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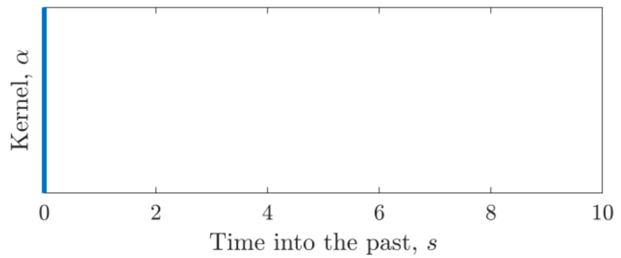
Estimation of absolute and distributed time delays in differential equations based on the linear chain trick

11.30 – 11.50, Friday, August 18th, 2023
24th Nordic Process Control Workshop
Norwegian University of Science and Technology

What are distributed delay differential equations?

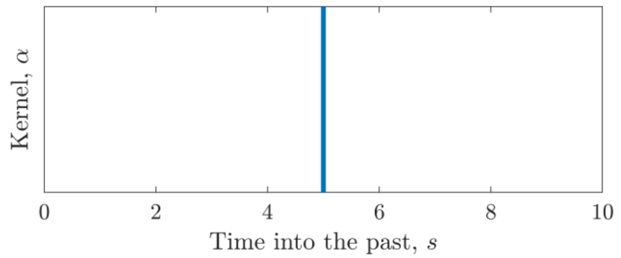
Ordinary differential equation (ODE)

$$\dot{x}(t) = f(x(t), p)$$



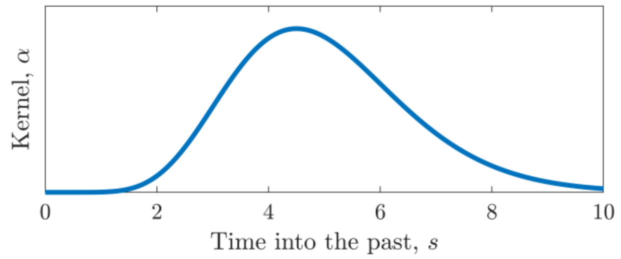
Delay differential equation (DDE) w. absolute/discrete delay

$$\dot{x}(t) = f(x(t), z(t), p)$$
$$z(t) = x(t - \tau)$$



Distributed delay differential equation (DDDE), i.e., w. distributed/continuous delay

$$\dot{x}(t) = f(x(t), z(t), p)$$
$$z(t) = \int_{-\infty}^{t} \alpha(t - s) x(s) \, \mathrm{d}s$$



System

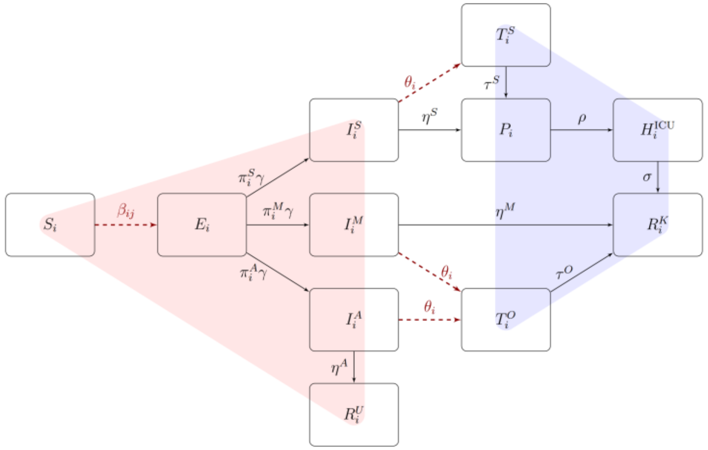
Distributed delay differential equation (DDDE), i.e., w. distributed/continuous delay

$$
\begin{aligned}
\dot{x}(t) &= f(x(t), z(t), p) \\
z(t) &= \int_{-\infty}^{t} \alpha(t-s) r(s) \, \mathrm{d}s \\
r(t) &= h(x(t), p) \\
y(t_k) &= g(x(t_k), p)
\end{aligned}
$$

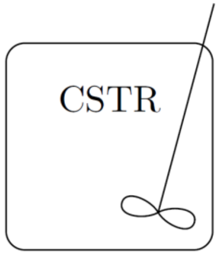
Why are we interested in delays?

Transport through pipes

Epidemiology (latency period)



Slow mixing



Why are we interested in distributed delays?

1. approximate the kernel

$$\dot{\hat{x}}(t) = f(\hat{x}(t), \hat{z}(t), p)$$
$$\hat{z}(t) = \int_{-\infty}^{t} \hat{\alpha}(t-s)\hat{r}(s)\,\mathrm{d}s$$
$$\hat{r}(s) = h(\hat{x}(s), p)$$

$$\hat{\alpha}(t) = \sum_{m=0}^{M} c_m \hat{\alpha}_m(t)$$
$$\hat{\alpha}_m(t) = b_m t^m e^{-at},$$
$$b_m = \frac{a^{m+1}}{m!}$$

2. transform to a set of ODEs (linear chain trick)

$$\dot{\hat{x}}(t) = f(\hat{x}(t), \hat{z}(t), p)$$
$$\dot{\hat{Z}}(t) = A\hat{Z}(t) + B\hat{r}(t)$$
$$\hat{z}(t) = C\hat{Z}(t)$$
$$\hat{r}(t) = h(\hat{x}(t), p)$$

$$A = a\begin{bmatrix} -I & & & \\ I & -I & & \\ & \ddots & \ddots & \\ & & I & -I \end{bmatrix} \qquad B = a\begin{bmatrix} I \\ \\ \\ \\ \end{bmatrix}$$

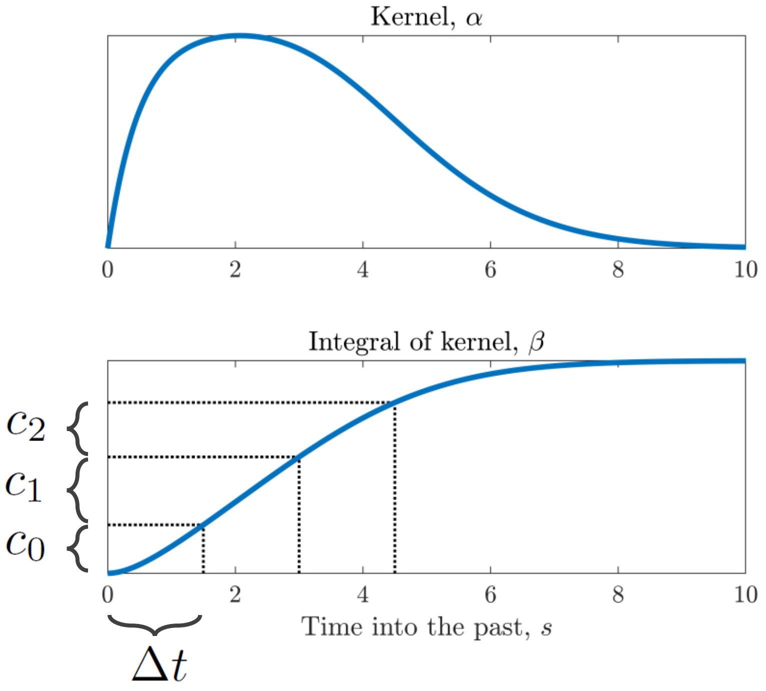
$$C = \begin{bmatrix} c_0 I & c_1 I & \dots & c_M I \end{bmatrix}$$

Is it justified?

