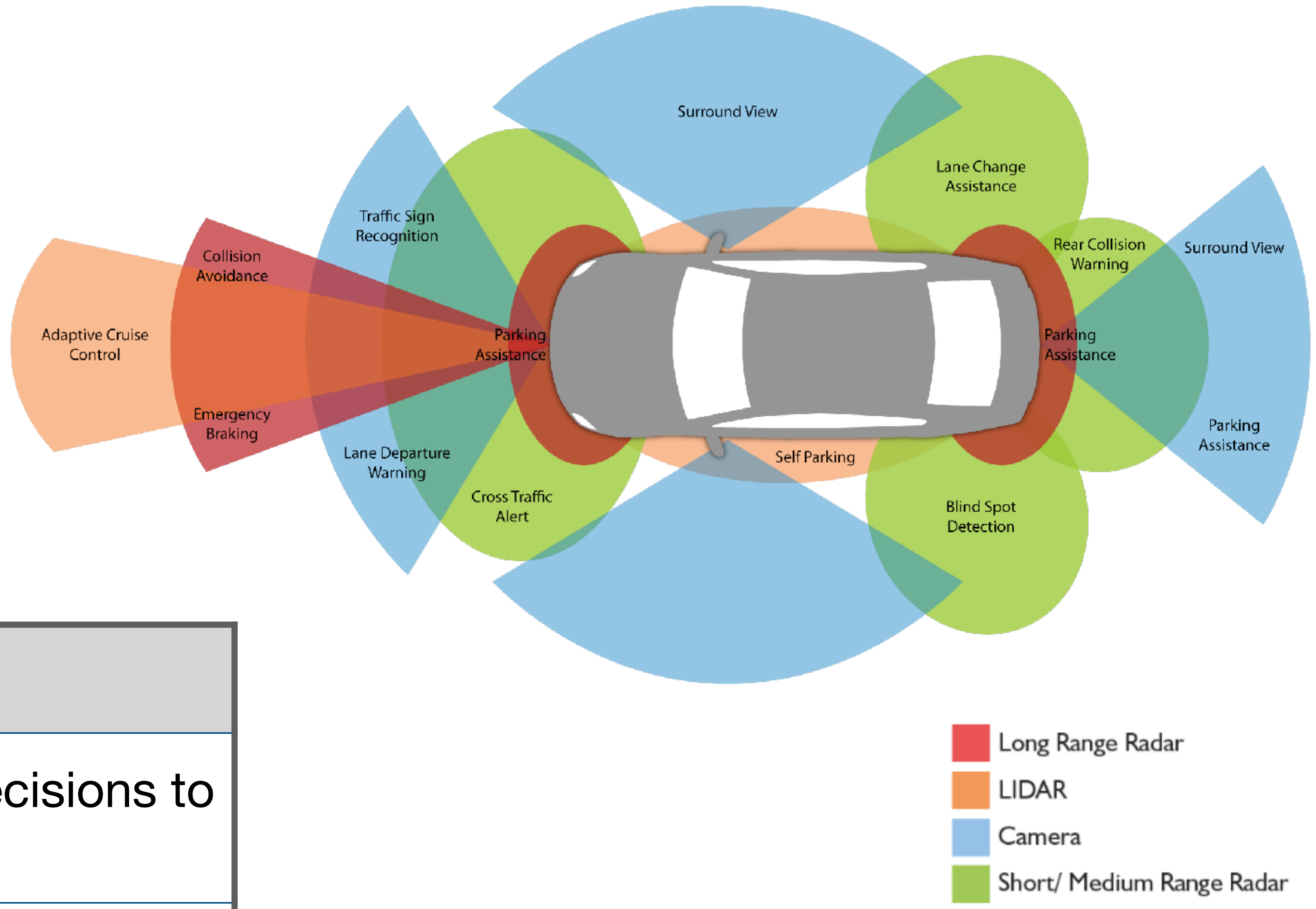

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This underlines the importance of strict regulation of these technologies

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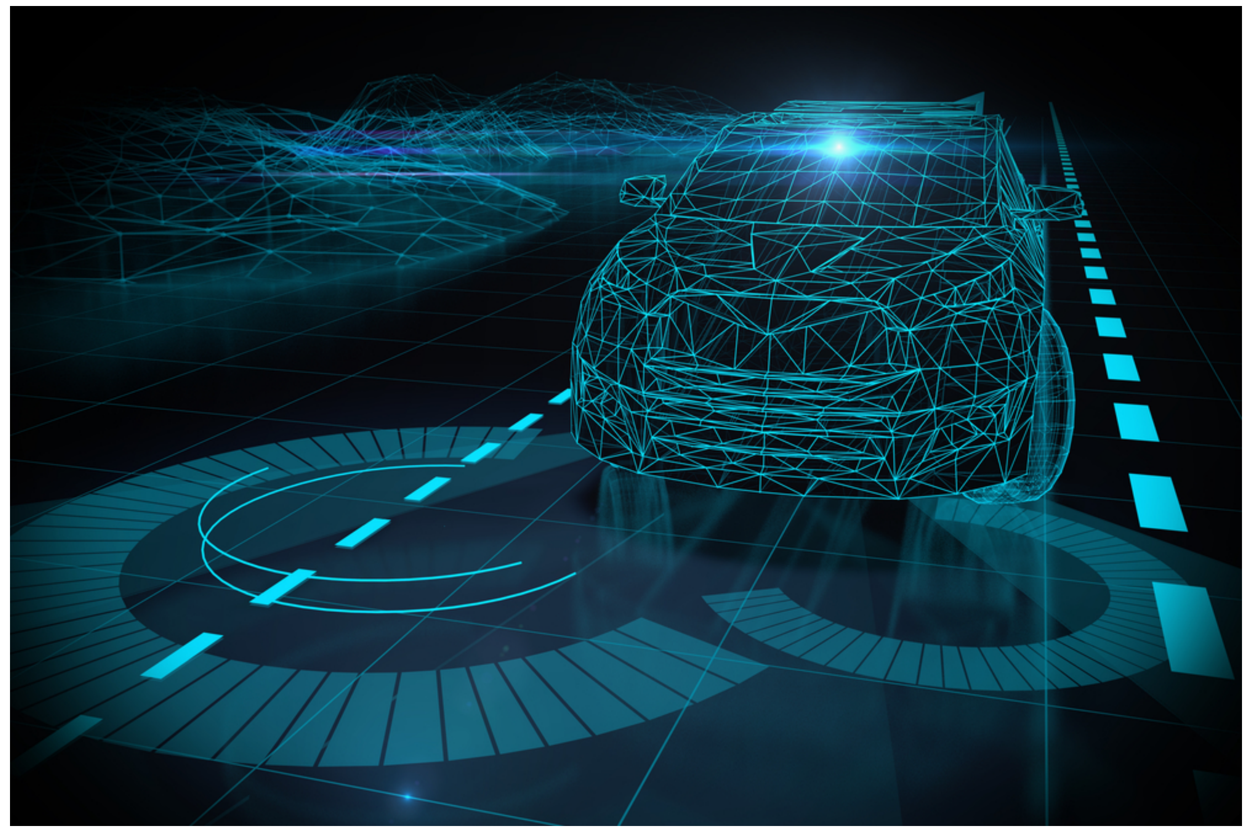
Validation and certification of ADAS

- Real-life on-track experiments are costly and time-consuming
- Use simulated experiments to integrate them into the vehicle homologation process



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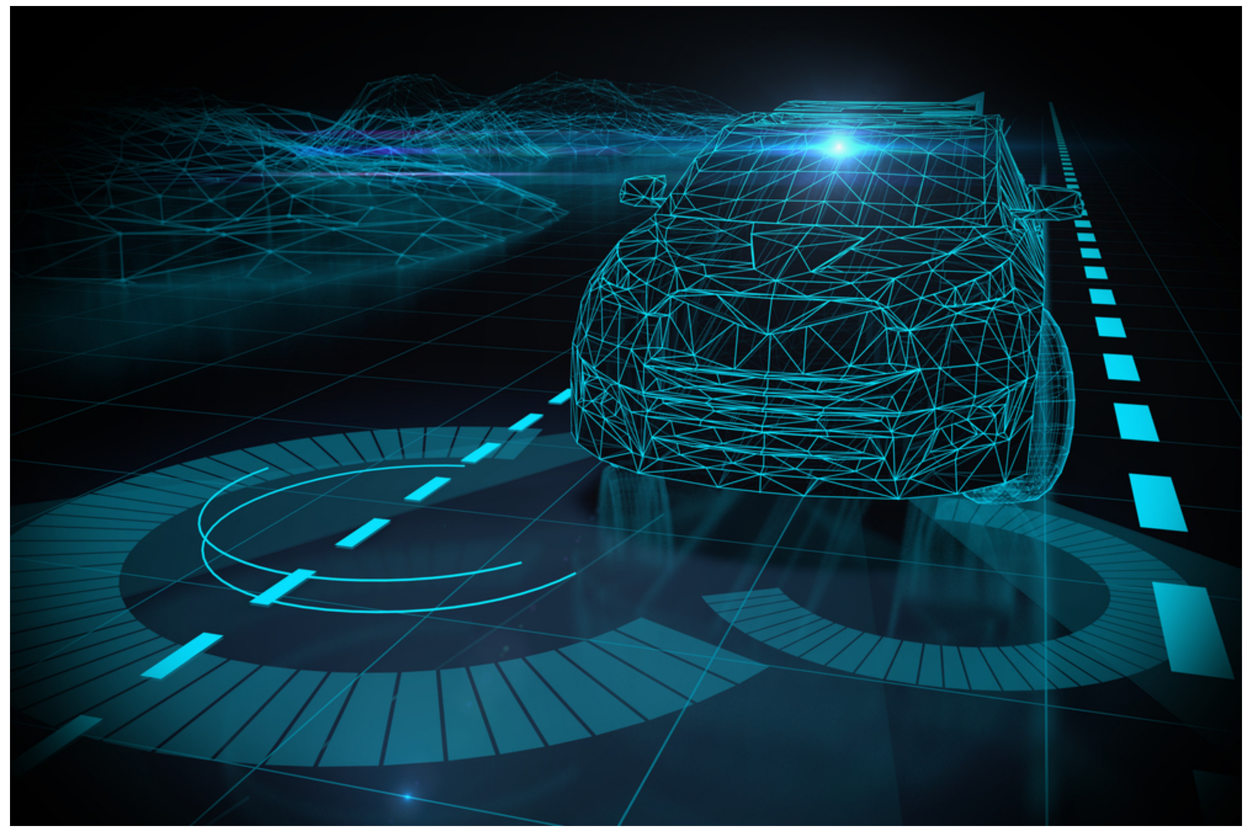
Are digital simulations sufficiently correlated with reality to be used legally?



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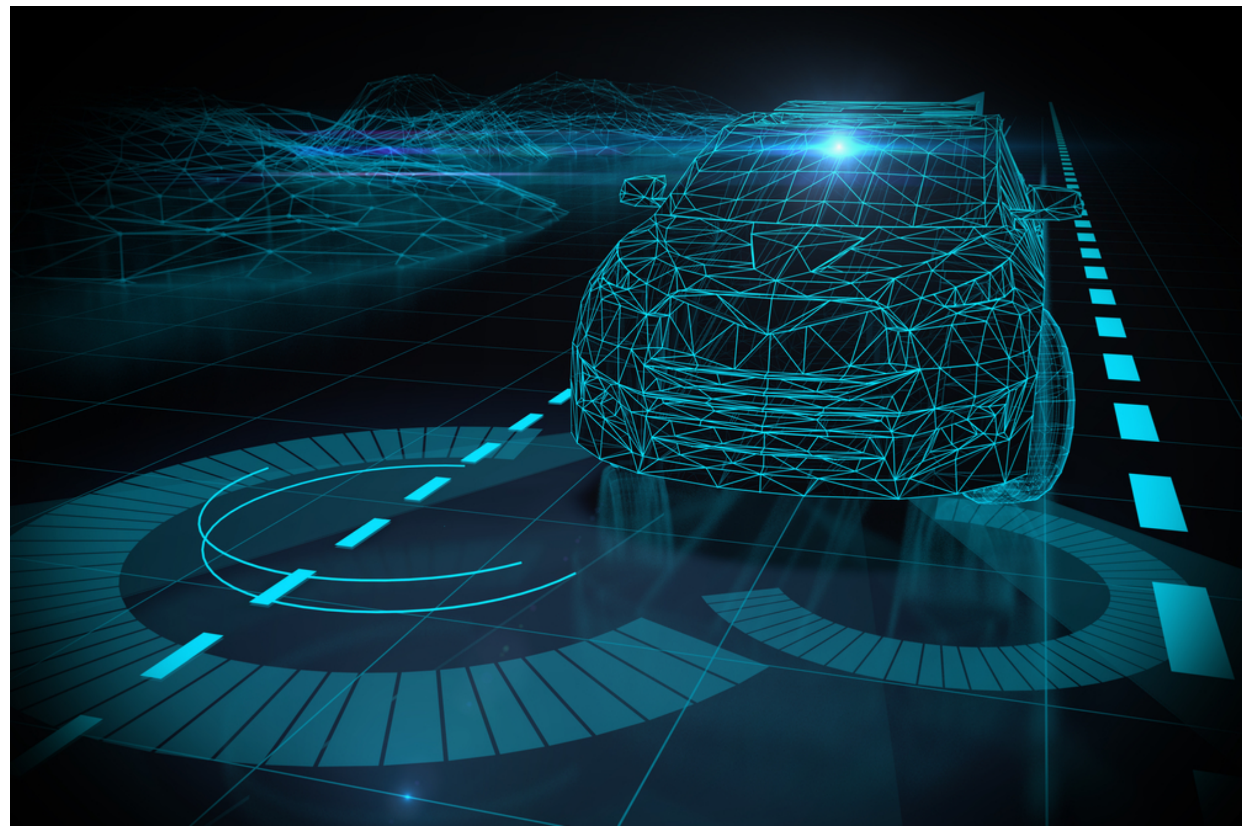
Global objective: calibrate the simulator

- Simulate time series most correlated with reality by identifying the input parameters used to generate it
- Develop a methodology for gauging the quality of simulations and modifying the input parameters to improve correlation automatically



General introduction

How the simulator works

Two primary types of experiments are used

- **Simulated ones:** generated using the digital simulator, offering great flexibility in experimental design
- **Real on-track ones:** physical tests performed on track, high cost and infrequently performed

Simulated time series

Reference on-track time series

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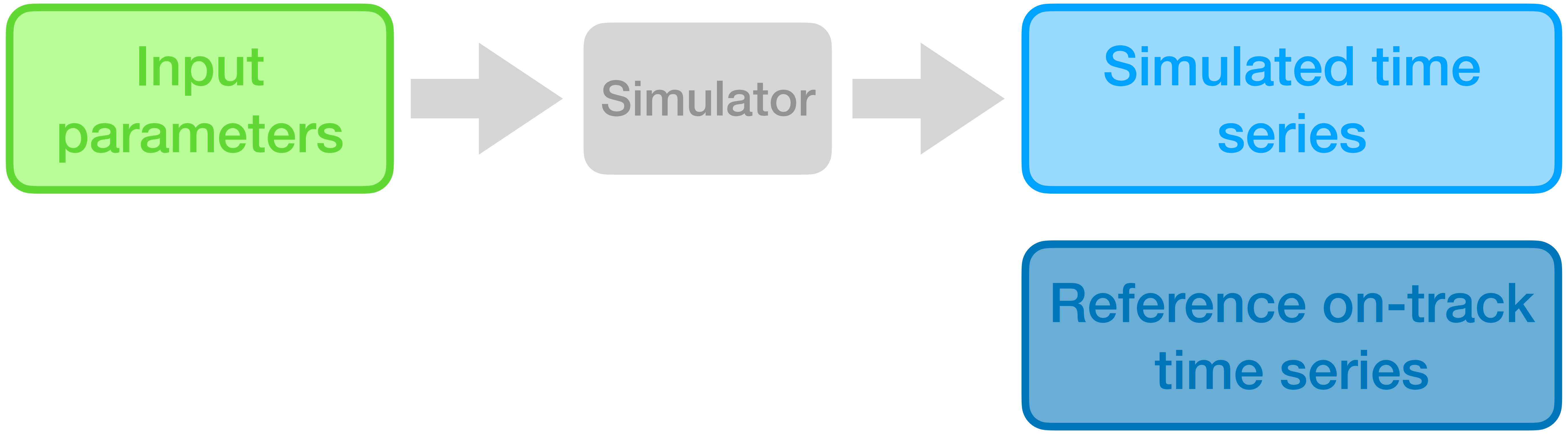
A **scenario** is defined as a combination of **two main components**

