Basic Concepts in the Methodology of Mathematical Modeling

Lecture 1: Basics

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Contents

I. Basic principles and guidelines

What is a model ?

MODEL . . . A model is an image of a sector of reality created in order to satisfy a given purpose or to accomplish a given task.

Guideline: Keep the structures which are essential for the Problem and neglect unnecessary details. This is the essence of modelling !!!

A model should be so simple as possible and only as complex as necessary!!

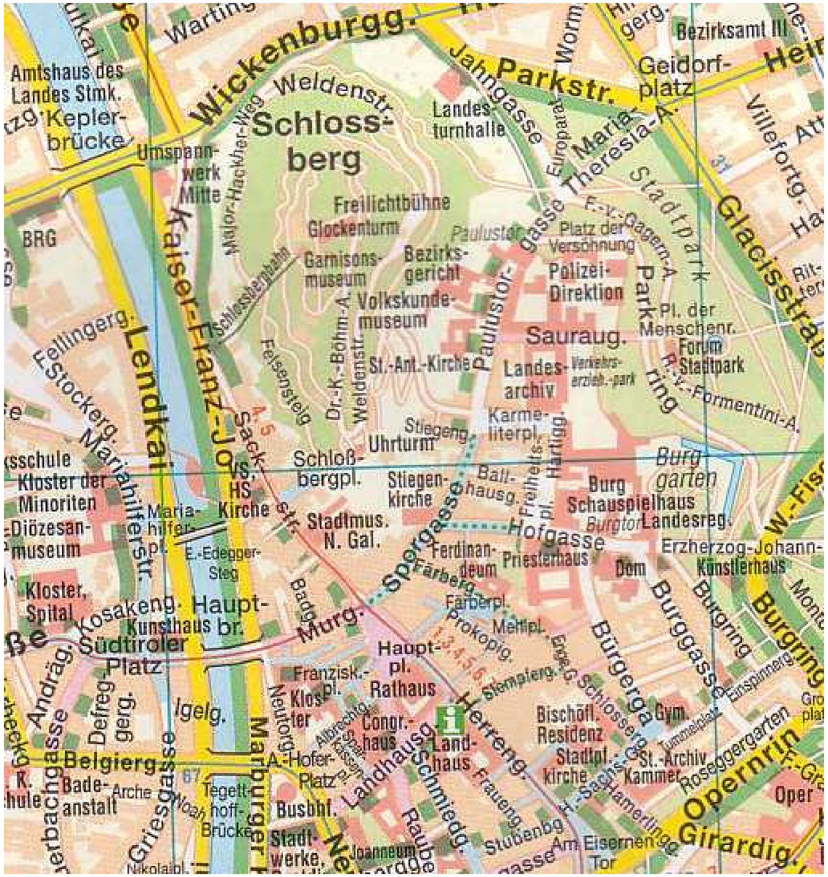
Examples for models

1. Verbal descriptions (news, witness reports etc.)

   Here the sector of reality could be a political event, like a session of parliament or a demonstration, and the image a text in a newspaper. Idealistically one would assume that the goal for writing the article is to give an unbiased report on the event which captures the politically relevant facts correctly. However, the purpose of the model (i.e., of the article) could also be different. For example the text should create the impression in the reader that the event demonstrates the superiority of the program of a certain party over the program of another party.

2. Structured lists of measurements (for classification purposes)

3. Maps:



4. “Real” models, as for instance models of airplanes for wind tunnel experiments.

5. Mathematical models
The image a the sector of reality is a set of equations or an other mathematical structure (as for instance a directed graph)

Another classification of models:

- Descriptive models
- Explanatory models (representation of causal relations)

Guidelines for modelling

- The purpose resp. the goal of the modelling process must be clear.
- In view of the goals the model has to be as simple as possible and only as complex as necessary.
- Variables and parameters of the models should have counterparts (resp. interpretations) in reality. In particular this is necessary for explanatory models.
- Does a model not achieve the given goals, then it has to be modified or even abandoned and replaced by a new one.

Never fall in love with your model !!!

Domain of validity

That sector of reality, which is represented by the model with sufficient accuracy.

The domain of validity is determined by the simplifying assumptions made during the modelling process and therefore is strongly and directly related with the goals of the modelling process.

Goals for modelling processes

a) Simulations (instead of experiments)

b) Determining quantities, which cannot be measured directly.