PDF and CDF of Erlang distribution

$$\hat{\alpha}_m(t) = b_m t^m e^{-at},$$

$$\hat{\beta}_m(t) = \int_0^t \hat{\alpha}_m(s)\,\mathrm{d}s = 1 - \frac{1}{a}\sum_{n=0}^{m} \hat{\alpha}_n(t)$$



Theorem 1 *Let $\alpha : \mathbb{R}_+ \to \mathbb{R}_+$ be a kernel that satisfies (3), and define*

$$\beta(t) = \int_0^t \alpha(s)\,\mathrm{d}s \tag{6}$$

as well as

$$\hat{\beta}^{(M)}(t) = \sum_{m=0}^{M} c_m \hat{\beta}_m(t), \tag{7}$$

where $t_{m+1} - t_m = \Delta t$, $a = 1/\Delta t$, and $c_m = \beta(t_{m+1}) - \beta(t_m)$. Note that $\hat{\beta}_m$ depends on the rate parameter, a. Then,

$$\lim_{\Delta t \to 0} \hat{\beta}^{(\infty)}(t) = \beta(t) \tag{8}$$

for any continuity point, $t \in \mathbb{R}_+$, of β.

H. C. Tijms. *Stochastic models: An algorithmic approach.* Wiley Series in Probability and Statistics. Wiley, 1995.

H. Cossette, D. Landriault, E. Marceau, and K. Moutanabbir. Moment-based approximation with mixed Erlang distributions. *Variance*, 10(1):166–182, 2016.

Estimation of model and time-delay parameters

Dynamical least-squares problem

$$\min_{p,q} \quad \phi = \frac{1}{2}\sum_{k=0}^{N}(y(t_k) - \hat{y}(t_k))^T(y(t_k) - \hat{y}(t_k))$$

subject to

$$\begin{aligned}
\hat{x}(t_0) &= \hat{x}_0(p), \\
\hat{Z}(t_0) &= \hat{Z}_0(p), \\
\dot{\hat{x}}(t) &= f(\hat{x}(t), \hat{z}(t), p), && t \in [t_0, t_N], \\
\dot{\hat{Z}}(t) &= A(q)\hat{Z}(t) + B(q)\hat{r}(t), && t \in [t_0, t_N], \\
\hat{z}(t) &= C(q)\hat{Z}(t), && t \in [t_0, t_N], \\
\hat{r}(t) &= h(\hat{x}(t), p), && t \in [t_0, t_N], \\
\hat{y}(t_k) &= g(\hat{x}(t_k), p), && k = 0, \ldots, N, \\
e^T q &= 1, \\
p_{\min} &\leq p \leq p_{\max}, \\
q_{\min} &\leq q \leq q_{\max}
\end{aligned}$$

Assumption on initial condition

$$\hat{Z}(t_0) = \left[\hat{z}_0(t_0); \; \cdots \; ; \; \hat{z}_M(t_0)\right]$$

$$\begin{aligned}
\hat{z}_m(t_0) &= \int_{-\infty}^{t_0} \hat{\alpha}_m(t_0 - s)\hat{r}(s)\,\mathrm{d}s \\
&= \hat{r}(t_0)
\end{aligned}$$

$$\hat{r}(t_0) = h(\hat{x}_0, p)$$

Single-shooting approach

Single-shooting objective function

$$\psi = \psi(p,q)$$
$$= \left\{ \phi = \frac{1}{2} \sum_{k=0}^{N} (y(t_k) - \hat{y}(t_k))^T (y(t_k) - \hat{y}(t_k)) : \right.$$

$$\left. \begin{aligned}
\hat{x}(t_0) &= x_0(p), \\
\hat{Z}(t_0) &= \hat{Z}_0(p), \\
\dot{\hat{x}}(t) &= f(\hat{x}(t), \hat{z}(t), p), \quad t \in [t_0, t_N], \\
\dot{\hat{Z}}(t) &= A(q)\hat{Z}(t) + B(q)\hat{r}(t), \quad t \in [t_0, t_N], \\
\hat{z}(t) &= C(q)\hat{Z}(t), \quad t \in [t_0, t_N], \\
\hat{r}(t) &= h(\hat{x}(t), p), \quad t \in [t_0, t_N], \\
\hat{y}(t_k) &= g(\hat{x}(t_k), p), \quad k = 0, \ldots, N
\end{aligned} \right\}$$

Single-shooting nonlinear program (NLP)

$$\begin{aligned}
\min_{p,q} \quad & \psi(p,q), \\
\text{subject to} \quad & e^T q = 1, \\
& p_{\min} \leq p \leq p_{\max}, \\
& q_{\min} \leq q \leq q_{\max}
\end{aligned}$$

- We use fmincon to solve this
- We provide gradients (but not Hessian)

- We use ode45 for nonstiff systems
- We use ode15s for stiff systems

Sensitivities

1. We derive the Jacobian of the right-hand side function
2. Can be parallellized ✗
3. **Sparsity can be exploited** ✓

$$\frac{\partial \psi}{\partial p_i}(p,q) = \sum_{k=0}^{N} (y(t_k) - \hat{y}(t_k)) S_{yp,i}(t_k)$$

$$\frac{\partial \psi}{\partial q_i}(p,q) = \sum_{k=0}^{N} (y(t_k) - \hat{y}(t_k)) S_{yq,i}(t_k)$$

$$\begin{aligned}
S_{xp,i}(t_0) &= \frac{\partial \hat{x}_0}{\partial p_i}(p), \\
S_{Zp,i}(t_0) &= \frac{\partial \hat{Z}_0}{\partial p_i}(p), \\
\dot{S}_{xp,i}(t) &= \frac{\partial f}{\partial x} S_{xp,i}(t) + \frac{\partial f}{\partial z} S_{zp,i}(t) + \frac{\partial f}{\partial p}, \\
\dot{S}_{Zp,i}(t) &= A(q) S_{Zp,i}(t) + B(q) S_{rp,i}(t), \\
S_{zp,i}(t) &= C(q) S_{Zp,i}(t), \\
S_{rp,i}(t) &= \frac{\partial h}{\partial x} S_{xp,i}(t) + \frac{\partial h}{\partial p}, \\
S_{yp,i}(t_k) &= \frac{\partial g}{\partial x} S_{xp,i}(t_k) + \frac{\partial g}{\partial p}
\end{aligned}$$

$$\begin{aligned}
S_{xq,i}(t_0) &= 0, \\
S_{Zq,i}(t_0) &= 0, \\
\dot{S}_{xq,i}(t) &= \frac{\partial f}{\partial x} S_{xq,i}(t) + \frac{\partial f}{\partial z} S_{zq,i}(t), \\
\dot{S}_{Zq,i}(t) &= \frac{\partial A}{\partial q_i} \hat{Z}(t) + A(q) S_{Zq,i}(t) \\
&\quad + \frac{\partial B}{\partial q_i} \hat{r}(t) + B(q) S_{rq,i}(t), \\
S_{zq,i}(t) &= \frac{\partial C}{\partial q_i} \hat{Z}(t) + C(q) S_{Zq,i}(t), \\
S_{rq,i}(t) &= \frac{\partial h}{\partial x} S_{xq,i}(t), \\
S_{yq,i}(t_k) &= \frac{\partial g}{\partial x} S_{xq,i}(t_k)
\end{aligned}$$