- **Input parameters:** establish the necessary conditions for conducting the simulations
- **Output time series:** capture the dynamic of the vehicles throughout the experience



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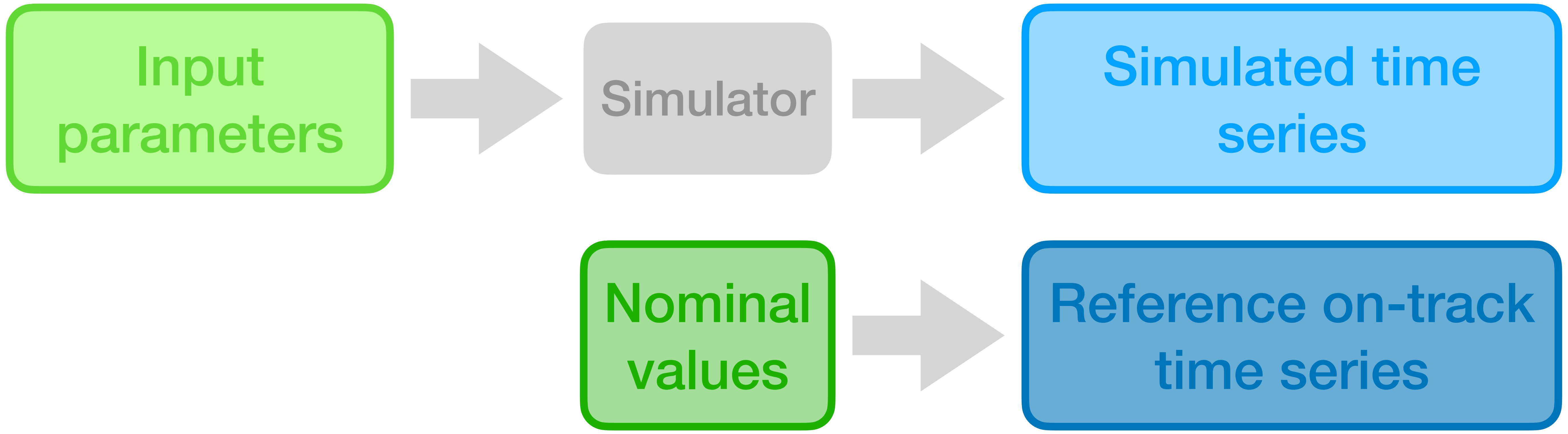
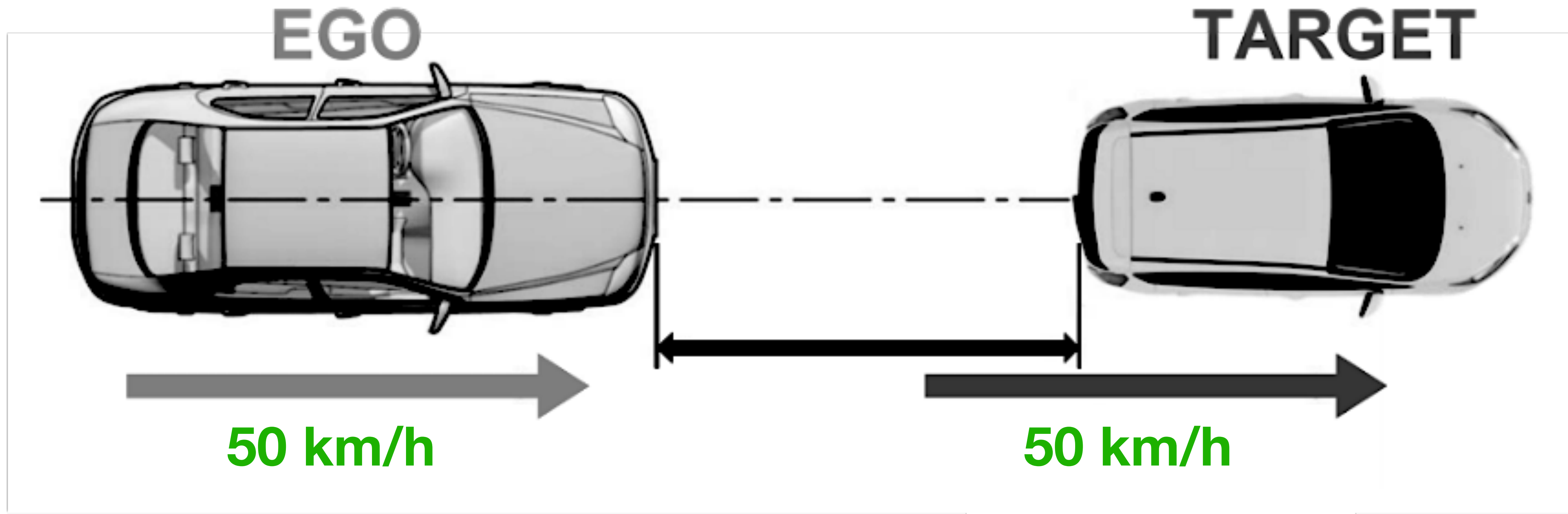
Nominal values

- Define the reference scenario to be tested and used as initial values during on-track experiments

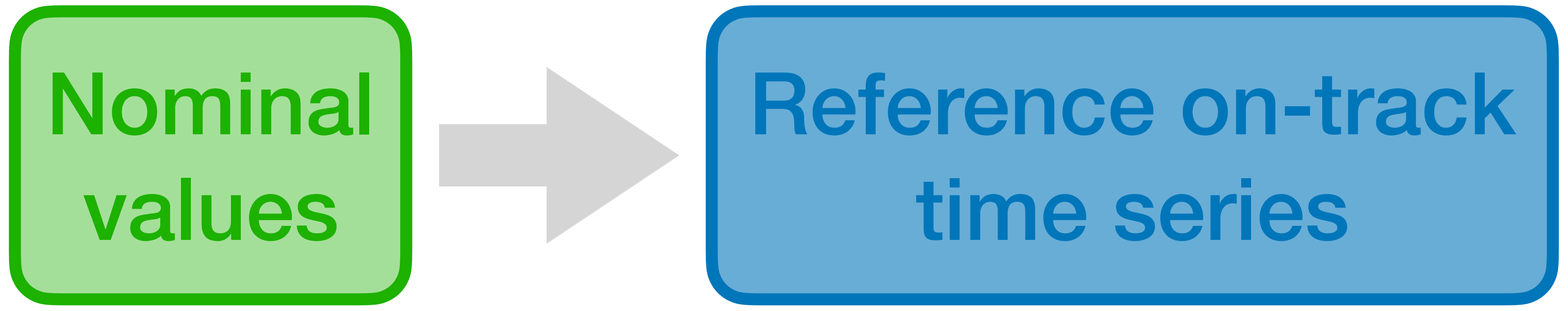


General introduction

Global objective of the thesis



- **For each** **real-life on-track time series:** **nominal values** are given



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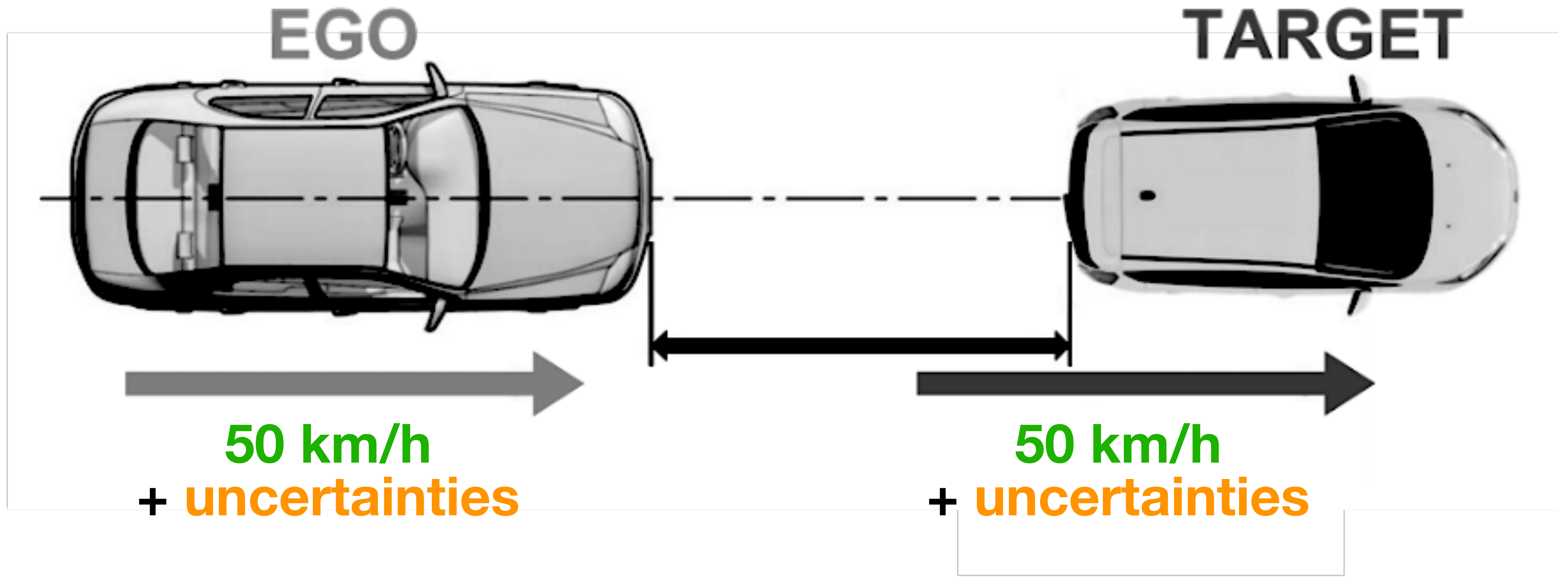
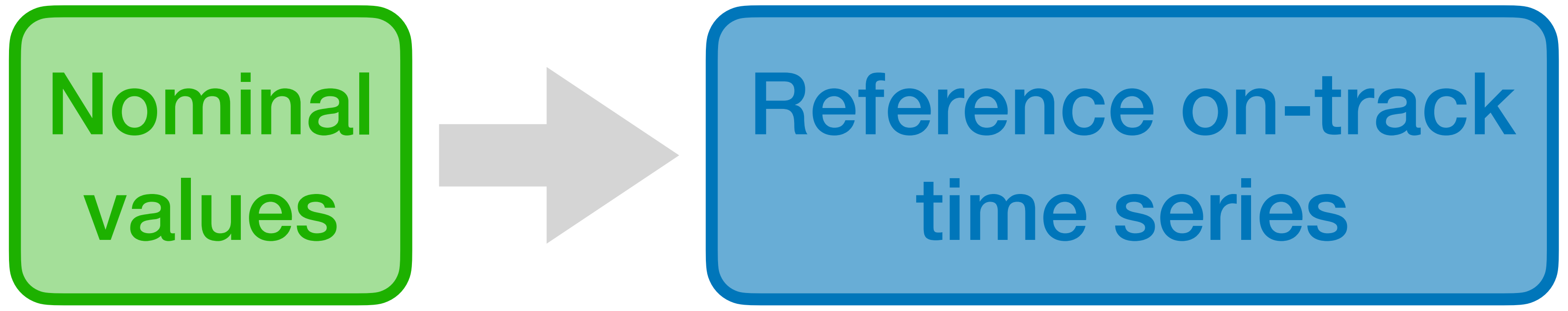


- **For each real-life on-track time series: nominal values** are given
- **Nominal values:** subject to uncertainties due to sensor errors and a certain tolerance

If the theoretical initial speed is 50 km/h, telling the simulation to start at 50.1 km/h can help simulate more realistic time series.



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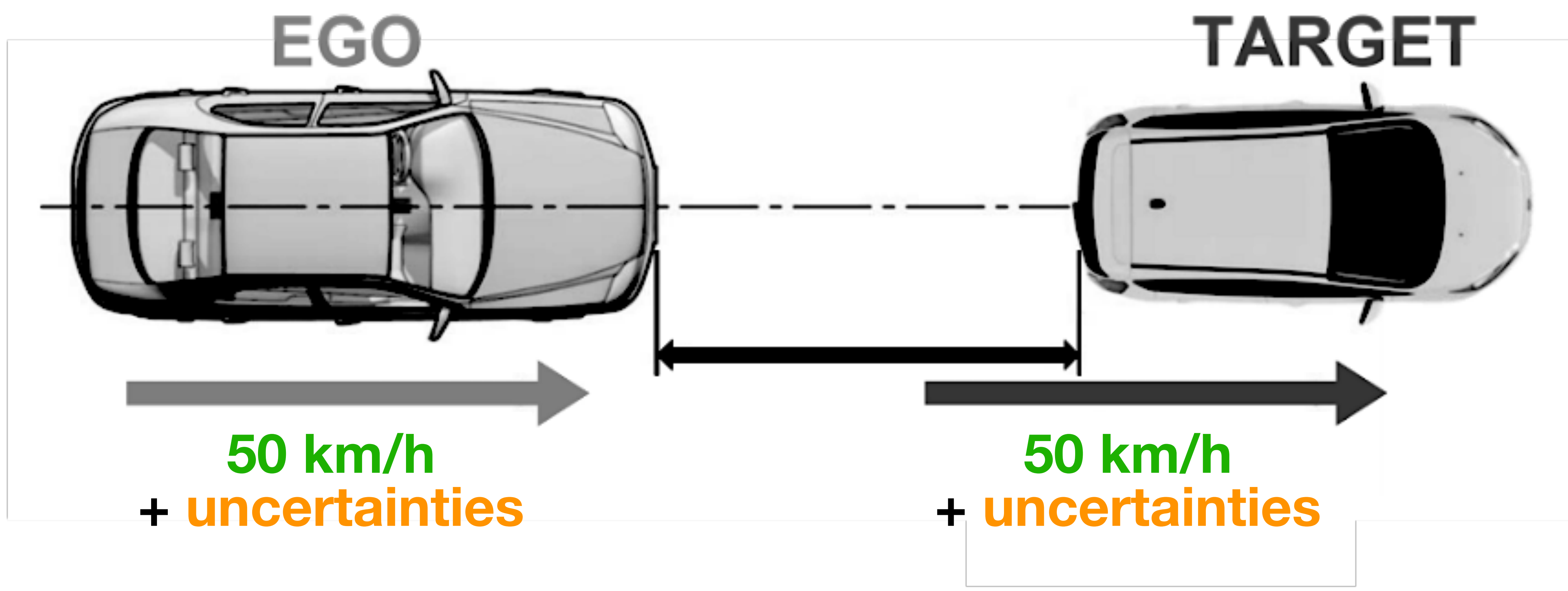

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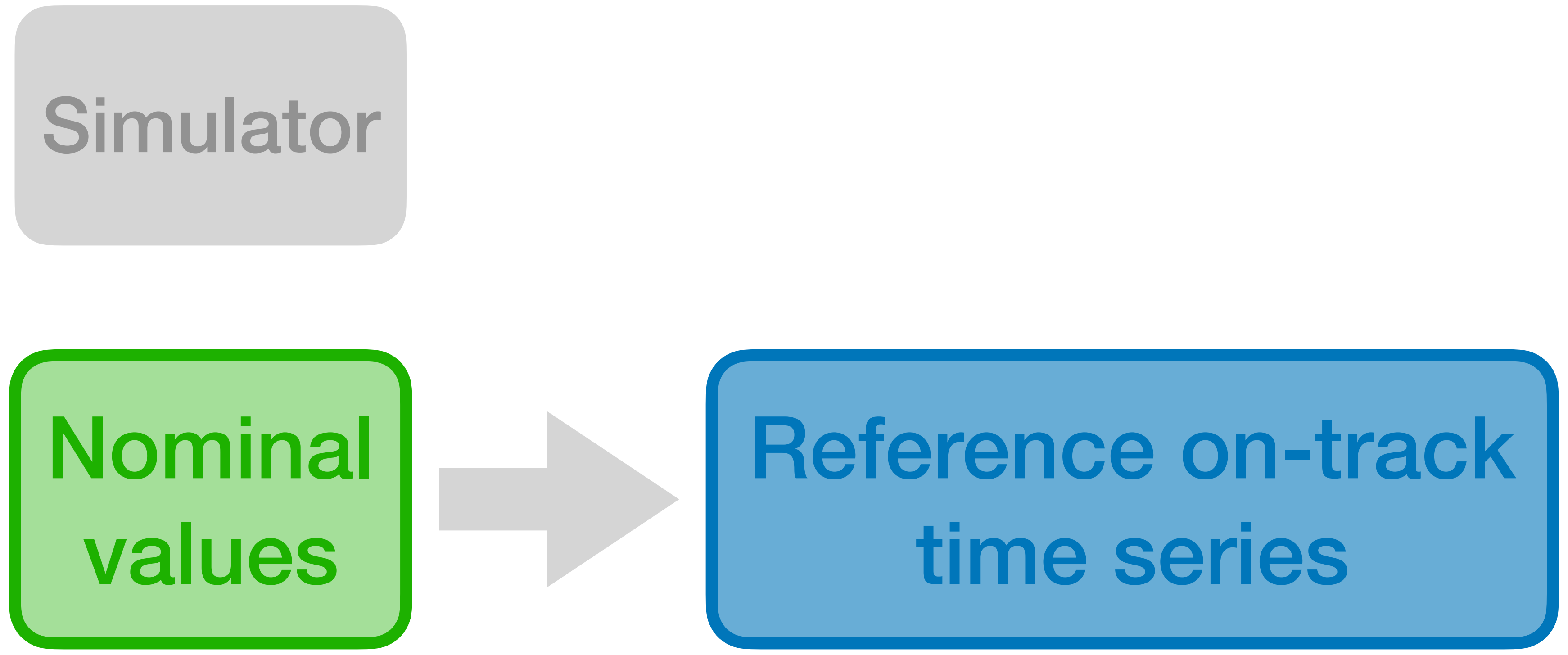