c) Control and optimal control

d) Gain of knowledge

Determining factors

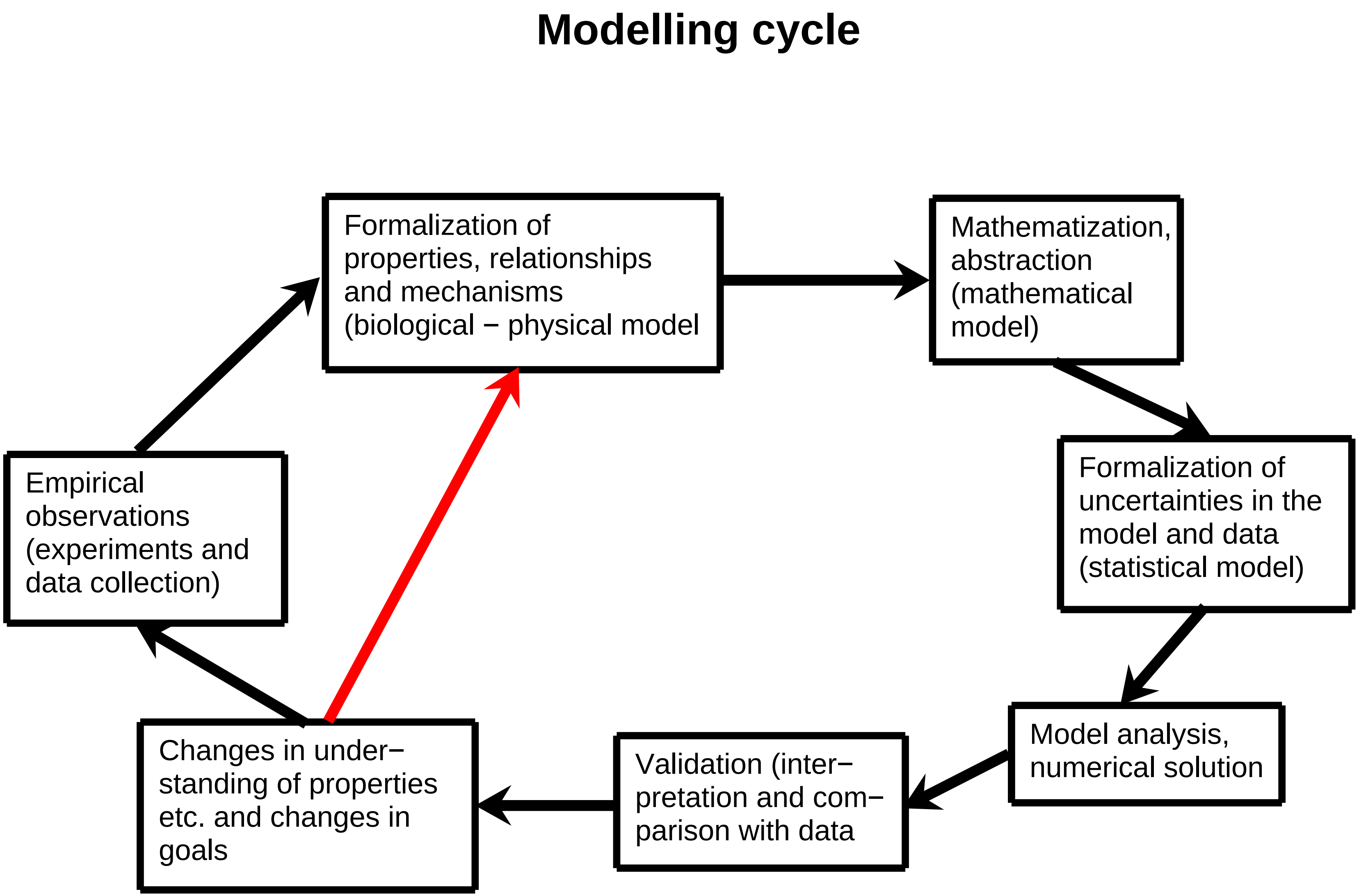
a) Development and Applications of new mathematical methodologies.

$$\text{Mathematics} \quad \Longleftrightarrow \quad \text{Applied areas}$$

b) Availability of enormous computing power (complex models, visualization).

c) New technologies for measuring devices.

II. Main steps of a modelling process



Dimensional Considerations

Physical quantities have a dimension.

"Basic" dimensions: M=[mass], L=[length], T=[time],
Q=[electrical charge]

f . . . physical variable $\Longrightarrow [f] = P_1^{a_1} \cdot \cdots \cdot P_n^{a_n}$, where P_i are
primary dimensions and $a_i \in \mathbb{Q}$.

Rules: 1. If $f_1 = f_2$, then $[f_1] = [f_2]$.
2. $[f_1 f_2] = [f_1][f_2]$
3. f_1 and f_2 can only by added if $[f_1] = [f_2]$.
4. Numbers are dimensionless (e.g. [2]=1).
5. Arguments of non-polynomial functions have to be dimensionless. E.g. $[e^{\omega t}] = 1$ if $[t] = T$, because $[\omega] = 1/T$ (frequency) so that $[\omega t] = 1$

Dimensional considerations and empirical formulae

$\boldsymbol{V}_{\text{tot}}$ ... total blood volume in the human body
$\boldsymbol{S}$ ... surface of the human body
$\boldsymbol{w}$ ... body weight in kg
$\boldsymbol{h}$ ... height of the person in cm

Empirical formula 1: $\boldsymbol{V}_{\text{tot}} = \mathbf{3\,290}\boldsymbol{S} - \mathbf{1\,229}$

Empirical formula 2: $\boldsymbol{S = kw^{\alpha}h^{\beta}}, \quad \boldsymbol{\alpha, \beta} \in \mathbb{Q}$

Both sides of the formula must have the same dimension:

$$\boldsymbol{L^2 = [k/\rho]L^{3\alpha+\beta}} \quad \Longrightarrow \quad \boldsymbol{\beta = 2 - 3\alpha}.$$

Instead of 3 parameters only 2 have to be determined:
$\boldsymbol{k = 0.007184,\ \alpha = 0.425} \quad \Longrightarrow$

$$\boldsymbol{S = 0.007184\, w^{0.425}\; h^{0.725}} \quad \text{(DuBois, 1916)}$$

Buckingham's π-Theorem

$Q_1, \ldots, Q_n$ ... physical quantities

dimension $Q_j = \delta_1^{m_{1,j}} \cdot \ldots \cdot \delta_k^{m_{k,j}}$

$\mathcal{M} = \left(m_{i,j}\right)_{i=1,\ldots,k,\ j=1,\ldots,n}$ ... dimensionality matrix of $Q_1, \ldots, Q_n$

rank $\mathcal{M} = p$

$$f(Q_1, \ldots, Q_n) = 0 \text{ "physically meaningfull" expression} \qquad (1)$$