Point reactor kinetics model (nuclear fission)

$$\dot{n}(t) = \frac{\rho(t) - \beta}{\Lambda} n(t) + \sum_{i=1}^{N_p} \lambda_i C_i,$$

$$\dot{C}_i(t) = \frac{\beta_i}{\Lambda} n(t) - \lambda_i C_i(t) - \frac{C_i}{\tau_c} + \frac{\tilde{C}_i(t) e^{-\lambda_i \tau_\ell}}{\tau_c},$$

$$\dot{\rho}(t) = -\alpha H n(t)$$

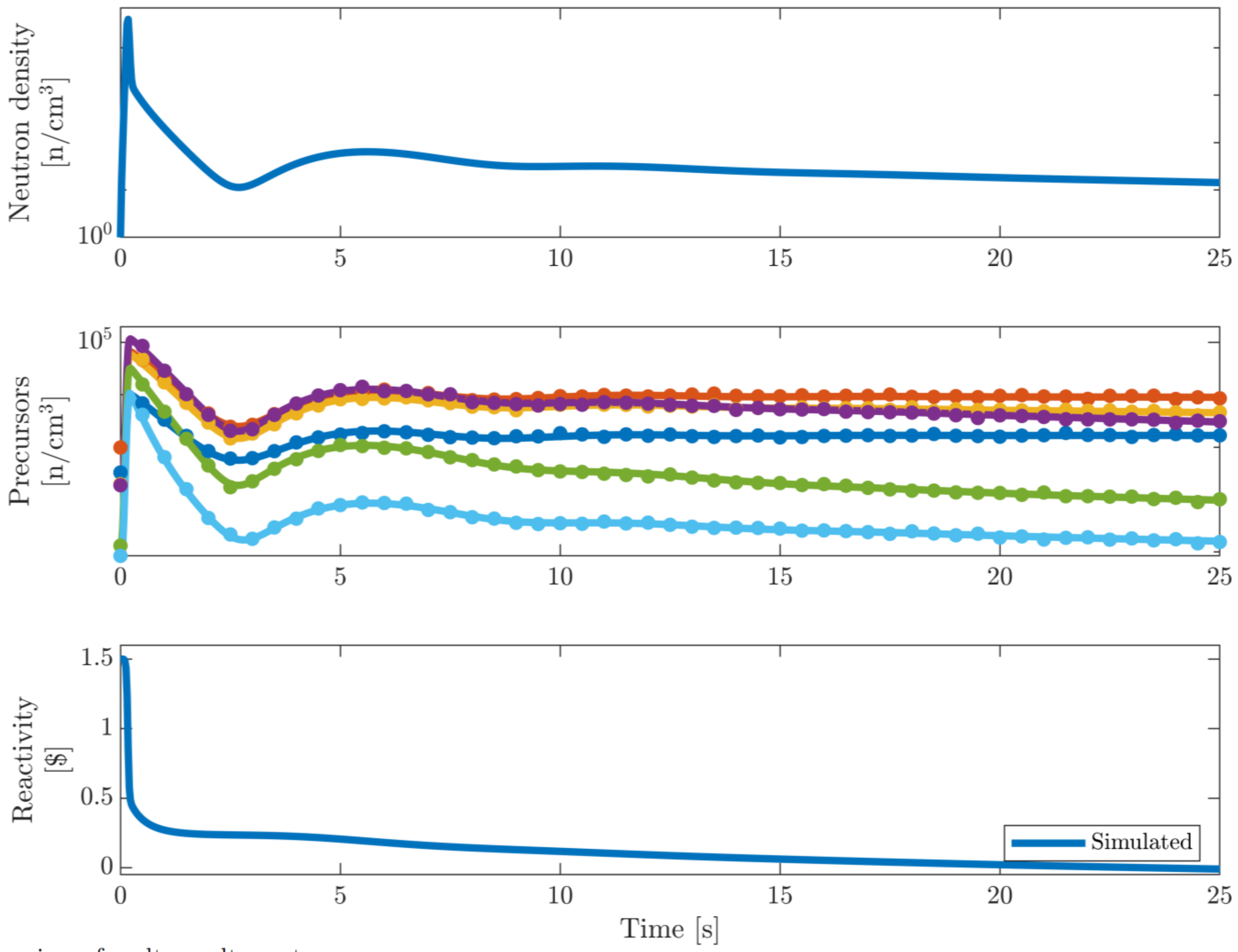
$$\tilde{C}_i(t) = \int_{-\infty}^{t} \alpha(t-s) C_i(s) \, \mathrm{d}s$$

$$N_p = 6$$

$$\beta = \textstyle\sum_{i=1}^{N_p} \beta_i$$

- Estimate model parameter α and kernel α

(U235-graphite reactor)