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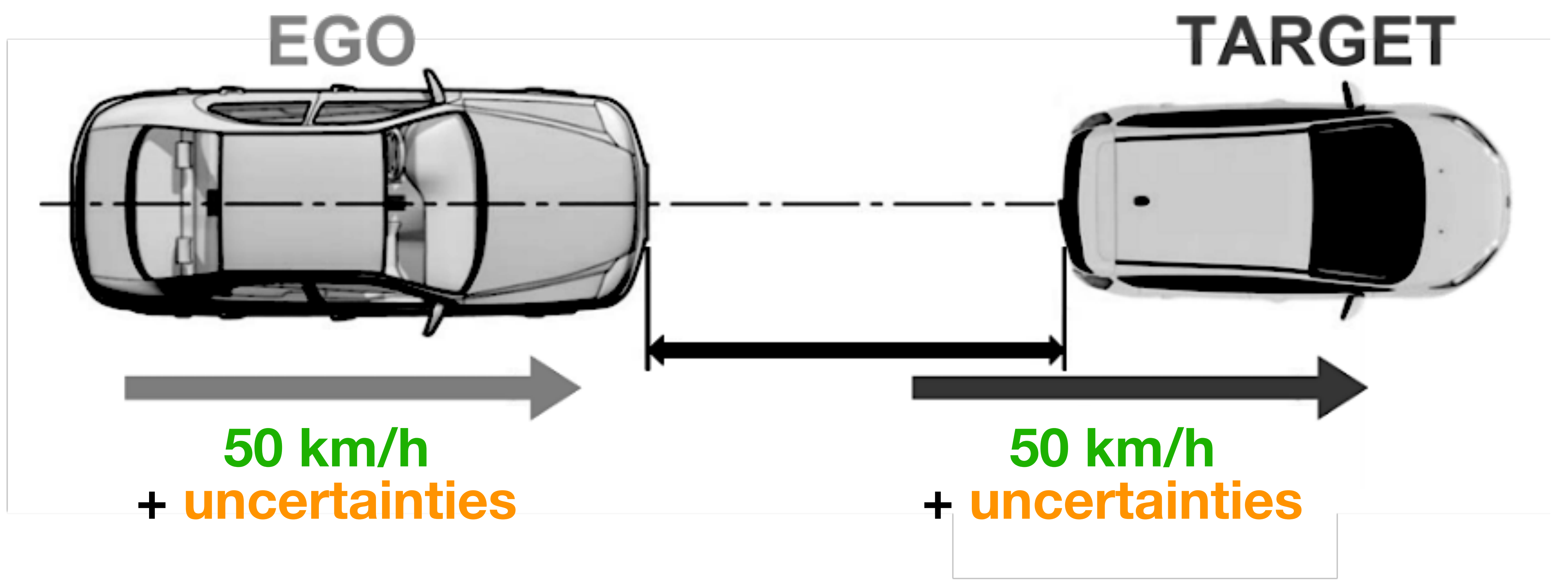

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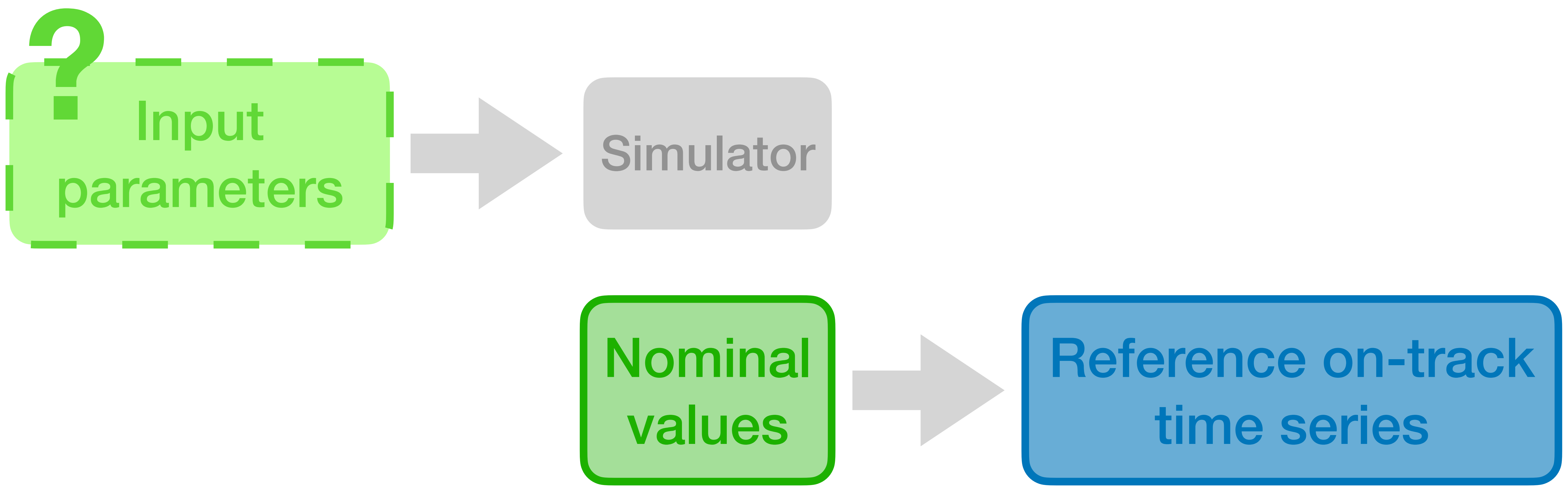

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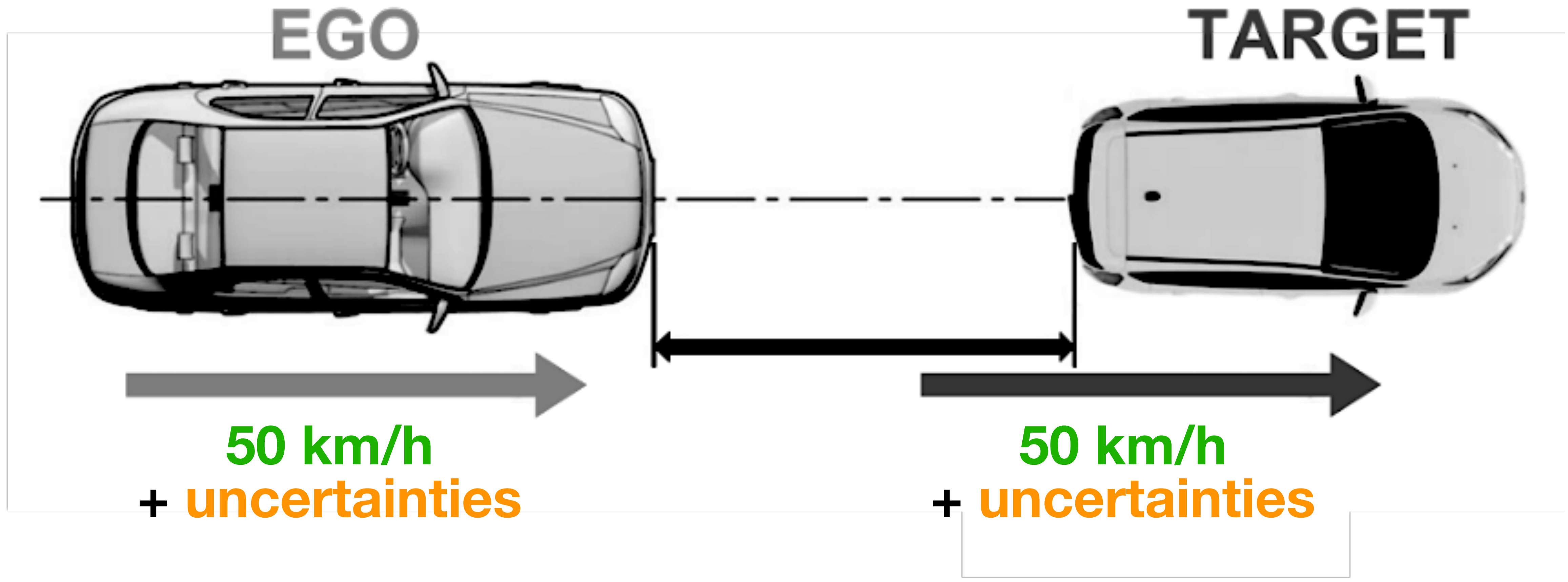

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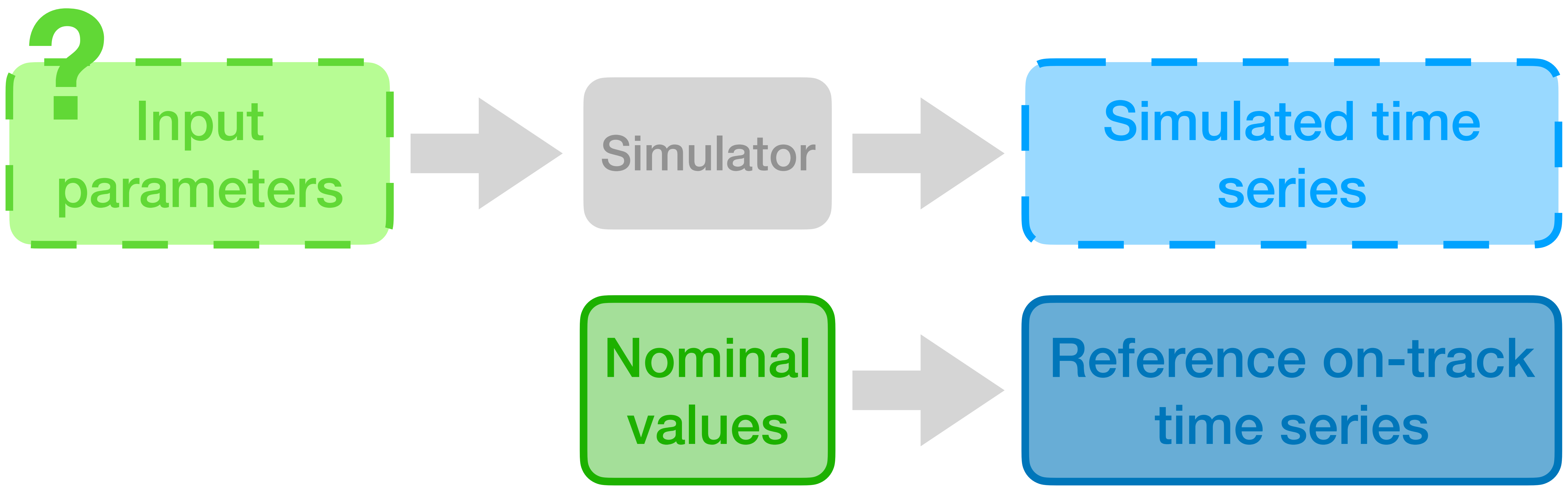

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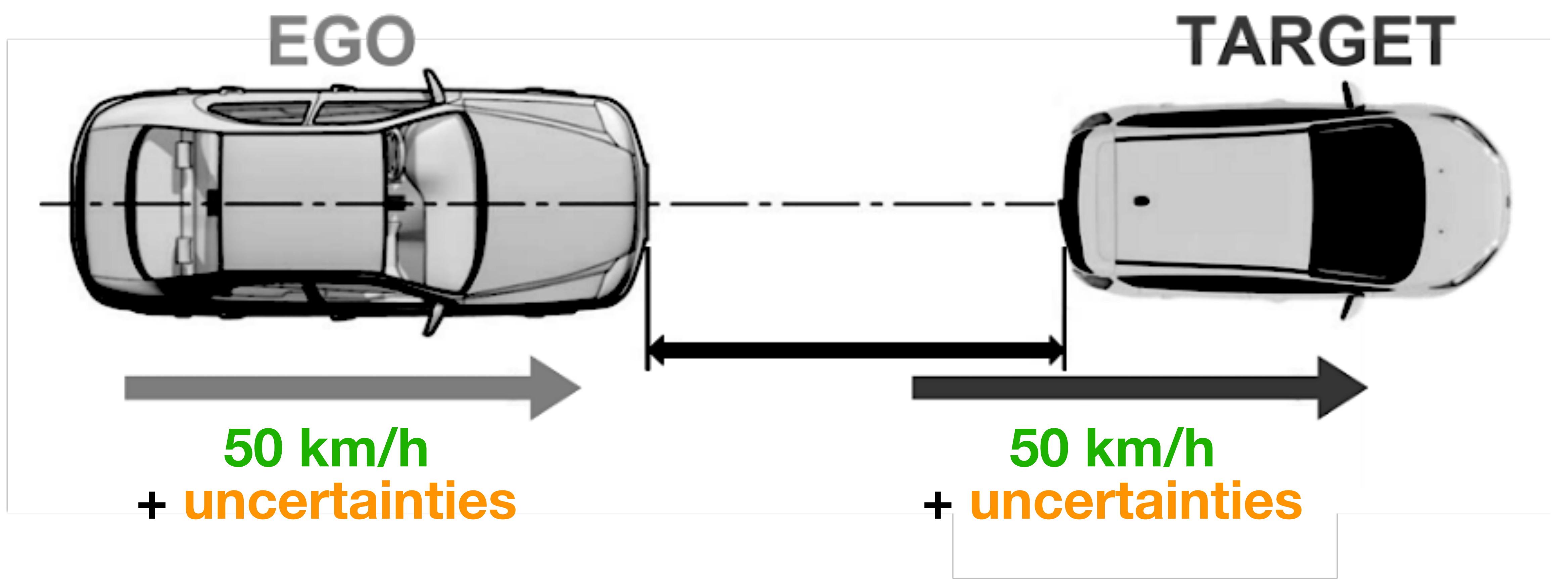

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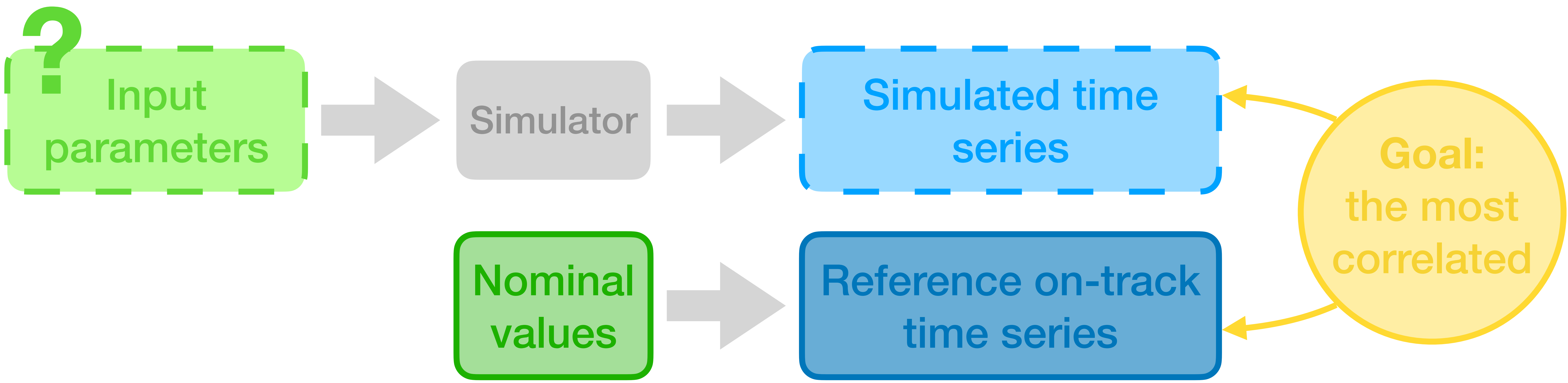
- **To calibrate the simulator:** by testing values around nominal values determine which **input parameters** provide the **simulated time series** the **most correlated** to real on-track ones