$\Longrightarrow$ (1) is equivalent to

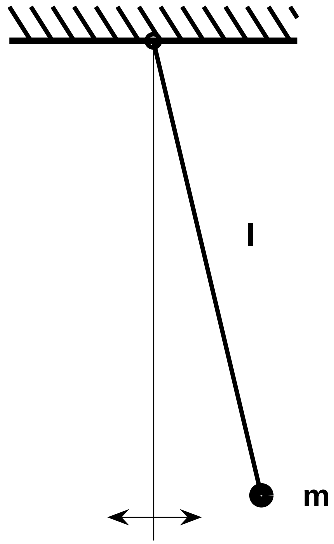
$$F(\pi_1, \ldots, \pi_{n-p}) = 0,$$

$\pi_i = Q_1^{\alpha_{1,i}} \cdot \ldots \cdot Q_n^{\alpha_{n,i}}$, $i = 1, \ldots, n-p$, are dimensionless

$a_i =$ col$(\alpha_{1,i}, \ldots, \alpha_{n,i}) \in \mathbb{Q}^n$, $i = 1, \ldots, n-p$

constitute a basis for the equation $\mathcal{M}a = 0$.

An example



m mass of the pendulum
ℓ length of the pendulum
g gravity
τ period of oscillations

Assume that $\tau = h(m, \ell, g)$, i.e., $f(\tau, m, \ell, g) = 0$.
Primary dimensions: T (time), M (mass) and L (length) $\Longrightarrow$ dimension $g = LT^{-2}$ and

$$\mathcal{M} = \begin{pmatrix} 1 & 0 & 0 & -2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix}$$

An example

$n - p = 4 - \text{rank}\,\mathcal{M} = 4 - 3 = 1$

$a = \text{col}\,(2, 0, -1, 1)$ is a basis of ker$,\mathcal{M}$

$\Longrightarrow f(\tau, , m, \ell, g) = 0$ is equivalent to

$$F(\pi) = 0, \quad \pi = g\tau^2/\ell = \tau^2 m^0 \ell^{-1} g^1$$

$\Longrightarrow g\tau^2/\ell = \kappa^2$, where κ^2 is a positive zero of F

$\Longrightarrow$

$$\tau = \kappa\sqrt{\ell/g}$$

The role of mathematicians

Strengths: Trained to attack problems in a formal and structured approach, knowledge of mathematical structures

Weaknesses: Little insight into the problems and peculiarities of the applied area

Requirements: Enter the applied area deep enough in order to understand the problems and to be able to communicate with the researchers in the applied area, adopt the goals of the applied area

Basic Concepts in the Methodology of Mathematical Modeling

Lectures 2&3: Cardiovascular Modelling

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The basic model

- Problem: Reaction of the CVS to an ergometric work-load (bicycle ergometer, 75 Watt for 10 min.)
- Focus: Control loops
- Data:
  - Heart rate (every 2 sec.),
  - mean arterial systemic pressure (every 2 sec., Finapress)
  - cardiac output of the left ventricle (irreg-ularly, Doppler-echocardiography)

The basic model

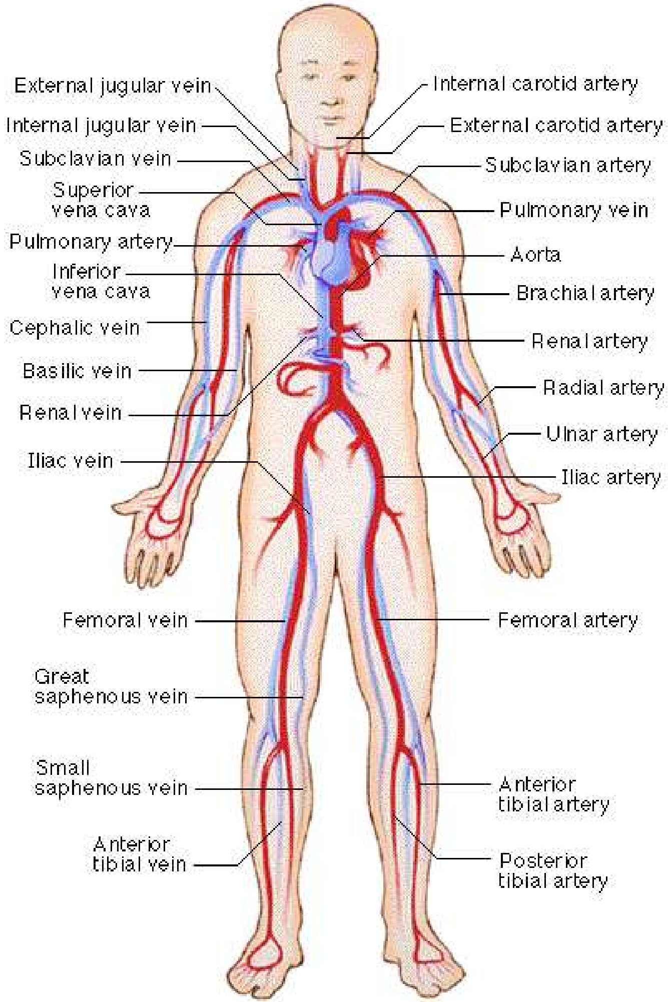
Model structure:

compartmental model

non-pulsatile flow

autoregulation

barorezeptor-loop



The basic model

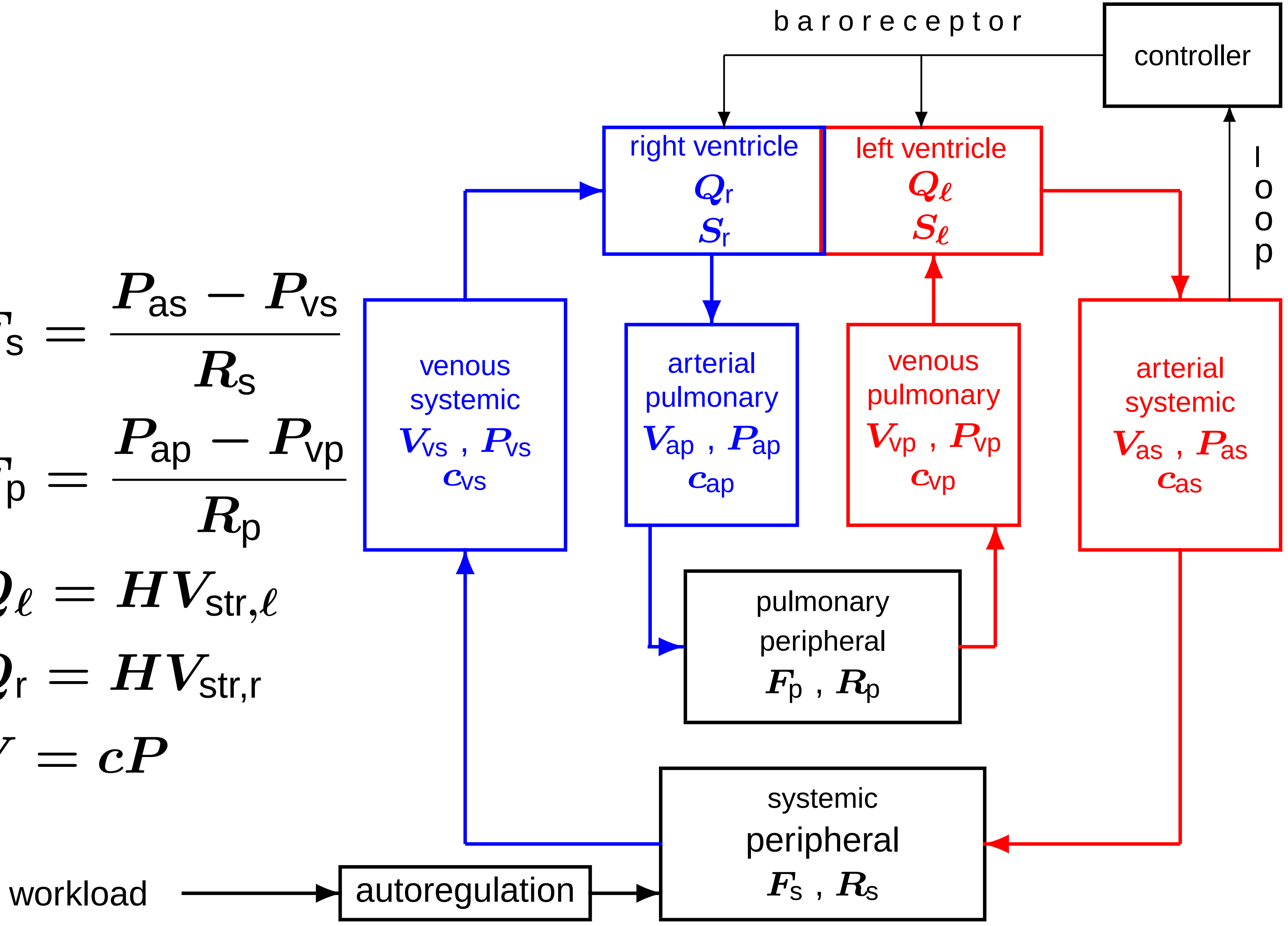
$$F_s = \frac{P_{as} - P_{vs}}{R_s}$$

$$F_p = \frac{P_{ap} - P_{vp}}{R_p}$$

$$Q_\ell = H V_{str,\ell}$$

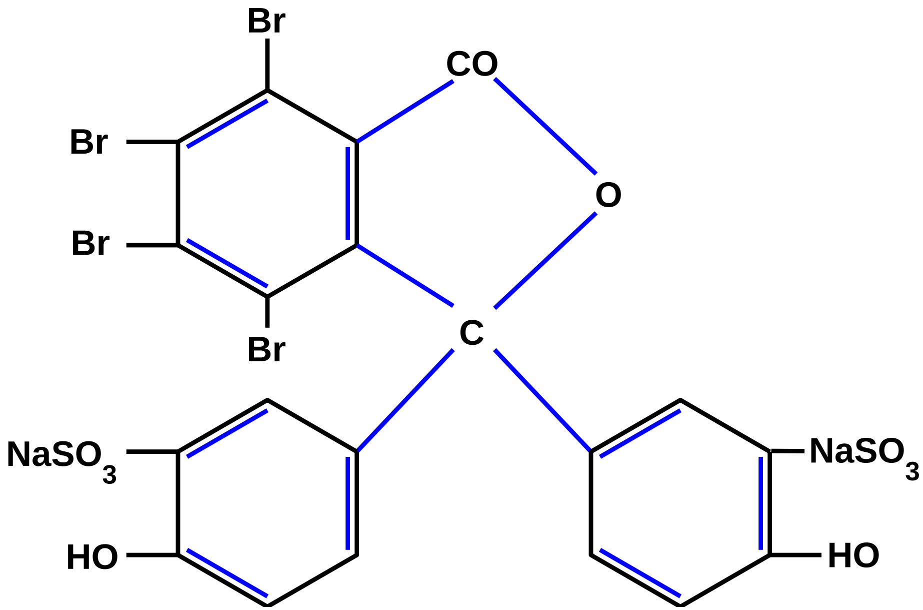
$$Q_r = H V_{str,r}$$

$$V = cP$$



Digression 1: Bromsulphalein test

Test for hepatic functions; the decay rate of bromsulphalein in the liver characterizes certain hepatic functions.