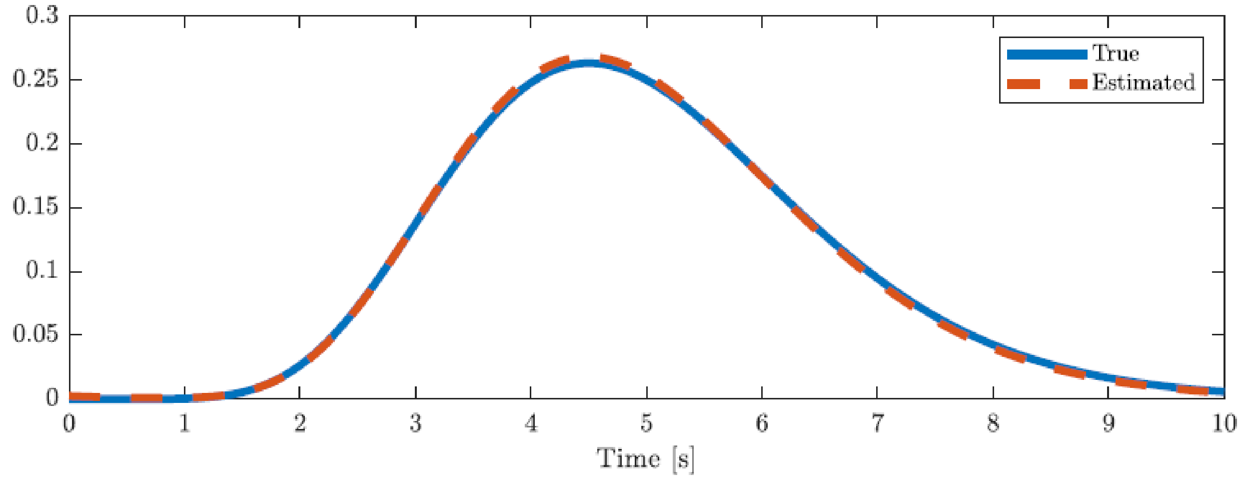


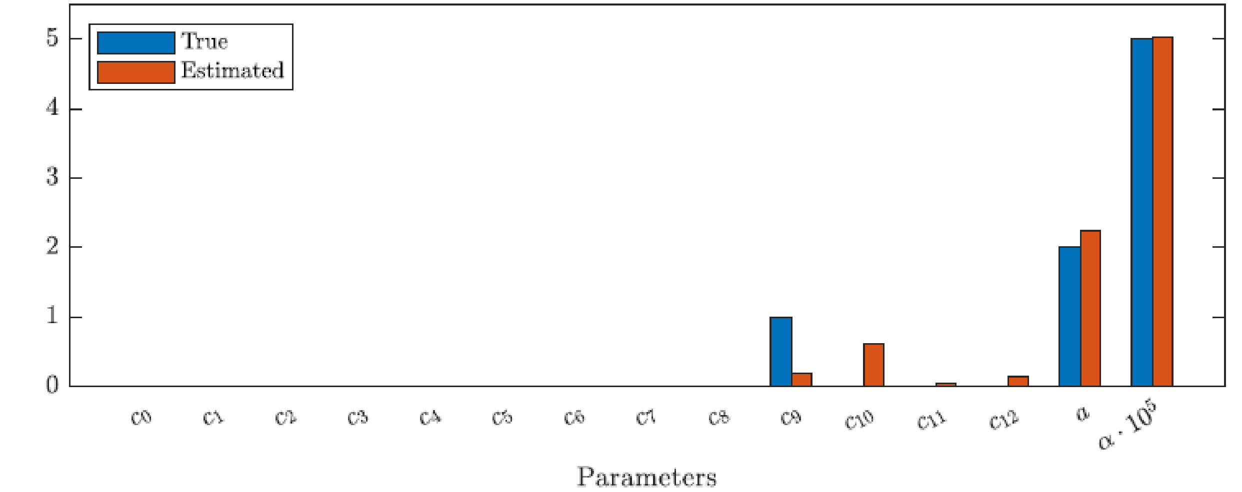
W. M. Stacey. *Nuclear reactor physics.* Wiley, 2nd edition, 2007.

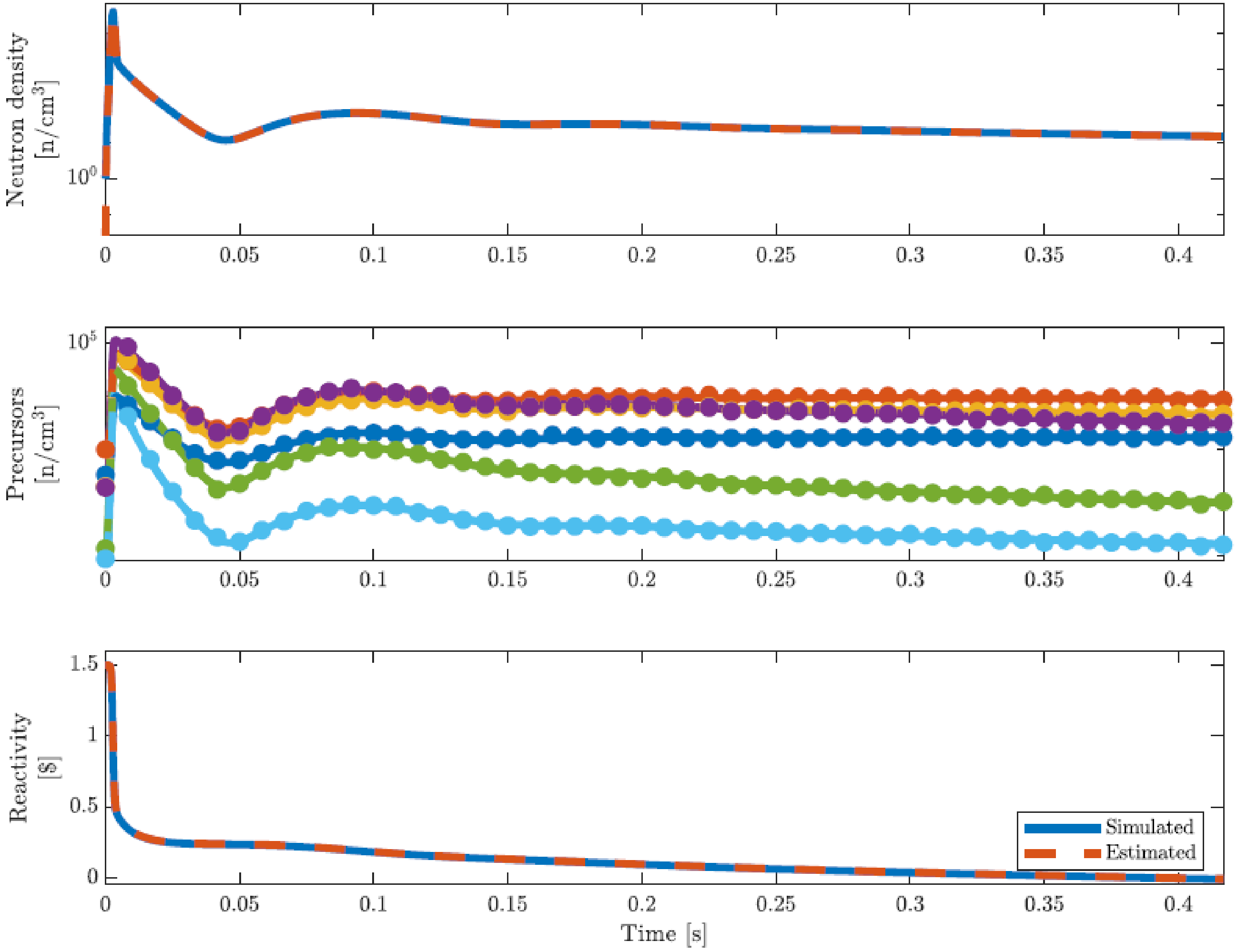
S. Q. B. Leite, M. T. de Vilhena, and B. E. J. Bodmann. Solution of the point reactor kinetics equations with temperature feedback by the ITS2 method. *Progress in Nuclear Energy*, 91:240–249, 2016.

D. Wooten and J. J. Powers. A review of molten salt reactor kinetics models. *Nuclear Science and Engineering*, 191:203–230, 2018.