General introduction

Global objective of the thesis

Input values
θ

Model
$y = S(\theta) + \varepsilon$

Output values
y

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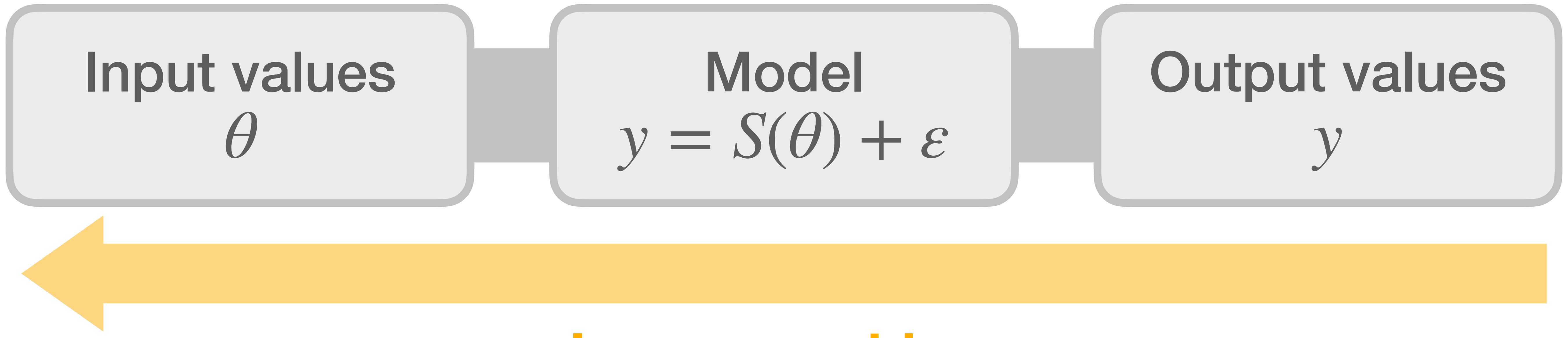
Inverse problem

Infer $\widehat{\theta}$ such that $y = S(\widehat{\theta})$

General introduction

Global objective of the thesis



Inverse problem

Infer $\hat{\theta}$ such that $y = S(\hat{\theta})$

Solve the following inverse problem

- For a reference on-track time series, recover the input parameters that simulate the closest time series

$$\underset{\theta \in \Theta}{\arg\min}\; d\big(S(\theta) + \varepsilon, y_\varphi\big)$$

Θ *: the parameter space to explore ;* d *: a distance ;* S *: the simulator ;* y_φ *: the on-track reference time series*

2. Solving the inverse problem

Solving the inverse problem

Introduction

Bayesian approach

- Estimate the posterior distribution given by Bayes' theorem

$$\pi(\theta \,|\, Y = y_\varphi) \propto p(Y = y_\varphi \,|\, \theta)\, \pi_0(\theta)$$

$\pi_0(\theta)$: *prior distribution* ; $p(Y = y_\varphi \,|\, \theta)$: *likelihood*

Solving the inverse problem

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When computing the likelihood function is impractical or intractable

- Use *likelihood-free* methods to generate a sample $\theta_1, \ldots, \theta_n$ of the posterior and then approximate it

$$\pi(\theta \,|\, y_\varphi) \approx \frac{1}{n} \sum_{i=1}^{n} \delta_{\theta_i}(\theta)$$

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How do you generate such a sample?

Solving the inverse problem

Approximate Bayesian computation (ABC)

Generic rejection sampler

Initialization:

- Draw the first particles according to the prior $\theta_1^{(0)}, \dots, \theta_n^{(0)} \sim \pi_0$

Iterations:

1: **for** $k = 0, \dots, K$ **do**

2: Generate the associated time series $y_i^{(k)} = S\big(\theta_i^{(k)}\big) \quad \forall i = 1, \dots, n$

3: Determine accepted particles $A_k = \{i : d(y_i^{(k)}, y_\varphi) \leq h_k\} \subseteq \{1, \dots, n\}$

4: **Update step:**

8: Generate the new particles with a *rejection sampling* method

$$\theta_1^{(k+1)}, \dots, \theta_n^{(k+1)} \sim \pi_0$$

Solving the inverse problem

Approximate Bayesian computation (ABC)

Weighted rejection sampler

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4: **Update step:**

6: Compute the weights $\omega_i^{(k)} = \exp\big(-d(y_i^{(k)}, y_\varphi)/h_k\big) \quad \forall i \in A_k$

8: Generate the new particles with a *rejection sampling* method

$$\theta_1^{(k+1)}, \dots, \theta_n^{(k+1)} \sim \pi_0$$

1) Assign importance weight to accepted particles

$$\exp\Big(-\frac{1}{h} d\big(S(\theta), y_\varphi\big)\Big)$$

Solving the inverse problem

Approximate Bayesian computation (ABC)

Sequential Monte Carlo sampler with weighted particles

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7: Construct the next distribution with a weighted KDE

$$\pi_{k+1}(\theta) = \frac{1}{|A_k|} \sum_{i \in A_k} \omega_i^{(k)} G_\rho\left(\theta - \theta_i^{(k)}\right)$$

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1) Assign importance weight to accepted particles

$$\exp\Big(-\frac{1}{h} d\big(S(\theta), y_\varphi\big)\Big)$$

2) Construct a sequence of slowly changing intermediary distibutions $\pi_1, \dots, \pi_{K-1}$ which bridge between the prior and the posterior

Solving the inverse problem

Approximate Bayesian computation (ABC)

Sequential Monte Carlo sampler with weighted particles and decreasing tolerance

Initialization:

- Initiate the changing tolerance $h_0 = h$
- Draw the first particles according to the prior $\theta_1^{(0)}, \ldots, \theta_n^{(0)} \sim \pi_0$

Iterations:

1: **for** $k = 0, \ldots, K$ **do**

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4: **Update step:**

5: Compute the new tolerance $h_{k+1} = h_0(k+1)^{-1/\gamma}$

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3) Monotonically decrease tolerance parameter

$$h_k = k^{-1/\gamma} h_0$$

Solving the inverse problem

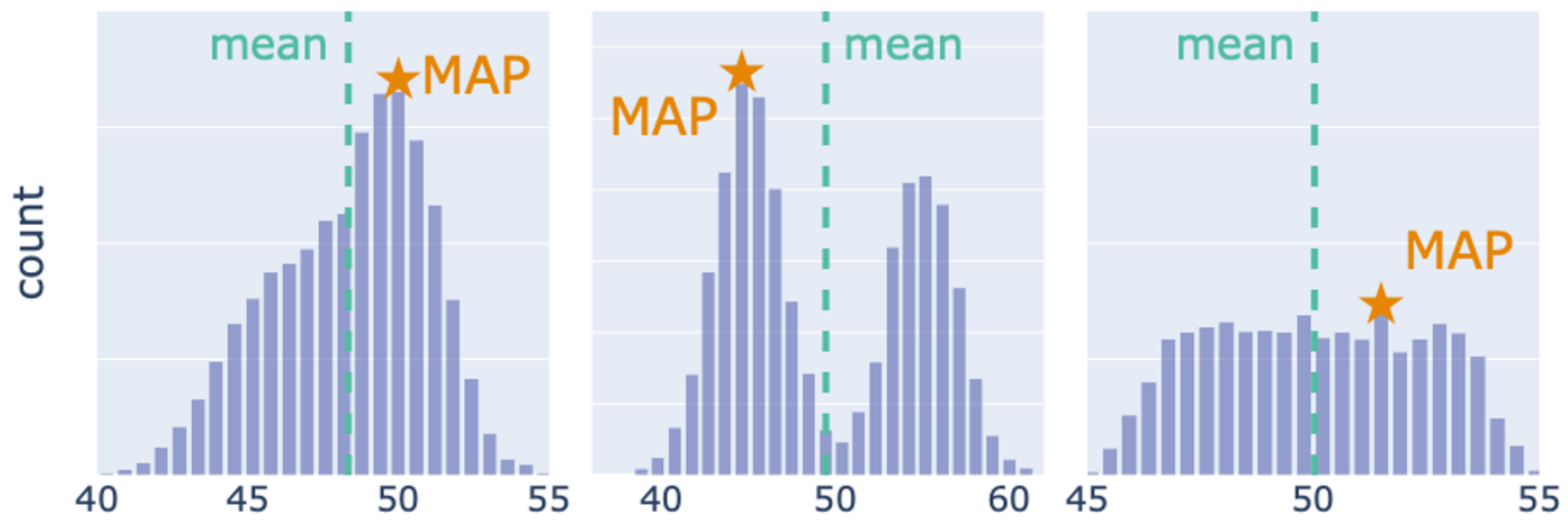
Constructing and evaluating estimators

How to transform posterior distribution into a point value estimation?

Solving the inverse problem

Constructing and evaluating estimators

How to transform posterior distribution into a point value estimation?



A single point value estimation

1) Weighted mean
2) Coordinate-wise maximum a posteriori

- Maximum a posteriori criterion

$$\hat{\theta}_{\text{MAP}} \in \underset{\theta \in \Theta}{\arg\max}\ \pi(\theta \mid Y = y_\varphi)$$

Solving the inverse problem

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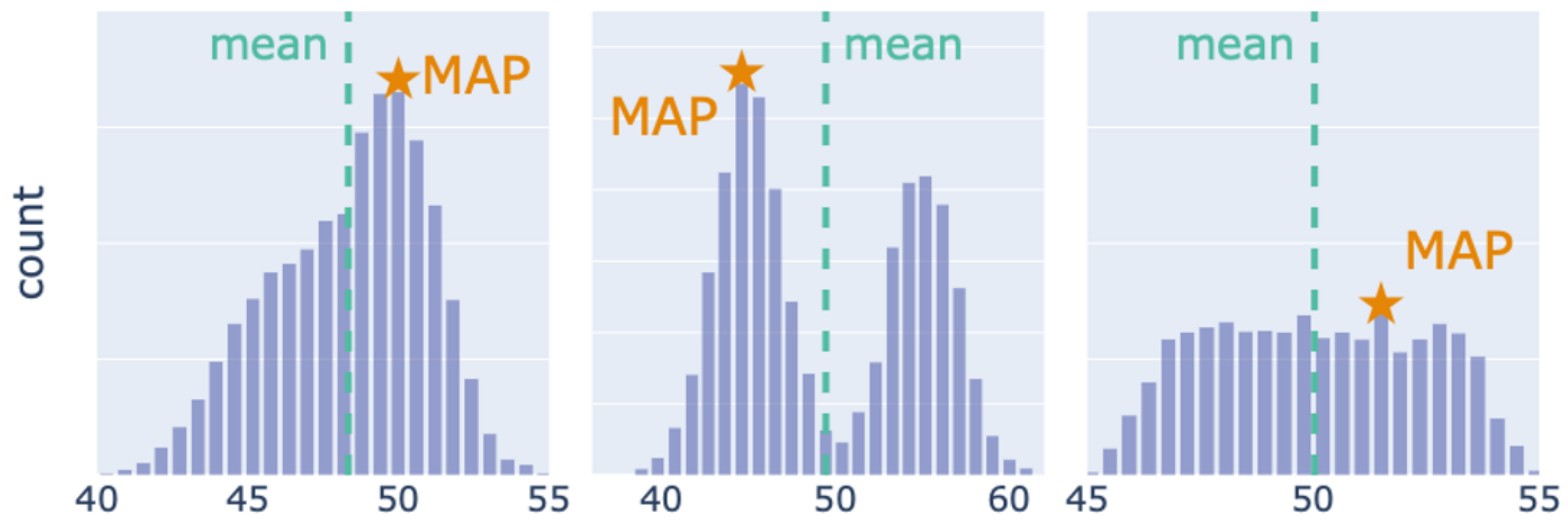

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How to evaluate the quality of the obtained results?

Simulator

y_φ

Solving the inverse problem

Constructing and evaluating estimators

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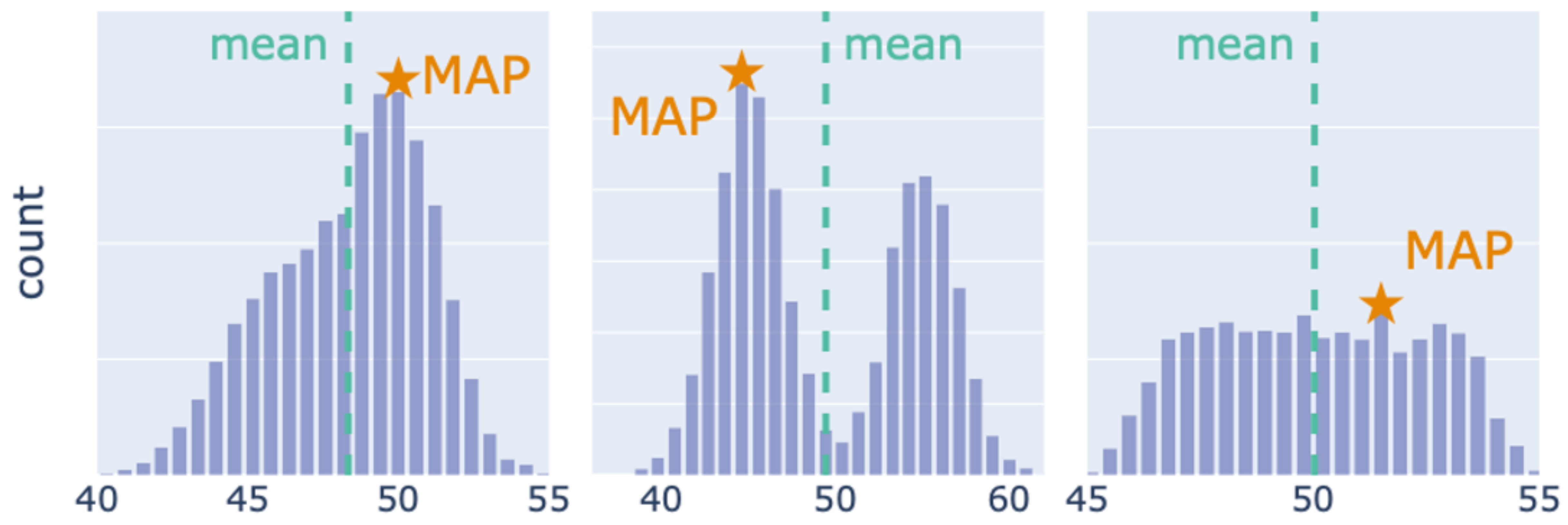

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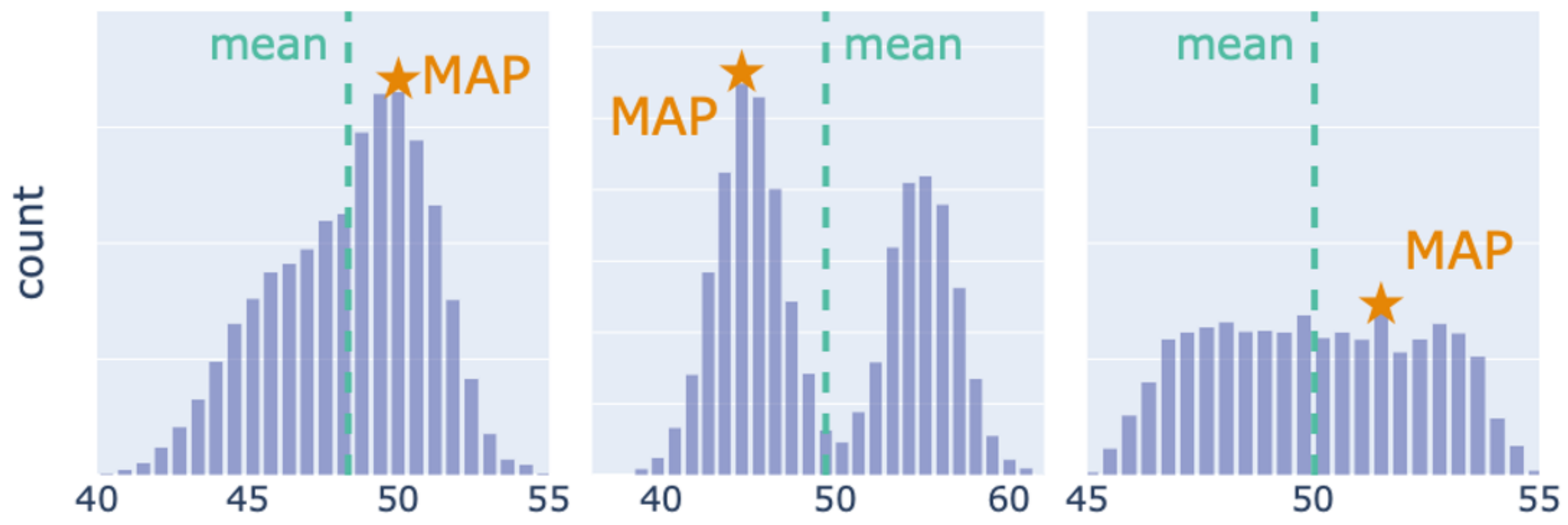