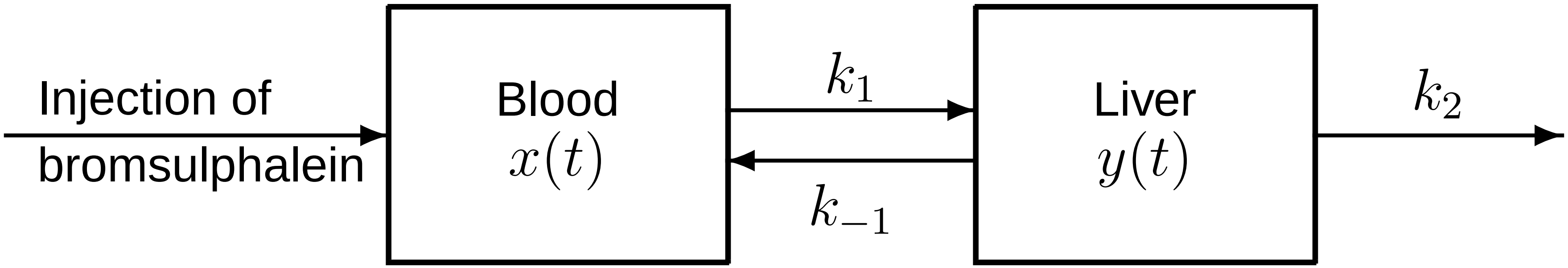


The bromsulphalein retention test:

a) Intravenous application of a dosage d of bromsulphalein at time $t = 0$.

b) Take blood samples approximately every 10 min. and determine the concentration of bromsulphalein in blood.

Compartment model:



$x(t)$ ... mass of BS in blood at time t

$y(t)$ ... mass of BS in liver at time t

k_1, k_{-1}, k_2 ... transition rates

Mass-balance:

$$\dot{x}(t) = -k_1 x(t) + k_{-1} y(t), \tag{1}$$

$$\dot{y}(t) = k_1 x(t) - (k_{-1} + k_2) y(t) \tag{2}$$

Initial conditions: $x(0) = d$, $y(0) = 0$.

Characteristic equation:

$$\lambda^2 + \big(k_1 + k_{-1} + k_2\big)\lambda + k_1 k_2 = 0.$$

$\Longrightarrow$

$$\lambda_{1,2} = -\frac{1}{2}\left(k_1 + k_{-1} + k_2 \pm \sqrt{(k_1 + k_{-1} + k_2)^2 - 4k_1k_2}\right)$$

$$\begin{aligned}
&(k_1 + k_{-1} + k_2)^2 - 4k_1k_2 \\
&\quad = k_1^2 + k_{-1}^2 + k_2^2 + 2k_1k_{-1} + 2k_{-1}k_2 - 2k_1k_2 \\
&\quad > k_1^2 + k_{-1}^2 + k_2^2 + 2k_1k_{-1} - 2k_{-1}k_2 - 2k_1k_2 \\
&\quad = (k_1 + k_{-1} - k_2)^2 \geq 0.
\end{aligned}$$

$\Longrightarrow \quad \lambda_1 < \lambda_2 < 0$

$\Longrightarrow$

$$x(t) = c_1 \frac{\lambda_1 + k_{-1} + k_2}{k_1} e^{\lambda_1 t} + c_2 \frac{\lambda_2 + k_{-1} + k_2}{k_1} e^{\lambda_2 t},$$
$$y(t) = c_1 e^{\lambda_1 t} + c_2 e^{\lambda_2 t}.$$

Initial condition $\Longrightarrow$

$$c_1\lambda_1 + c_2\lambda_2 + (k_{-1} + k_2)(c_1 + c_2) = k_1 d,$$
$$c_1 + c_2 = 0.$$

$$\Longrightarrow \quad c_1 = \frac{k_1 d}{\lambda_1 - \lambda_2}, \quad c_2 = -\frac{k_1 d}{\lambda_1 - \lambda_2}.$$

$$x(t) = x(t; k_1, k_{-1}, k_2), \qquad y(t) = y(t; k_1, k_{-1}, k_2)$$

Task: Identification of k_2 (and k_1, k_{-1})

Data: ξ_i, $i = 1, \ldots, N$,... concentration of Bromsulphalein in blood at times $t_1 < \cdots < t_N$.