Point reactor kinetics – Noisy measurements

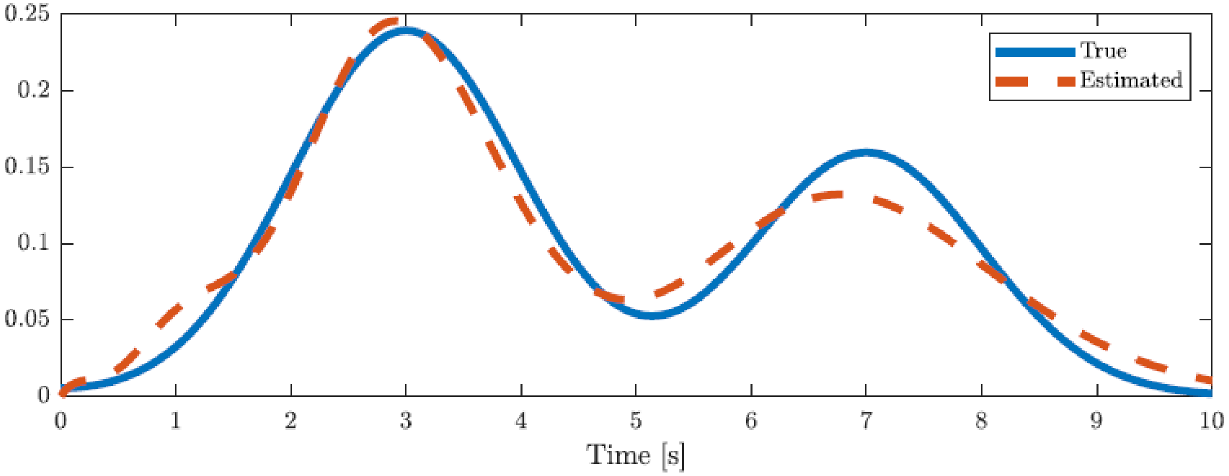


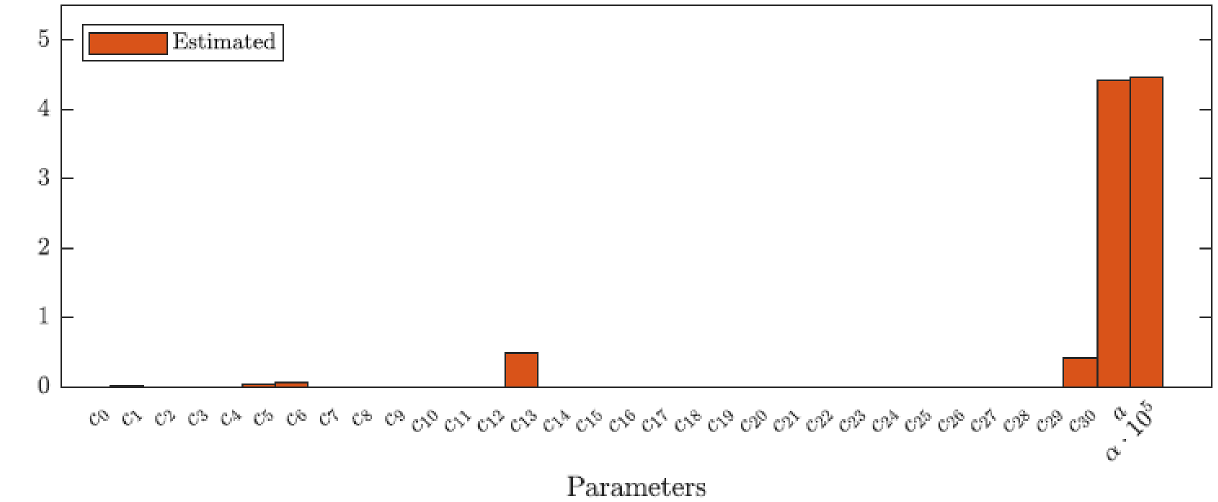


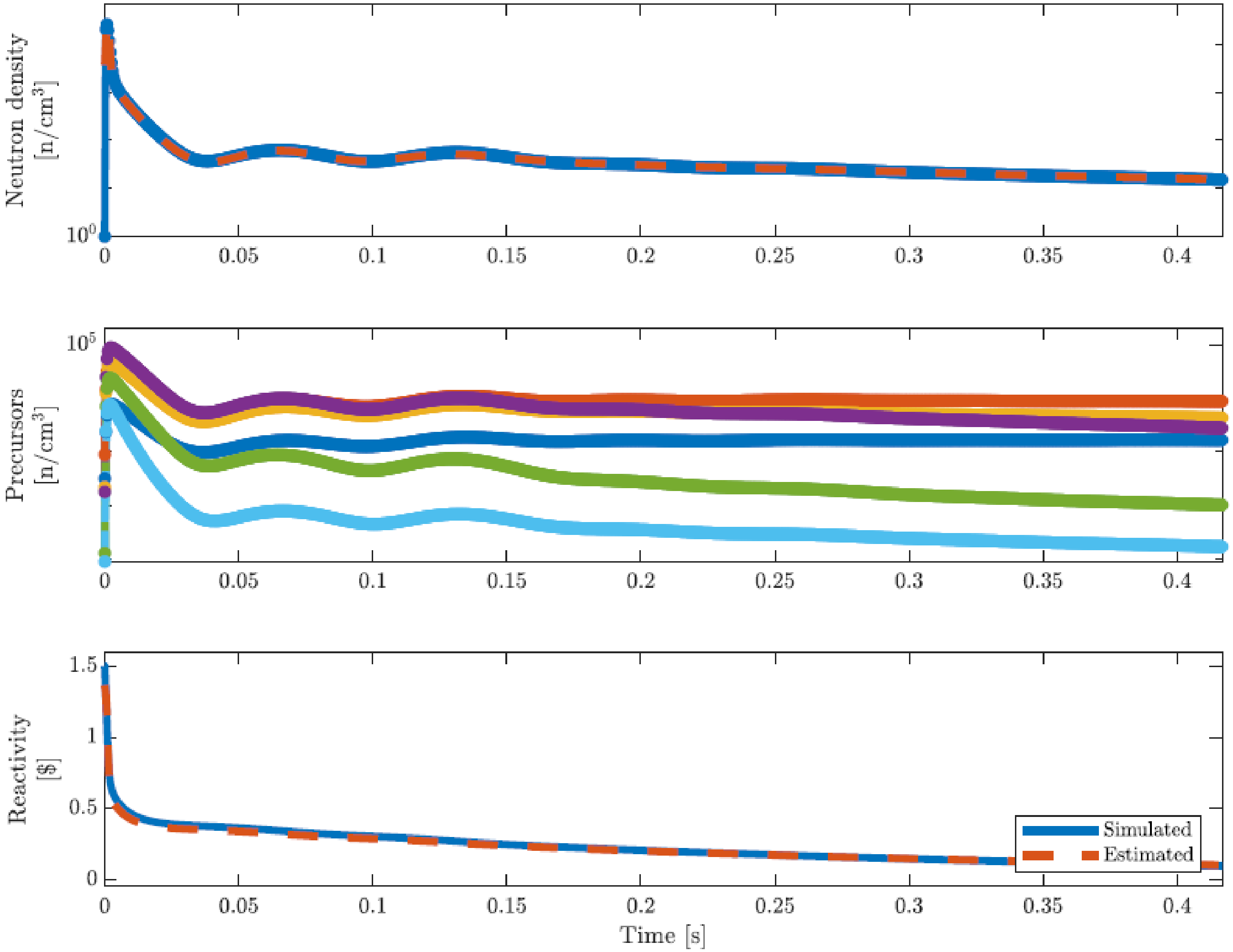


Top left: True (blue solid) and estimated (red dashed) kernel. **Bottom left**: The coefficients, c_m and a, for the true (blue) and estimated (red) kernel. **Right (top, middle, and bottom):** Simulation based on the true (solid) and the estimated (dashed) kernel as well as the measurements (circles).

Point reactor kinetics – Exact meas., non-Erlang kernel







Top left: True (blue solid) and estimated (red dashed) kernel. **Bottom left**: The coefficients, c_m and a, for the estimated (red) kernel. **Right (top, middle, and bottom):** Simulation based on the true (solid) and the estimated (dashed) kernel as well as the measurements (circles).