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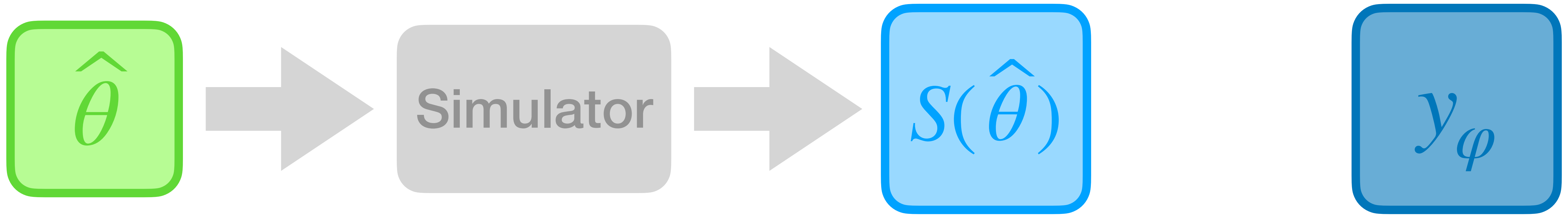

Solving the inverse problem

Constructing and evaluating estimators

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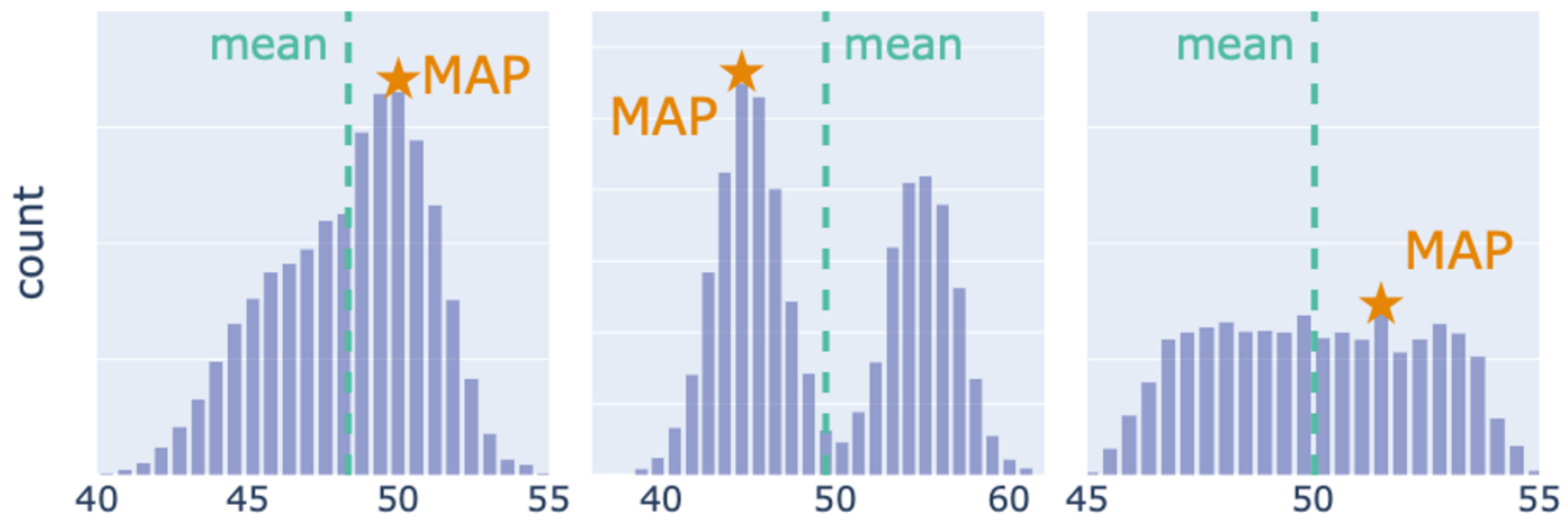

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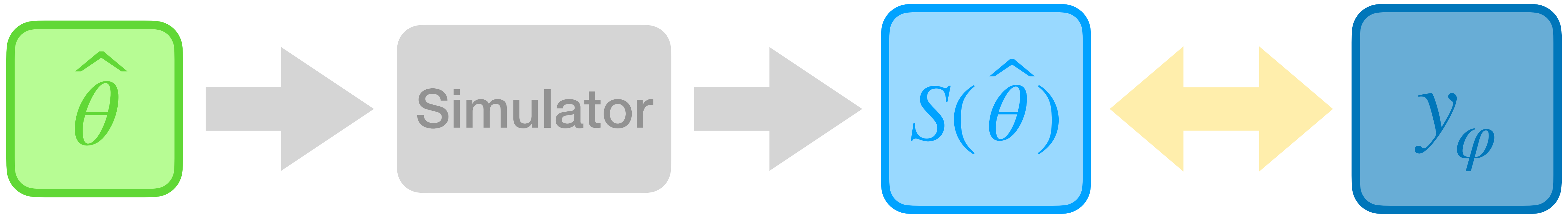

Solving the inverse problem

Conclusion

	generic rejection	SMC	SMC
option	mean	mean	MAP
s-RMSE	0.1787	0.1673	**0.1628**
time	9 min	2 min	2.5 min

Conclusion

- Our SMC sampler performs better
- Computing the MAP provides a better result
- Reasonable computation times

Solving the inverse problem

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Solving the inverse problem

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Model

$$y = S(\theta) + \varepsilon$$

Other possibilities

- Optimization techniques with *gradient-free* methods
- Depending on the nature of the noise ε : Bayesian synthetic likelihood (BSL)

Solving the inverse problem

A new problematic

Input values θ → Model $y = S(\theta) + \varepsilon$ → Output values y

One difficulty araises

- *Likelihood-free* methods require the generation of numerous outputs y
- The simulator is computationally too expensive

Solving the inverse problem

A new problematic

Input values	Model	Output values
θ	$y = S(\theta) + \varepsilon$	y

One difficulty araises

- *Likelihood-free* methods require the generation of numerous outputs y
- The simulator is computationally too expensive

For example

- We generated 2000 outputs to obtain the previous result with SMC sampler

	1 output	**2000 outputs** *
time	5 minutes	7 days

* *stop and restard the simulator at each step*

Solving the inverse problem

A new problematic

Forward problem

Predict $\widehat{y} = \widehat{S}(\theta)$

Input values θ → Model $y = S(\theta) + \varepsilon$ → Output values y

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For example

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- We need to train a surrogate model $\widehat{S}$ which mimics the simulator S
- Predicts y for a given θ using $\widehat{y} = \widehat{S}(\theta)$

* *stop and restard the simulator at each step*

3. Construction of the surrogate model

Construction of the surrogate model

Introduction

Objectives

- Construct a surrogate model $\widehat{S}$ which mimics the simulator S
- For a given set of parameters θ, predict simulated time series y by $\widehat{y} = \widehat{S}(\theta)$
- Accurately replicates the simulator's behavior while maintaining reasonable calculation times

Construction of the surrogate model

Introduction

Objectives

- Construct a surrogate model $\widehat{S}$ which mimics the simulator S
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- In traditionnal time series forecasting, the objective is to predict the future from the past
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What to do

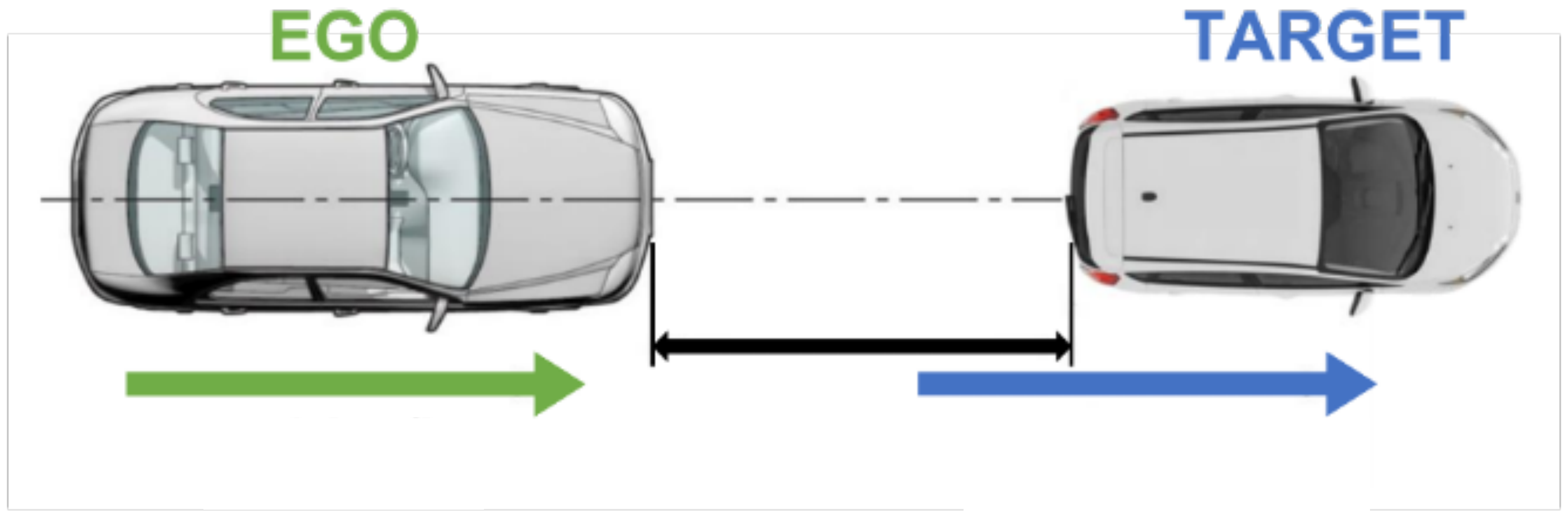
- Construct a dataset to build the model: beforehand simulated scenarios output by the simulator
- Choosing the right input parameter spaces

Construction of the surrogate model

Data description

Considered scenario

- Two vehicles in motion, the **target** vehicle is in front and the **ego** vehicle behind
- We test the automatic emergency braking of the ego vehicle following sudden braking by the target vehicle



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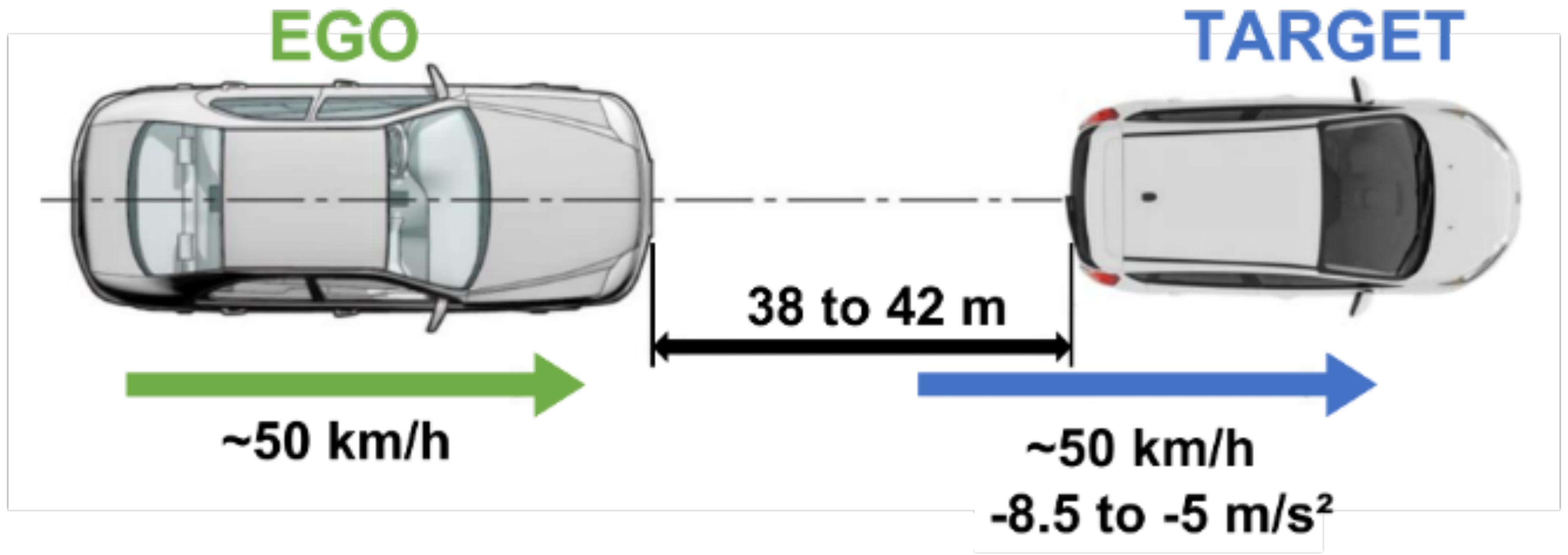

Input parameters: a total of 8 values

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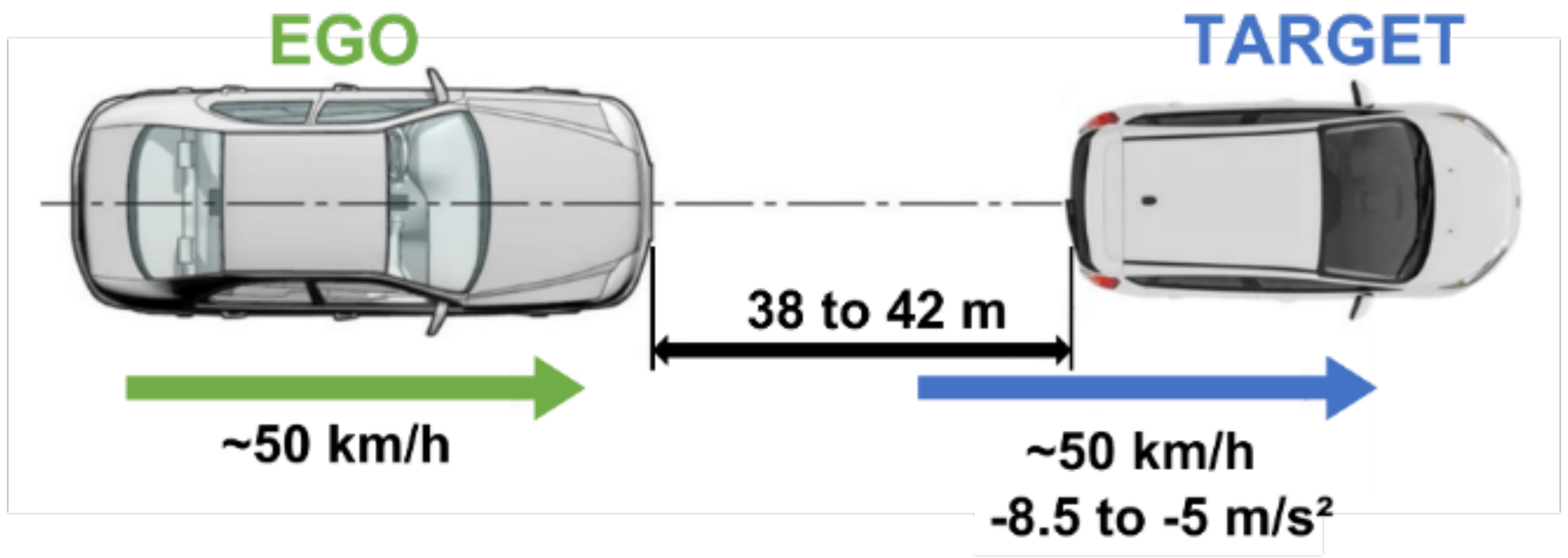
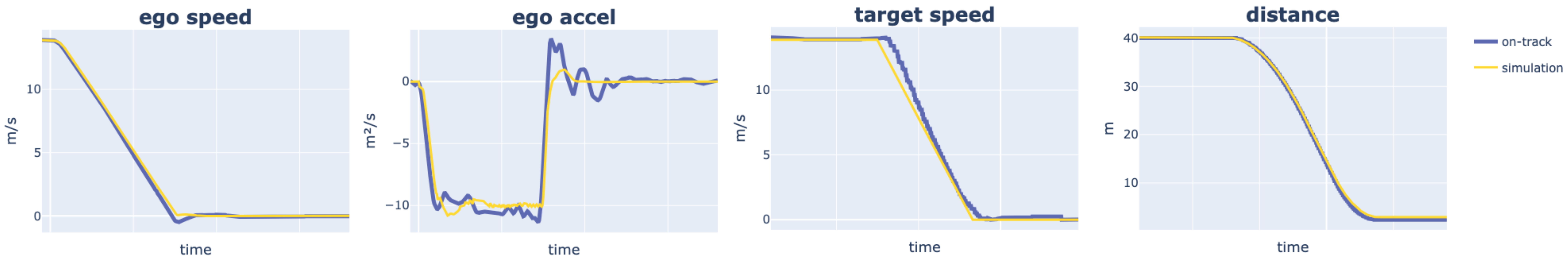