$$\xi_i = \frac{x(t_i)}{V},$$

V ... blood volume

Model equations

$$c_{\mathrm{as}}\dot{P}_{\mathrm{as}} = Q_\ell - F_{\mathrm{s}},$$

$$c_{\mathrm{vs}}\dot{P}_{\mathrm{vs}} = F_{\mathrm{s}} - Q_{\mathrm{r}},$$

$$c_{\mathrm{ap}}\dot{P}_{\mathrm{ap}} = Q_{\mathrm{r}} - F_{\mathrm{p}},$$

$$\boxed{\dot{x}(t) = \mathcal{F}(x(t), q) + Bu(t)}$$

$$c_{\mathrm{vp}}\dot{P}_{\mathrm{vp}} = F_{\mathrm{p}} - Q_\ell,$$

$$\ddot{S}_\ell + \gamma_\ell \dot{S}_\ell + \alpha_\ell S_\ell = \beta_\ell H,$$

$$\ddot{S}_{\mathrm{r}}r + \gamma_{\mathrm{r}} \dot{S}_{\mathrm{r}} + \alpha_{\mathrm{r}} S_{\mathrm{r}} = \beta_{\mathrm{r}} H,$$

$$\dot{R}_{\mathrm{s}} = \frac{1}{K}\Big(A_{\mathrm{pesk}}\big(F_{\mathrm{s}} C_{\mathrm{a,O_2}} - M\big) - (P_{\mathrm{as}} - P_{\mathrm{vs}})\Big),$$

$$\dot{H} = u(t)$$

Model equations

Formula for Q_ℓ: $\quad Q_\ell = HV_{\text{str}}$ (V_{str} ... stroke volume)

Assumption:

$V_{\text{str}} = g(V_{\text{diast}}, P_v, P_a) \;\Leftrightarrow\; f(V_{\text{str}}, V_{\text{diast}}, P_v, P_a) = 0$

Primary dimensions: M, L, T

$[V_{\text{str}}] = [V_{\text{diast}}] = L^3, \; [P_v] = [P_a] = ML^{-1}T^{-2}$

$\Longrightarrow$

$$\mathcal{M} = \begin{pmatrix} 0 & 0 & 1 & 1 \\ 3 & 3 & -1 & -1 \\ 0 & 0 & -2 & -2 \end{pmatrix}, \quad \text{rank}\,\mathcal{M} = 2$$

Basis for $\ker \mathcal{M}$: $a = \text{col}\,(1, -1, 0, 0), \; b = \text{col}\,(0, 0, -1, 1)$

$\Longrightarrow \pi_1 = V_{\text{str}}/V_{\text{diast}}, \quad \pi_2 = P_a/P_v$ and $F(\pi_1, \pi_2) = 0$

$\Longrightarrow V_{\text{str}}/V_{\text{diast}} = h(P_a/P_v) \overset{h \text{ linear}}{\Longrightarrow} V_{\text{str}} = S\frac{P_a}{P_v}V_{\text{diast}}$

(Frank-Starling)

Model equations

Filling process: $\dot{V}(t) = \frac{1}{R_\ell}(P_{\text{vp}} - P(t))$ and

$$V(t) = c_\ell P(t)$$

$$\Longrightarrow \dot{V}(t) = \frac{1}{c_\ell R_\ell}(c_\ell P_{\text{vp}} - V(t)),\ V(0) = V_{\text{syst}}$$

$$V_{\text{diast}} = V(t_d),\ t_d = t_d(H) = \frac{1}{H} - \frac{\kappa}{H^{1/2}}$$

Bazett 1920

$$\Longrightarrow Q_\ell = Hf(P_{\text{vp}}, P_{\text{as}}, S_\ell, H)$$

Optimal control

Choose $u(t)$ such that:

$$J(u(\cdot), x^{\text{rest}}) = \int_0^\infty \left(q_{\text{as}}^2 (P_{\text{as}}(t) - P_{\text{as}}^{\text{exer}})^2 + u(t)^2\right) dt \to \min$$

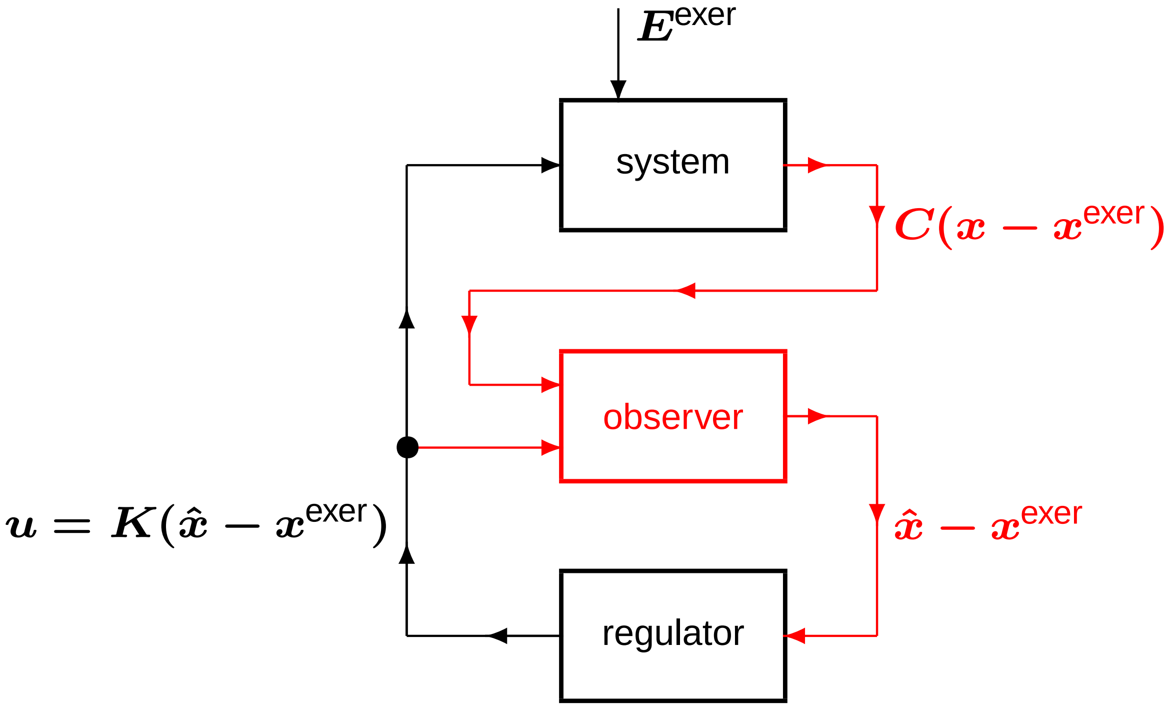
$$x(0) = x^{\text{rest}}$$

$$\Longrightarrow \qquad u(t) = K(x(t) - x^{\text{exer}}), \quad K = -B^{\top} X,$$