Summary

Approximate delay using a mixed Erlang PDF

Convert to ODEs

Estimate time delay parameters as ordinary parameters

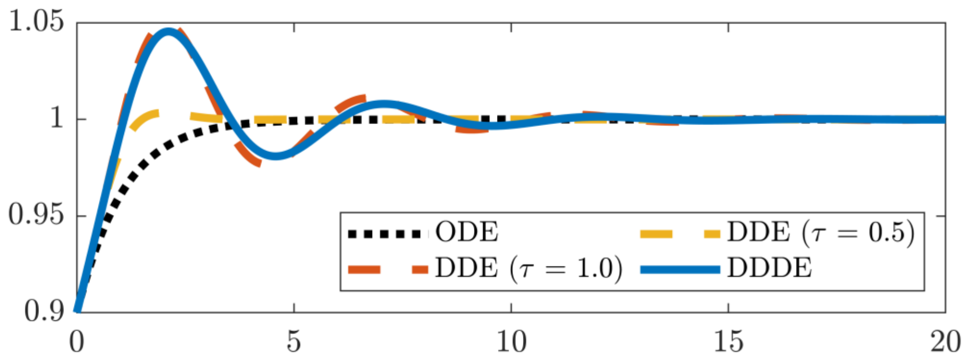
Thank you

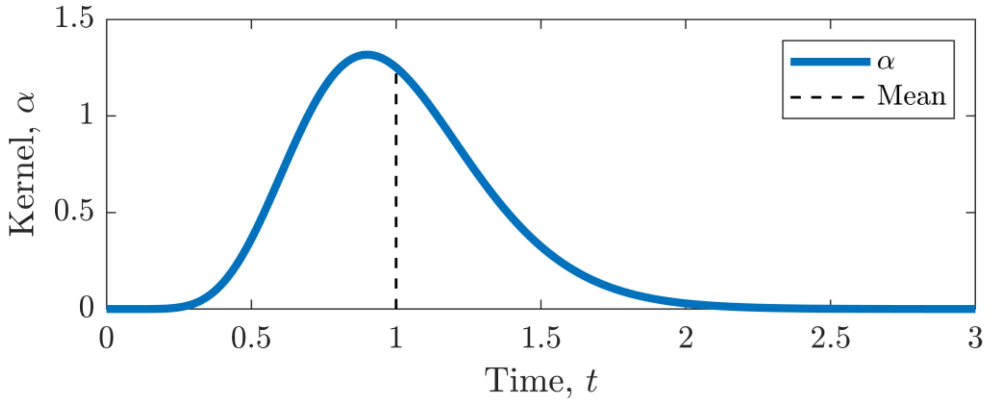
Logistic equation

$$\dot{N}(t) = \sigma N(t)\left(1 - \frac{\tilde{N}(t)}{K}\right)$$

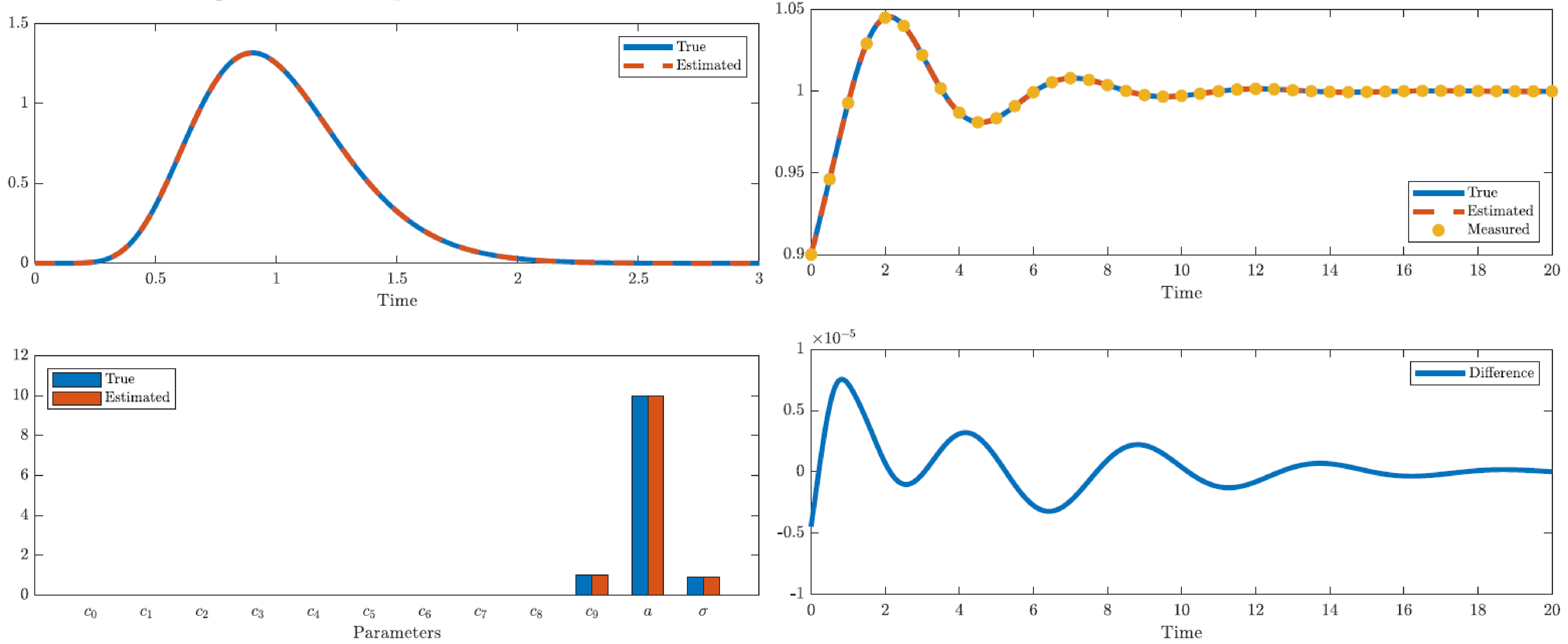
$$\tilde{N}(t) = \int_{-\infty}^{t} \alpha(t-s)N(s)\,\mathrm{d}s$$