Input parameters: a total of 8 values

Output time series: 4 distinct types of time series, each one has a different number of time steps



Construction of the surrogate model

Expert aggregation model

To deal with time series, we consider expert aggregation

- We have M experts noted $(f_m)_{m=1,\ldots,M}$
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- At each time step t, a weight vector ω_t is constructed to predict

$$\hat{y}_t = \sum_{m=1}^{M} \omega_{m,t} f_{m,t}(\theta)$$

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Aggregated model

- Exponentially weighted aggregation (EWA) is used to compute weight vectors sequentially

$$\omega_{m,t} = \frac{\exp(-\eta L_{m,t-1}(\theta))}{\sum_j \exp(-\eta L_{j,t-1}(\theta))} \qquad \text{where} \qquad L_{m,T}(\theta) := \sum_{t=1}^{T} \ell(f_{m,t}(\theta), y_t)$$

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Hybrid model

- Select a single method per time step
- Only one value of the weight vector is equal to 1, and the rest is equal to 0

Construction of the surrogate model

Choice of experts

Classical machine learning

Construction of the surrogate model

Choice of experts

Classical machine learning

- k-nearest neighbors (k-NN)
  - One of the most fundamental and straightforward algorithm
  - 2 parameters: k and the norm $||.||$ to mesure distances between points

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  - 2 main parameters: λ the regularization strength and the kernel mapping used

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Dimensionality reduction

- Principal component analysis (PCA)
  - Classical: decomposes the covariance matrix into its eigenvalues
  - Functional: eigenfunctions instead of eigenvalues
  - Sparse: introduces sparsity structures to the variables

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Neural networks

- Convolutionnal neural network (CNN)
  - Effective with image data
  - Spatial feature extraction capabilities are used to adapt visual analysis assets to the analysis of temporal data

Construction of the surrogate model

Construction of hybrid and aggregated models

Scaled RMSE $(\times 10^{-2})$ between true and predicted values

	Ego speed (m/s)	Ego accel (m/s^2)	Target speed (m/s)	Distance (m)
k-NN	11.00	64.77	8.02	36.83
1-RF	1.36	9.54	4.86	13.31
4-RF	**0.12**	**1.47**	2.34	10.84
KRR	2.20	7.14	1.63	17.86
PCA-RF	2.33	20.53	5.58	20.96
CNN	0.18	3.85	**1.06**	**4.16**

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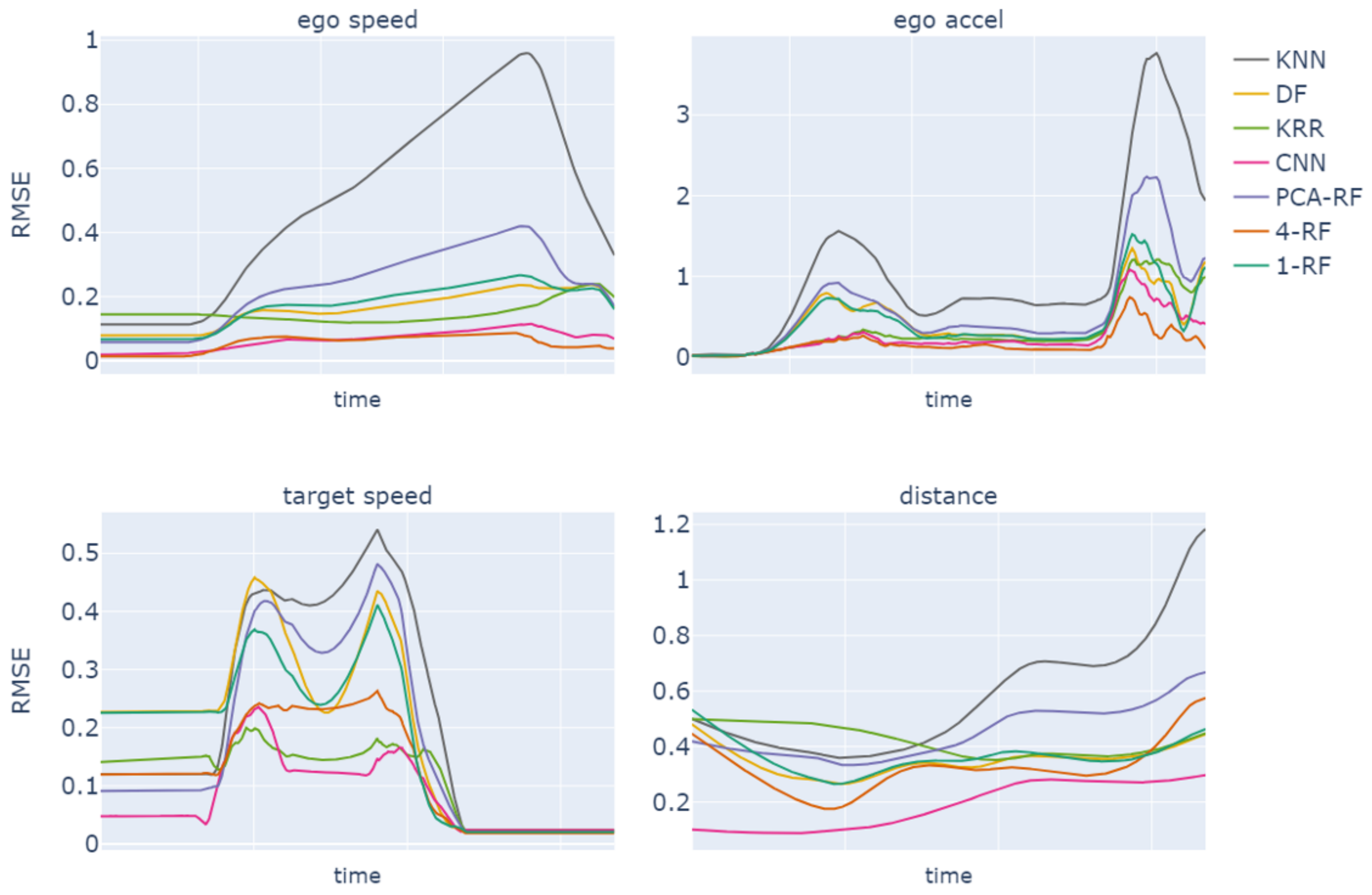

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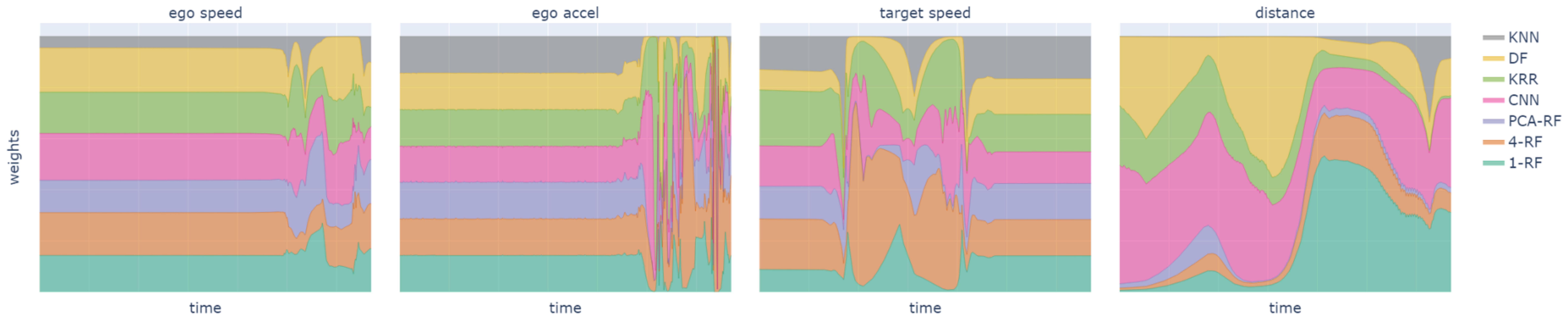
Construction of hybrid and aggregated models

Weight vectors for the aggregated model (EWA algorithm)



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Two hybrid models

Construction of the surrogate model

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Two hybrid models

- Hybrid 1: select best method for each time step

Hybrid 1

Construction of the surrogate model

Construction of hybrid and aggregated models

Two hybrid models

- Hybrid 1: select best method for each time step
- Hybrid 2: select best method for each time step among the three best ones

Construction of the surrogate model

Results of hybrid and aggregated models

Validation set: used to compute weights

	Ego speed	Ego accel	Target speed	Distance	mean
CNN	0.18	3.85	1.06	4.16	2.31
hybrid 1	0.11	1.46	0.93	4.16	1.66
hybrid 2	0.11	1.46	1.04	4.16	1.69
aggregated	**0.07**	**0.59**	**0.24**	**1.36**	**0.56**

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Test set: unknown data

	Ego speed	Ego accel	Target speed	Distance	mean
CNN	0.23	3.34	1.00	2.52	1.77
hybrid 1	0.12	1.35	1.12	2.52	1.28
hybrid 2	0.12	1.35	**1.00**	2.52	**1.25**
aggregated	0.64	3.81	1.35	4.97	2.69

Construction of the surrogate model

Results of hybrid and aggregated models

Calculation times

	CNN	hybrid 1 (+)	hybrid 2 (+)	aggregated (+)	simulation
training time	59 min	0.29 sec	0.18 sec	2 min 13	
100 outputs	1.39 sec	10.25 sec	8.59 sec	2 min 17	
2000 outputs	30 seconds	3.5 minutes	3 minutes	46 minutes	7 days *

(+) *add the prediction times for each method*

***** *stop and restard the simulator at each step*

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- Aggregated model is disapointing because of its poor generalization to unknown data
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Goal: define a framework that incorporates this functional setting to ensure algorithm convergence

4. Theoretical guarantees for functional expert aggregation

Theoretical guarantees for functional expert aggregation

Introduction

Expert aggregation

- We have M experts noted $(f_m)_{m=1,\ldots,M}$
- For a given input parameter θ, each one provides a prediction $f_{m,t}(\theta)$ for each time step t
- Construct a temporal weight vector ω_t to predict y_t by

$$\widehat{y}_t = \sum_{m=1}^{M} \omega_{m,t} f_{m,t}(\theta) \quad \text{with} \quad \sum_{t=1}^{T} \ell\left(f_{m,t}(\theta), y_t\right)$$

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- Need to generate the entire time series from a non-temporal input parameter
- Discretization is numerically necessary but should not be included in the theoritical analysis

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Theoretical analysis

- Need to generate the entire time series from a non-temporal input parameter
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Solution

- Consider time series and experts' weights as continuous functions in time

Theoretical guarantees for functional expert aggregation

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- Define a new framework to generalize expert aggregation to a functional setting with specific
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It will permit to use existing optimization tools and guarantee convergence rates of algorithms despite this pseudo-linearity

Theoretical guarantees for functional expert aggregation

Optimization setting

Solve the following optimization problem

$$\operatorname*{arg\,min}_{w \in \mathscr{C}} \left\{ \mathscr{R}(w) \right\} \quad \text{where} \quad \mathscr{R}(w) = \mathbb{E}[\nabla \ell(w)] = \mathbb{E} \int_0^1 \left(\hat{y}(t) - y_\varphi(t) \right)^2 \mathrm{d}t$$

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The stochastic projected gradient descent (PGD) algorithm

- The k-th iteration is given by

$$W_{k+1} = \Pi_{\mathscr{C}}\left(W_k - \eta g_k\right)$$

  - g_k is an unbiased estimator of $\nabla \mathscr{R}(W_k)$
  - $\Pi_{\mathscr{C}}$ is the standard orthogonal projection operator on $\mathscr{C}$

Stochastic case: we only have access to $\nabla \ell(w)$ for all w

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Specific framework

+

Needed conditions

1. *Hilbert space to permit convex optimization techniques*
2. *A closed set of contraints*
3. *A μ-strongly convex and ν-smooth loss function*

Theoretical guarantees for functional expert aggregation

Main results with the stochastic PGD algorithm

Proposition 3.5. *Let* $\Pi_{\mathcal{C}}$ *be the orthogonal projection on* $\mathcal{C}$ *and let us assume that*

(i) $\mathbb{E}[g_k]$ *is a subgradient of* $\mathcal{R}$ *at* W_k*,*

(ii) $\mathbb{E}[\|g_k\|^2] \leq B^2$ *for some* $B > 0$*.*

Then, for all $k \geq 1$*,*

$$\mathbb{E}\|W_k - W^*\|^2_{\mathcal{H}} \leq \frac{4B^2}{\mu^2(k+1)}\,.$$

Theoretical guarantees for functional expert aggregation

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Guarantees can be demonstrated

- In deterministic case
- With mirror gradient descent algorithm

5. General conclusion

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Solving the inverse problem

- The sequential Monte Carlo sampler we created specifically for our problem returns very good results, with a clear improvement in the correlation between simulation and reality

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Surrogate model

- We have proposed various solutions to solve our forward problem
- Among traditional methods, the best method is convolutional neural networks
- We improved the results by making the approach more complex through the use of hybrid models
- We offer a wide choice of models and each one can decide to focus on either quality or speed

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Theoretical guarantees for functional expert aggregation

- We have developed a framework to generalize expert aggregation to weights and functional experts
- It allows the use of classical optimization algorithms (PGD) while maintaining the same convergence rates in deterministic and stochastic cases
- The application of the mirrror gradient descent and the corresponding proofs are still in progress
- Numerical experiments will be carried out to test the model's performance

Thank you

Appendix

A - Loss function study

- To solve forward or inverse problems, we need to compare time series

What does « two similar time series » means ?

A - Loss function study

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What does « two similar time series » means ?

- We need to provide a quantification method adapted to our problem

A - Loss function study

- To solve forward or inverse problems, we need to compare time series

What does « two similar time series » means ?

- We need to provide a quantification method adapted to our problem

There are many possibilities, including

RMSE	**MAE**	**Scaled RMSE**	**Derivative**
$\left(\frac{1}{T}\sum_{t=1}^{T}(y_t - z_t)^2\right)^{1/2}$	$\frac{1}{T}\sum_{t=1}^{T}\lvert y_t - z_t\rvert$	RMSE$(\widetilde{y}, \widetilde{z})$ where $\widetilde{y}$ denotes the scaled vector	$\ell(y, z) + \ell(y', z')$ where y' stands for the discrete derivative
DTW and soft-DTW	**Cross-correlation**	**DILATE**	**Mean, variance, kurtosis and skewness**
$\min_{A \in \mathscr{A}_{T,T}} \langle A, \Delta(y, z)\rangle$ $\min^{\gamma}_{A \in \mathscr{A}_{T,T}} \langle A, \Delta(y, z)\rangle$	$\frac{1}{2T-1}\sum_{k=0}^{2T-2}\sum_{i=0}^{T-1} y_i\, z_{i-k+T-1}$	$\alpha\, \ell_{\text{shape}}(y, z)$ $+(1-\alpha)\, \ell_{\text{temporal}}(y, z)$	$\Big((\mu_y - \mu_z)^2 + (\sigma_y^2 - \sigma_z^2)^2$ $+(k_y - k_z)^2 + (s_y - s_z)^2\Big)^{1/2}$

A - Loss function study

How do we decide which is best?