$$XA + A^{\top} X - XBB^{\top} X + C^{\top} C = 0,$$

where $A = (\partial \mathcal{F}/\partial)(x^{\text{exer}}, q)$, $B = \text{col}(0, \ldots, 1)$,
$C = (q_{\text{as}}, 0, \ldots, 0)$.

Dynamical observer



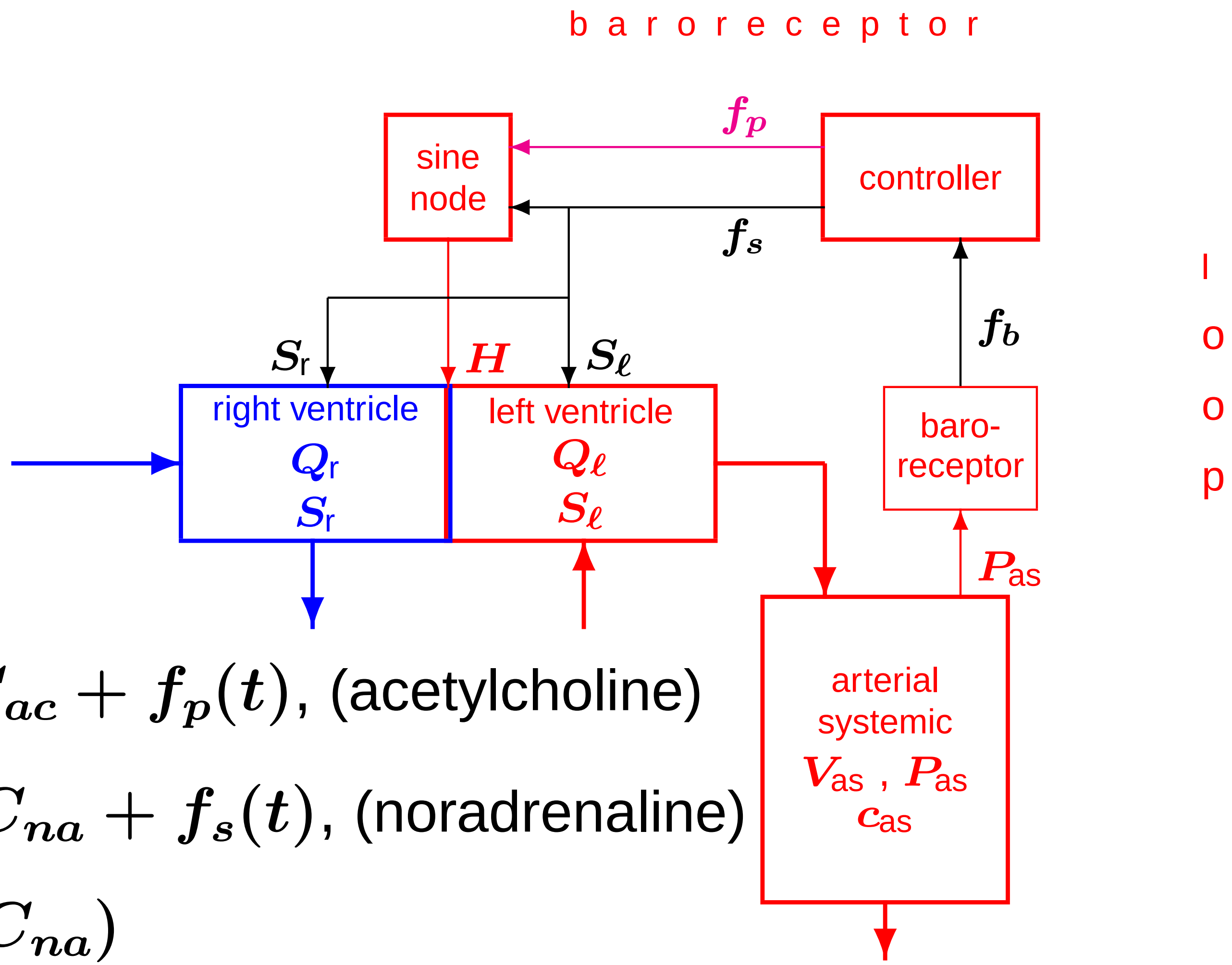
$$\dot{\hat{x}}(t) = (A + BK - LC)(\hat{x}(t) - x^{\text{exer}}) + LC(x(t) - x^{\text{exer}}), \quad t \geq 0,$$