- Estimate σ and α



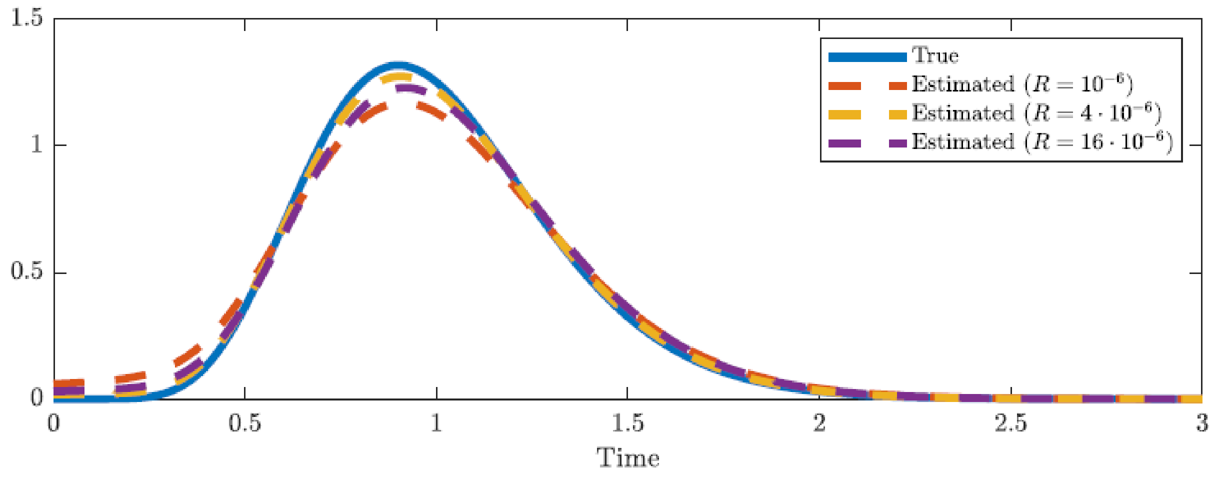


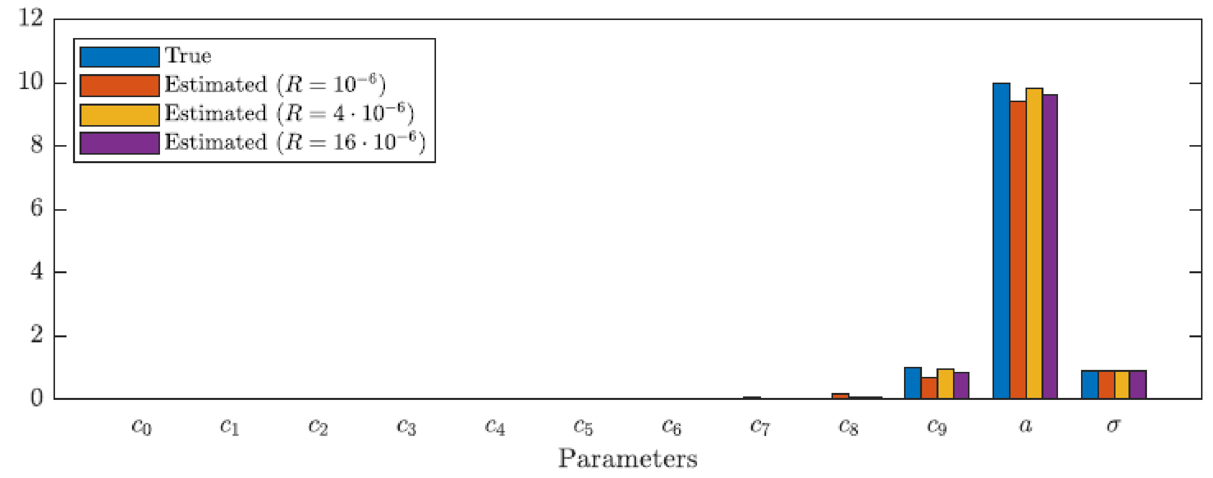
Logistic equation – Exact measurements, correct M



Top left: Identified kernel based on 21 measurements without noise (i.e., $R = 0$). **Bottom left**: The true (blue) and estimated (red) time-delay and model parameters, c_m, a, and σ. **Top right**: Simulation based on the true (blue solid) and estimated (red dashed) parameters as well as the measurements (yellow circles). **Bottom right**: Difference between simulations with true and estimated parameters.

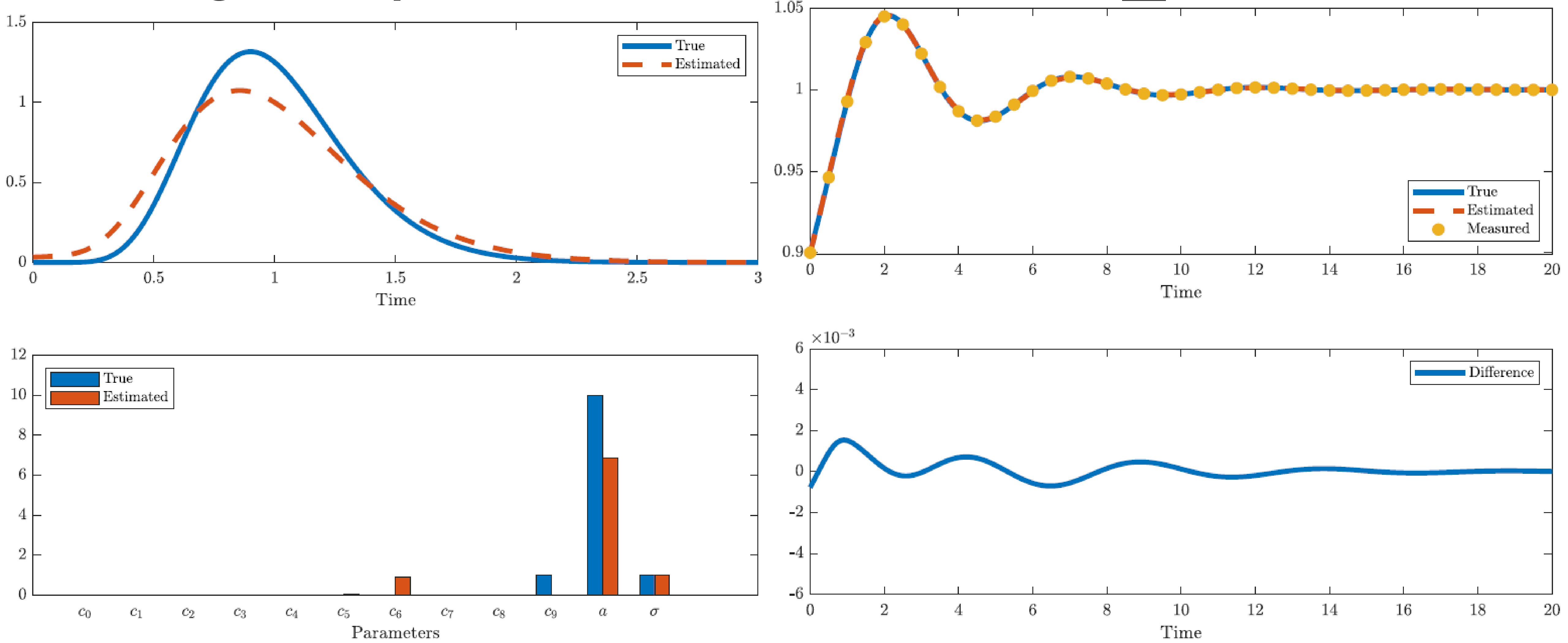
Logistic equation – Noisy measurements, correct M