- For each loss ℓ, among $y_1, \ldots, y_n$, we will determine the best y_i such that
$$\underset{y_i,\ i=1,\ldots,n}{\text{arg min}}\ \ell(y_i, y_\varphi)$$
- We look at the eight selected scenarios and compare them

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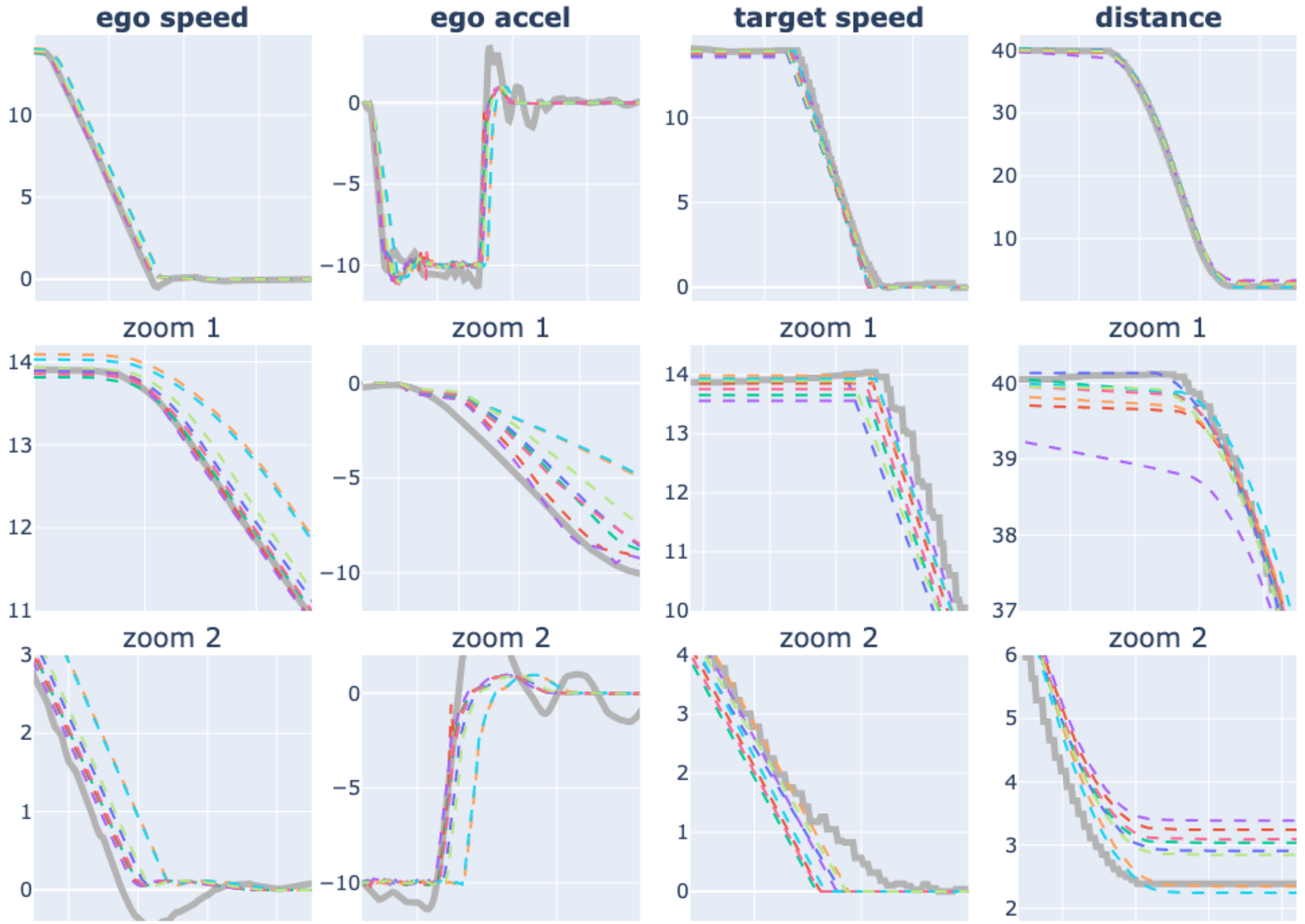

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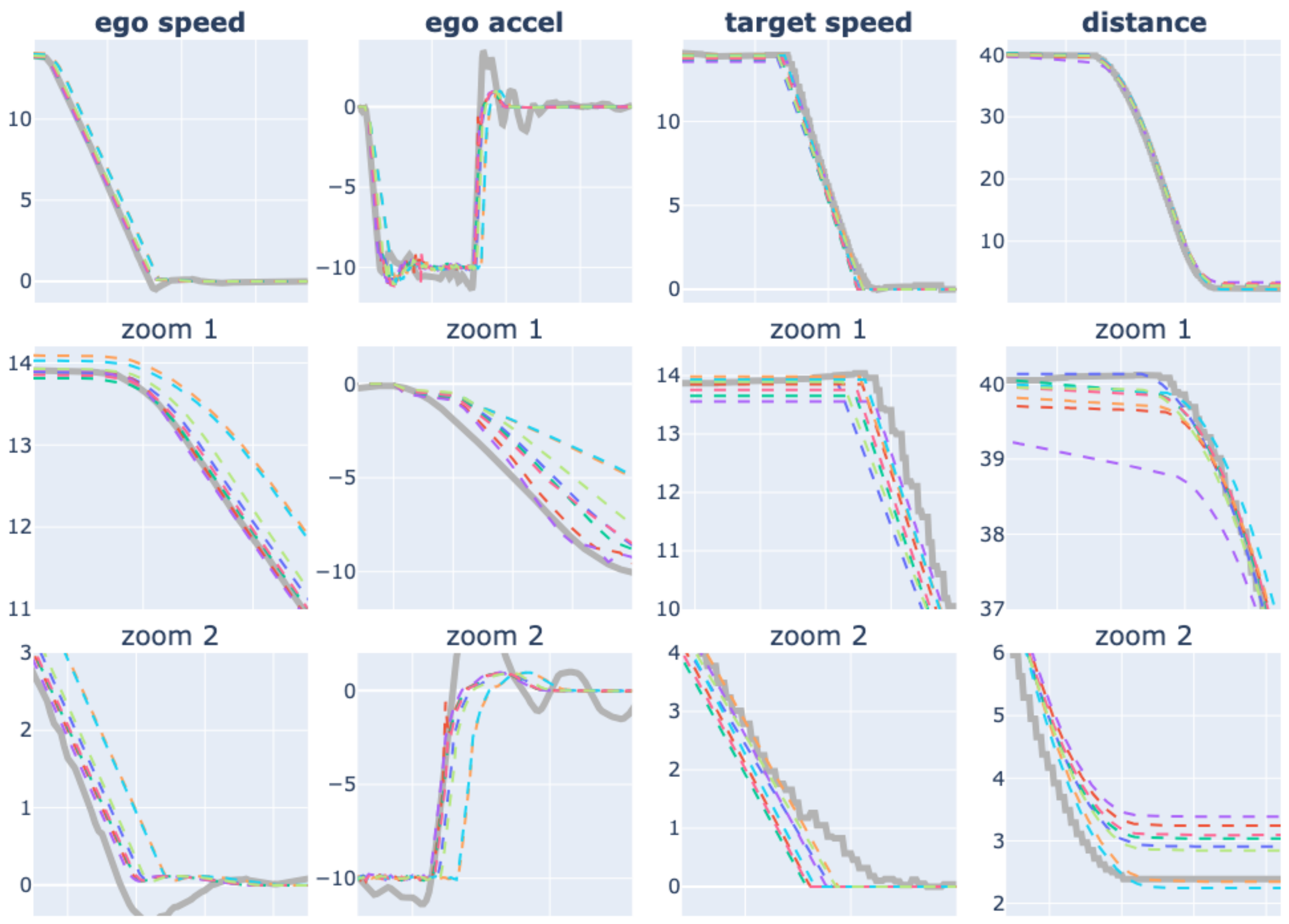
Overall best choice: scaled RMSE

- By pre-processing the time series to give each one the same weight
- Each one has the same importance in decision making



B - Solving the inverse problem

Mathematical description

Two hypotheses about the nature of the statistical model noise

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Mathematical description

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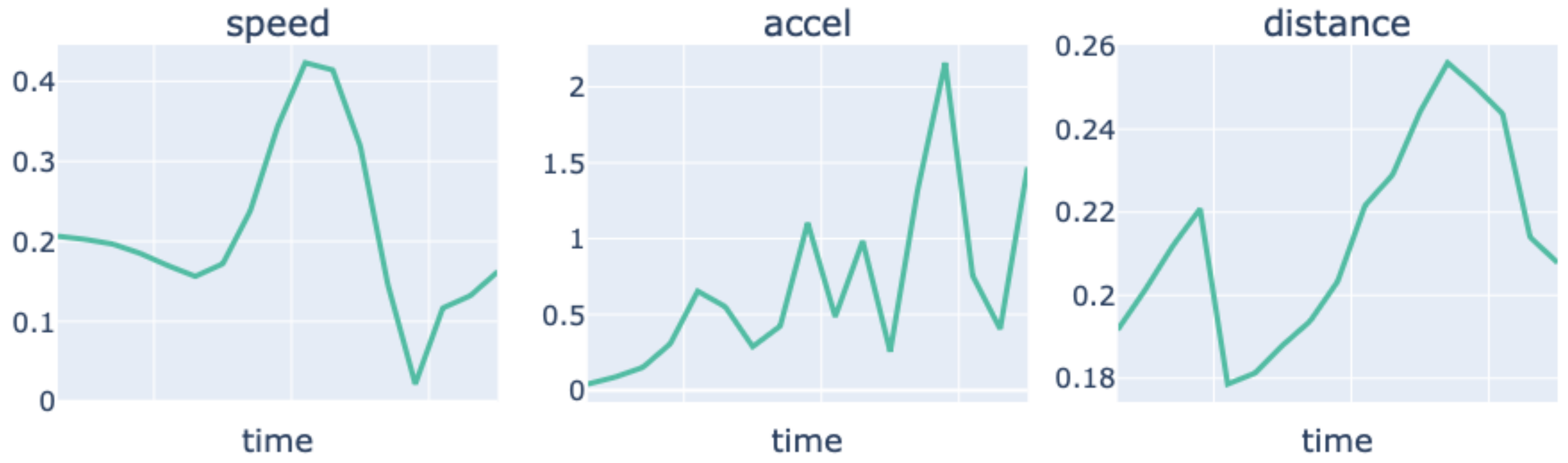
1) Gaussian noise assumption



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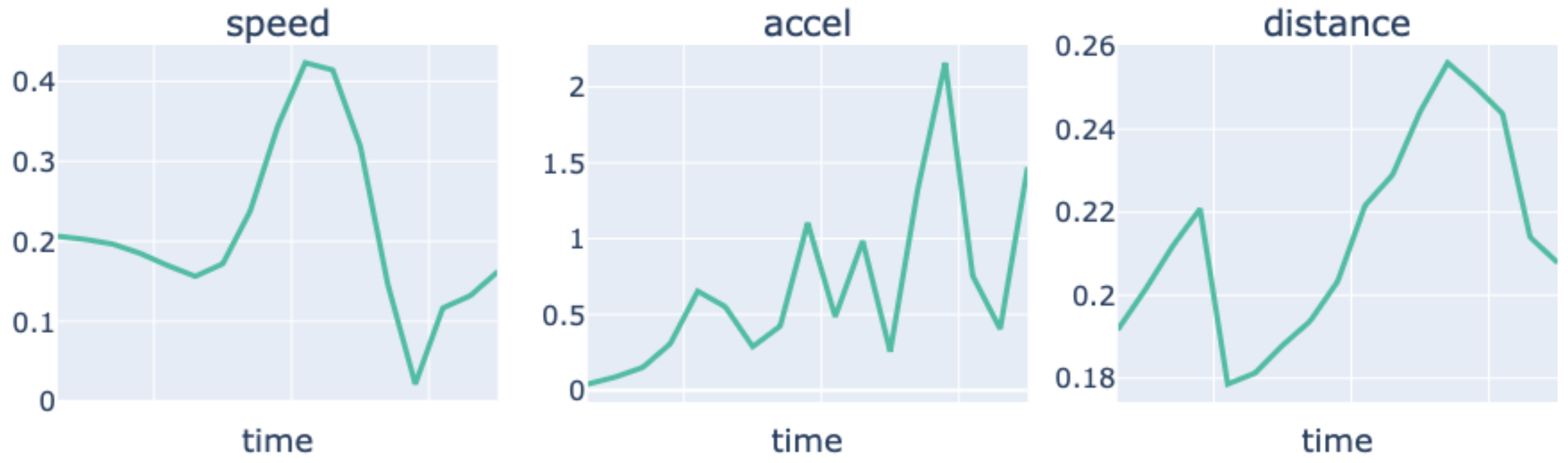
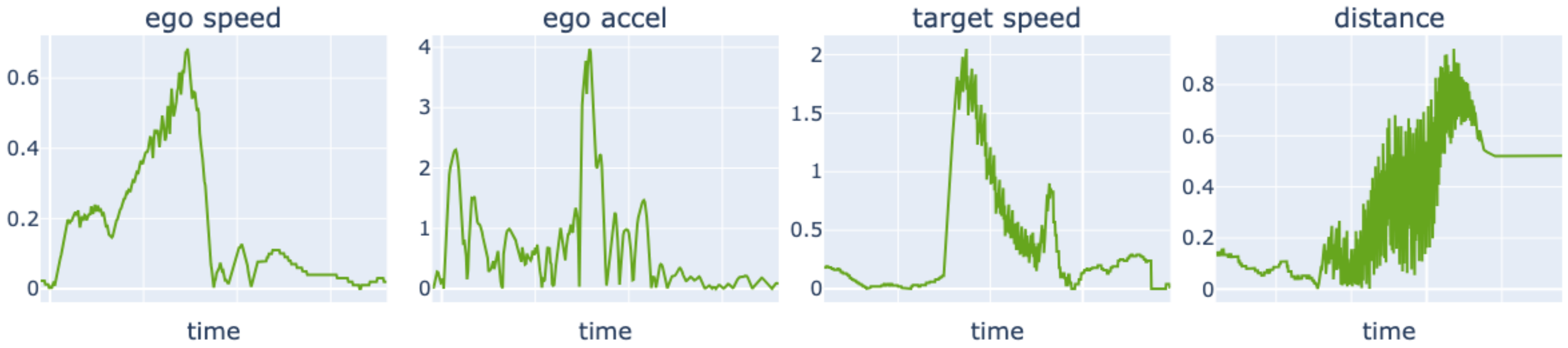


2) Assumption free



B - Solving the inverse problem

Mathematical description

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Let assume that the noise follows a Gaussian distribution

$$\varepsilon \sim \mathcal{N}(0,\Sigma)$$

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(a) If $\Sigma = \sigma^2 I_d$, then computing the maximum likelihood estimator is the ordinary least-squares estimator

$$\hat{\theta}_{\text{MLE}} = \text{arg min}_{\theta \in \Theta} \left\{ \sum_{i=1}^{n} \|Y_i - S(\theta)\|_{2,T}^2 \right\} = \text{arg min}_{\theta \in \Theta} \left\{ \sum_{i=1}^{n} \text{MSE}\big(Y_i, S(\theta)\big) \right\}$$

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B - Solving the inverse problem

Bayesian approaches - *Bayesian synthetic likelihood (BSL)*

$$\pi(\theta \,|\, y_\varphi) \propto p(y_\varphi \,|\, \theta)\pi_0(\theta)$$

- Likelihood distribution $p(y_\varphi \,|\, \theta)$ is assumed to be Gaussian $\mathcal{N}\left(y_\varphi; S(\theta), \Sigma\right)$

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$$S_n = \frac{1}{n}\sum_{i=1}^{n} y_i \qquad \text{and} \qquad \Sigma_n = \frac{1}{n-1}\sum_{i=1}^{n}(y_i - S_n)(y_i - S_n)^\mathsf{T}$$

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$$\pi_{\mathsf{BSL},n}(\theta \mid y_\varphi) \propto p_n(y_\varphi \mid \theta)\pi_0(\theta)$$

$$\text{where } p_n(y_\varphi \mid \theta) = \int \mathcal{N}(y_\varphi; S_n, \Sigma_n)\prod_{i=1}^{n} p(y_i \mid \theta)\,\mathrm{d}y_{1:n}$$

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- **Algorithm used:** waste-free sequential Monte Carlo sampler with a tempering version

B - Solving the inverse problem

Constructing and evaluating estimators

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How to evaluate the quality of the obtained results?