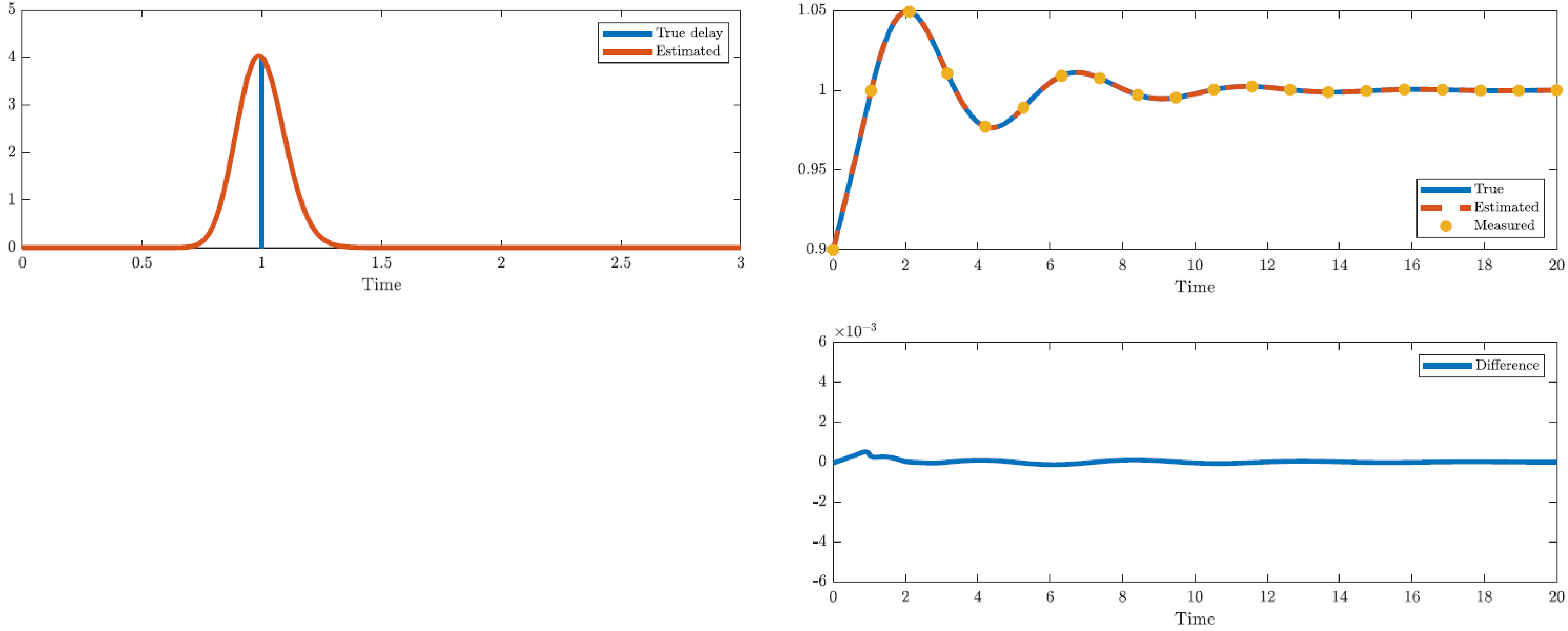
Identified kernels based on 161 measurements with varying values of the measurement noise variance, *R*.

Logistic equation – Exact measurements, incorrect M



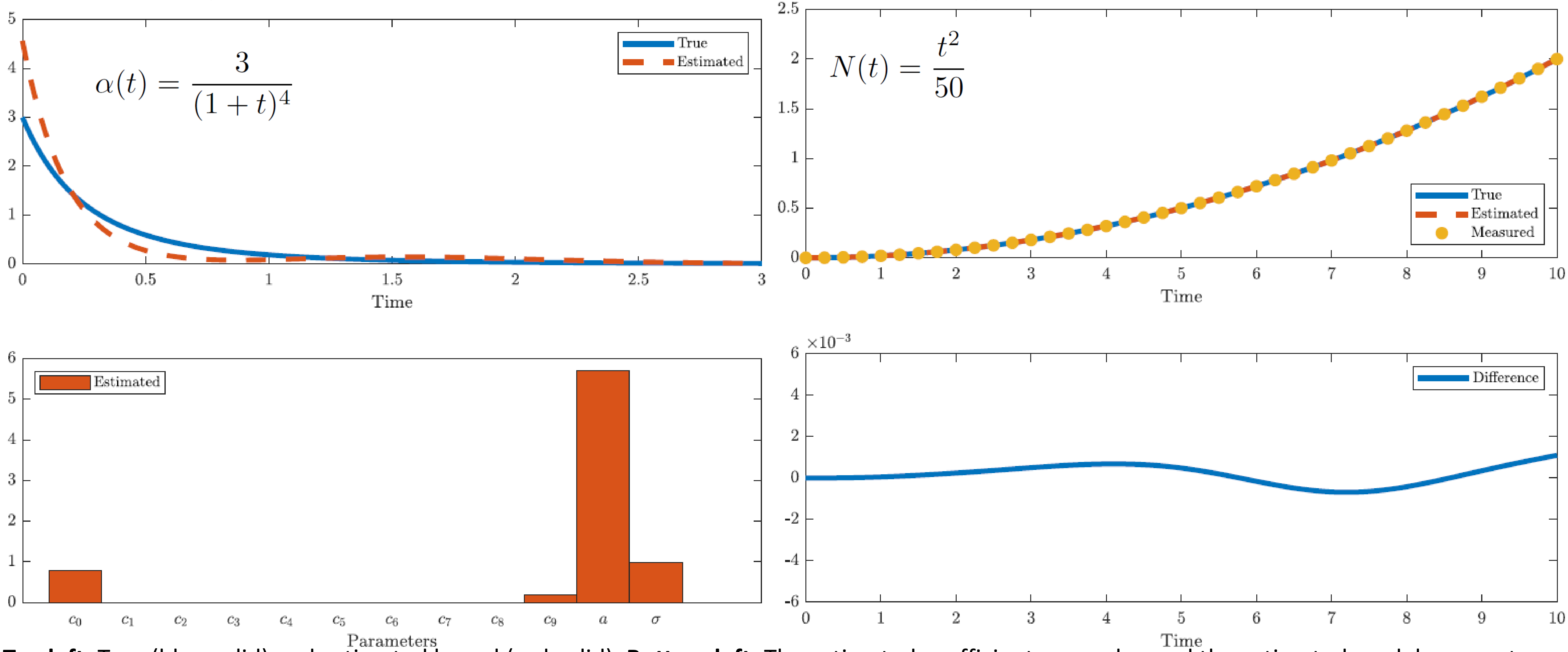
Top left: True (blue solid) and estimated (red dashed) kernel. **Bottom left**: The coefficients, c_m and a, for the true (blue) and estimated (red) kernel. **Top right**: Simulation based on the true (blue solid) and the estimated (red dashed) kernel as well as the measurements (yellow circles). **Bottom right**: Difference between simulations with true and estimated parameters.

Logistic equation – Absolute delay



Top left: True delay (blue solid) and estimated kernel (red solid). **Top right**: Simulation based on the true absolute delay (blue solid) and the estimated (red dashed) kernel as well as the measurements (yellow circles). **Bottom right**: Difference between simulations with true and estimated parameters. Bottom:

Logistic equation – ”Nonconforming” kernel



Top left: True (blue solid) and estimated kernel (red solid). **Bottom left**: The estimated coefficients, c_m and a, and the estimated model parameter σ. **Top right**: Simulation based on the true (blue solid) and the estimated (red dashed) kernel as well as the measurements (yellow circles). **Bottom right**: Difference between simulations with the true and estimated parameters.