- Let $\hat{\theta}$ be the point value estimation obtained at the end and d being the s-RMSE
- Look at the time series generated from $\hat{\theta}$ with the surrogate model and the simulator by computing

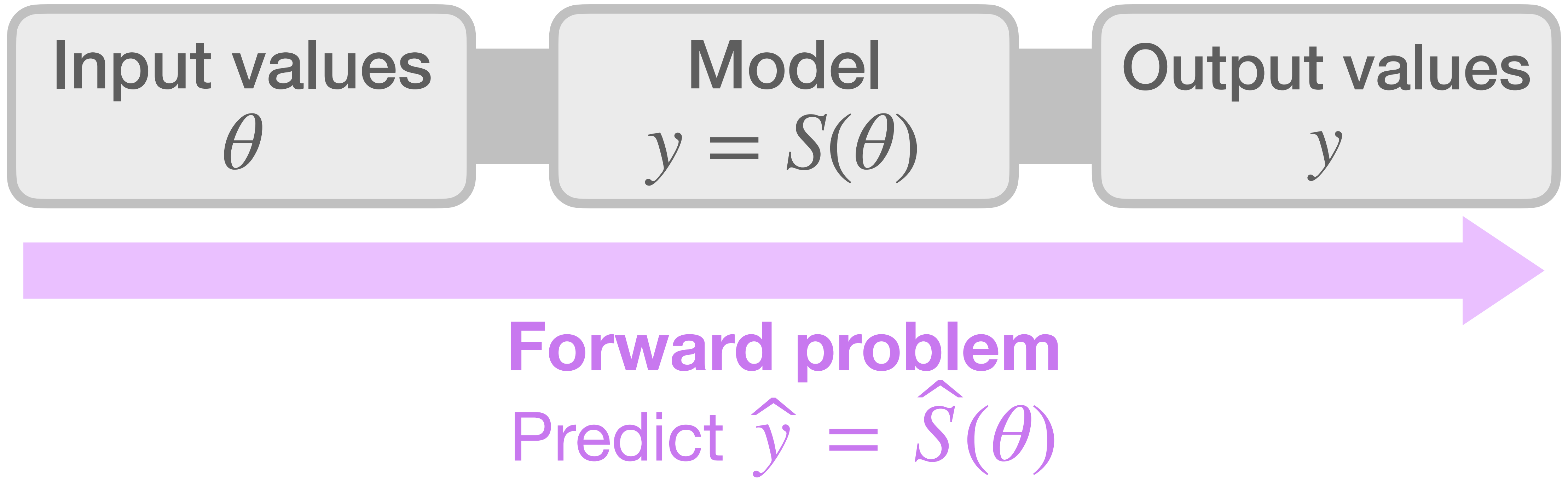
$$d\left(\hat{S}(\hat{\theta}), y_\varphi\right) \quad \text{and} \quad d\left(S(\hat{\theta}), y_\varphi\right)$$

- To better understand why some estimators work better than others, compute

$$\left| d\left(S(\hat{\theta}), y_\varphi\right) - d\left(\hat{S}(\hat{\theta}), y_\varphi\right) \right| \quad \text{and} \quad d\left(S(\hat{\theta}), \hat{S}(\hat{\theta})\right)$$

C - Construction of the surrogate model

Context and objectives of the thesis



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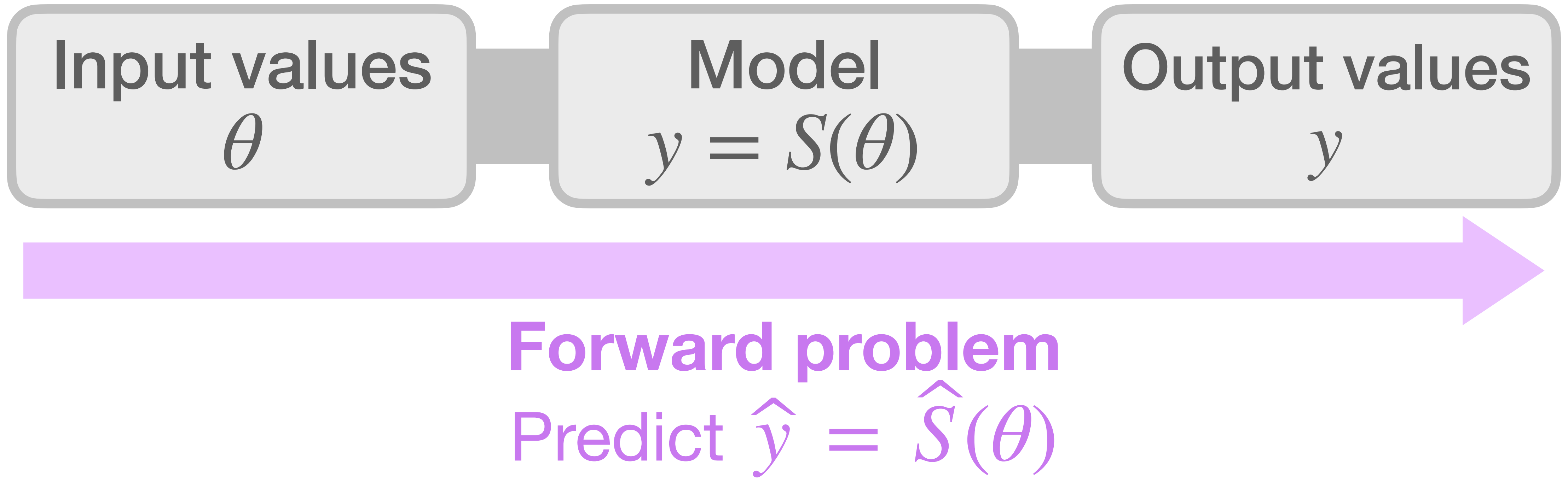

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$$y = S(\theta)$$

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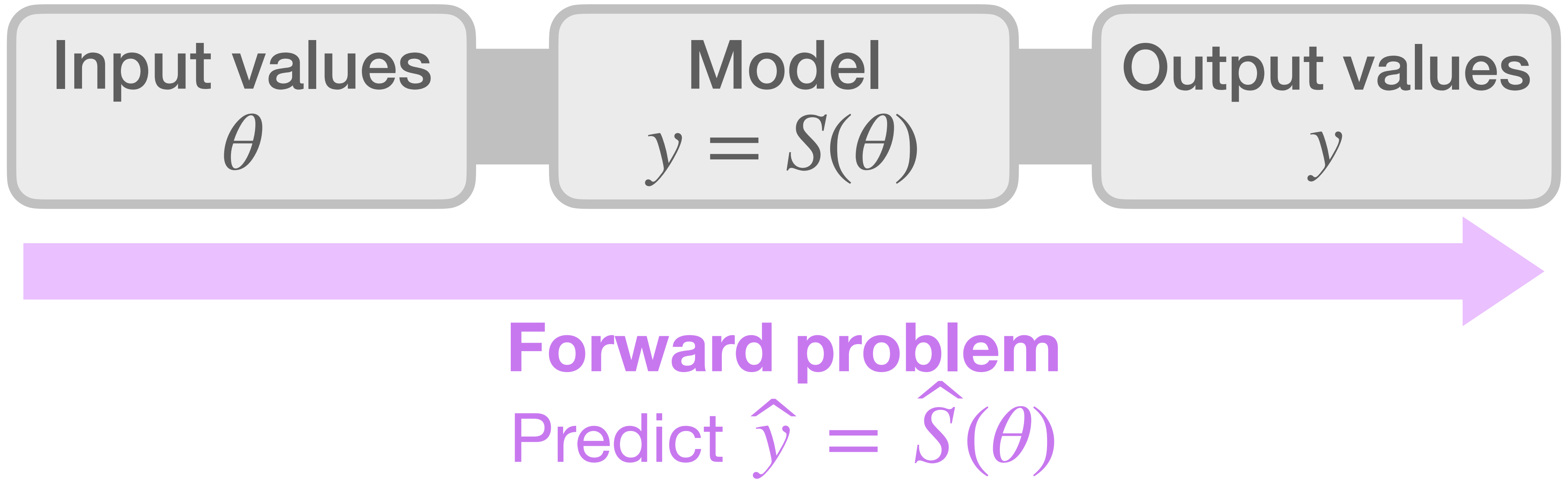

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How do we generate large amounts of time series?

- Using the simulator S would be optimal but it requires excessive computational resources
- We substitute the simulator S with a pre-trained surrogate model $\widehat{S}$ which mimics it

Predicts y *for a given* θ *using* $\widehat{y} = \widehat{S}(\theta)$

We need to construct a surrogate model using supervised statistical learning to solve a forward problem

C - Construction of the surrogate model

Different data formats

What are the data? How to use it?

C - Construction of the surrogate model

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Considered outputs are time series

- Time dependency must be taken into account when building our model
- Choose a format that's not too expensive and not too large

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- Vector format

$$\begin{pmatrix} \theta_{1,1} & \dots & \theta_{1,p} \\ \theta_{2,1} & \dots & \theta_{2,p} \\ \vdots & & \vdots \\ \theta_{n,1} & \dots & \theta_{n,p} \end{pmatrix} \left(\begin{array}{ccc|c|ccc} y^{(1)}_{1,1} & \dots & y^{(1)}_{1,T_1} & \dots & y^{(R)}_{1,1} & \dots & y^{(R)}_{1,T_R} \\ y^{(1)}_{2,1} & \dots & y^{(1)}_{2,T_1} & \dots & y^{(R)}_{2,1} & \dots & y^{(R)}_{2,T_R} \\ \vdots & & \vdots & & \vdots & & \vdots \\ y^{(1)}_{n,1} & \dots & y^{(1)}_{n,T_1} & \dots & y^{(R)}_{n,1} & \dots & y^{(R)}_{n,T_R} \end{array}\right)$$

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\end{array}\right)
$$

- Matrix format

$$
\left(\begin{array}{ccccc}
\theta_{1,1} & \theta_{1,2} & \cdots & \theta_{1,p} & 1 \\
'' & '' & \cdots & '' & 2 \\
\vdots & \vdots & & \vdots & \vdots \\
'' & '' & \cdots & '' & T \\
\hline
 & & \cdots & & \\
\hline
\theta_{n,1} & \theta_{n,2} & \cdots & \theta_{n,p} & 1 \\
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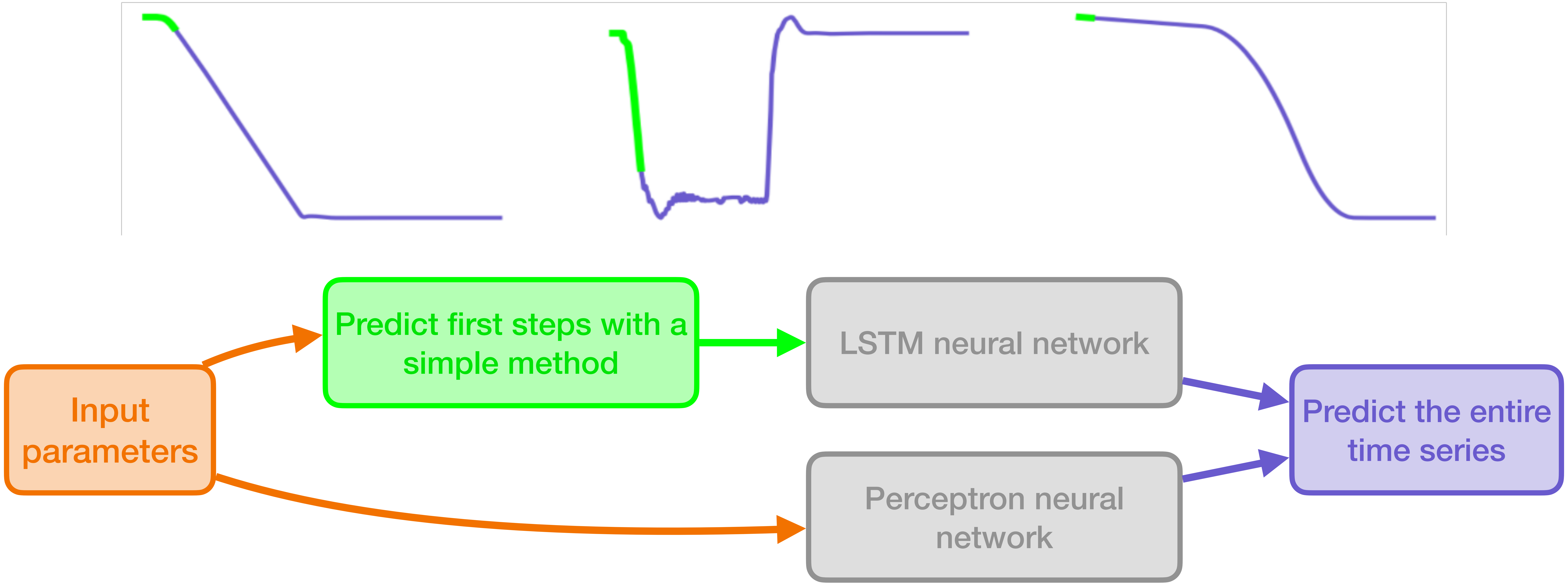
C - Construction of the surrogate model

Neural networks

- Long short-term memory (LSTM)
  - Handles sequential data
  - Maintains a hidden space which acts as a memory of previous inputs



C - Construction of the surrogate model

Conclusion - *Numerical results*

RMSE ($\times 10^{-1}$)	1-RF	4-RF	matrix 1-RF	matrix 4-RF	PCA 4-RF	Sparse PCA 4-RF	fPCA 4-RF
train	1.108	0.998	0.310	**0.201**	1.051	1.136	1.050
validation	2.535	2.243	2.688	2.692	2.572	2.598	2.583
test	3.308	3.047	4.012	3.999	3.465	3.481	3.473

RMSE ($\times 10^{-1}$)	k-NN	KRR	DF	CNN	multi LSTM	hybrid	aggre-gated
train	2.693	0.917	1.221	0.500	0.463	$\times$	$\times$
validation	2.966	3.234	1.791	0.500	0.507	**0.422**	0.996
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Traditional ML

C - Construction of the surrogate model

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Traditional ML

Neural networks

Hybrid and aggregated

C - Construction of the surrogate model

Conclusion - *Computation times*

time	1-RF	4-RF	matrix 1-RF	matrix 4-RF	PCA 4-RF	Sparse PCA 4-RF	fPCA 4-RF
training	2 min	2 min	30 min	2 hours	$<$ 1 min	16 min	$<$ 1 min
prediction	5 ms	8 ms	144 ms	484 ms	44 ms	412 ms	436 ms

time	k-NN	KRR	DF	CNN	multi LSTM	hybrid	aggre-gated
training	1 sec	1 sec	21 min	6 hours	33 min	5 sec (+)	4 min (+)
prediction	1 ms	$<$ 1 ms	26 ms	3 ms	27 ms	40 ms	6 sec

D - Theoretical guarantees for functional expert aggregation

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- Use the existing optimization tools to compute the best W such as

$$W^* = \operatorname*{arg\,min}_{W \in \mathscr{C}} \left\{ \mathscr{R}(W) := \mathbb{E}_P[\ell(W, X)] \right\}$$

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- Guarantee convergence rates of deterministic and stochastic algorithms with little or no proof modification

Needed conditions

1. Embed the space $\mathscr{W}$ in which W resides into a Hilbert space to permit convex optimization techniques
2. The set of contraints $\mathscr{C}$ needs to be closed
3. The loss function ℓ needs to be μ-strongly convex and ν-smooth

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- **Data**: (x, y) where $x \in \mathbb{R}^p$ is a non-temporal input and $y \in \mathcal{S}$ is a function of time where $\mathcal{S}$ is the set of real-valued twice constinuously differentiable functions on the interval $[0,1]$

$$\mathcal{S} = C^2([0,1], \mathbb{R})$$

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- **Renault's digital simulator**: Consider an unknown functional defined as follows

$$\begin{array}{cccc} F^* : & \mathbb{R}^p & \to & \mathcal{S} \\ & x & \mapsto & F^*(x) =: F^*_x \end{array}$$

which maps non-temporal input values x to output time series F^*_x

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To estimate F^*, we aggregate experts with weights

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We need to take into account this pseudo-linearity and update arguments if needed

D - Theoretical guarantees for functional expert aggregation

Framework overall description

Loss to consider

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$$\forall y \in \mathcal{S} \quad \|y\|_{L^2}^2 = \int_0^1 y(t)^2 \mathrm{d}t$$

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$$\forall y \in \mathcal{S} \quad \|y\|_{L^2}^2 = \int_0^1 y(t)^2 \mathrm{d}t$$

- For any $W \in \mathscr{W}$ and observation $z = (x, y)$, the loss of the aggregate F_W is

$$\ell(W, z) = \left\| F_{W,x} - y \right\|_{L^2}^2 = \left\| \sum_{j=1}^{M} w_j f_{j,x} - y \right\|_{L^2}^2$$

D - Theoretical guarantees for functional expert aggregation

Framework overall description

Loss to consider

- The set $\mathcal{S} = C^2([0,1], \mathbb{R})$ is endowed with the L^2-norm

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- The risk function is defined by

$$\mathcal{R}(W) = \mathbb{E}\|F_{W,X} - Y\|_{L^2}^2$$

where the expectation is taken with respect to the joint distribution of the random vector X and random function Y