$$x(0) = \hat{x}(0) = x^{\text{rest}},$$

where

$$YA^{\mathsf{T}} + AY - YC^{\mathsf{T}}CY + BB^{\mathsf{T}} = 0.$$

Baroreceptor-loop

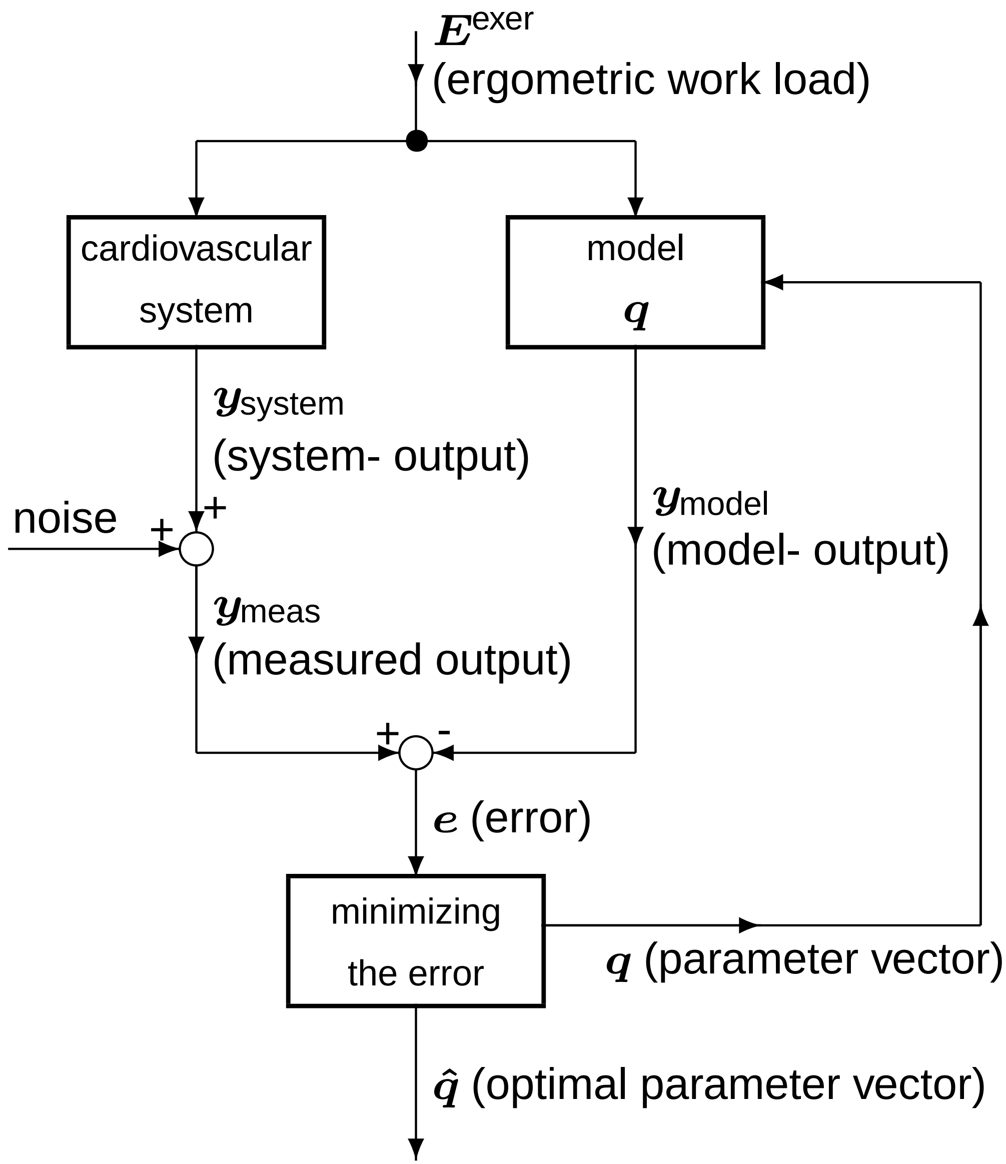


$$\dot{C}_{ac} = -\tau_{ac} C_{ac} + f_p(t), \text{ (acetylcholine)}$$

$$\dot{C}_{na} = -\tau_{na} C_{na} + f_s(t), \text{ (noradrenaline)}$$

$$H = h(C_{ac}, C_{na})$$

Parameter identification



Parameter identification

Output-least-squares formulation:

$\mathcal{Q}$ . . . *admissible parameter set*

Find $\hat{q} \in \mathcal{Q}$ *such that* $G(\hat{q}) = \min_{q\in\mathcal{Q}} G(q)$, *where*

$$G(q) = a_1^{\text{rest}} \sum_{i=N_{\text{start}}}^{-1} \left(P_{as}^{\text{rest}}(q) - \xi_i\right)^2 + a_1^{\text{exer}} \sum_{i=0}^{N_{\text{end}}} \left(P_{as}(t_i;q) - \xi_i\right)^2$$

$$+ a_2^{\text{exer}} \sum_{i=0}^{N_{\text{end}}} \left(H(t_i;q) - \eta_i\right)^2$$

$$+ a_3^{\text{rest}} \sum_{i=\tilde{N}_{\text{start}}}^{-1} \left(Q_\ell^{\text{rest}}(q) - \zeta_i\right)^2 + a_3^{\text{exer}} \sum_{i=0}^{\tilde{N}_{\text{end}}} \left(Q_\ell(\tilde{t}_i;q) - \zeta_i\right)^2.$$

Digression 2: Bromsulfalein test

Comparison of model-output and data:

$$J(k_1, k_{-1}, k_2, V) = \sum_{i=1}^{N} \left(\xi_i - \frac{1}{V} x(t_i; k_1, k_{-1}, k_2)\right)^2$$

$$\longrightarrow \text{ Min}$$

$$\Longrightarrow \quad \hat{k}_1,\ \hat{k}_{-1},\ \hat{k}_2,\ \hat{V}$$

Another possibility:

$$\tilde{J}(k_1, k_{-1}, k_2, V) = \sum_{i=1}^{N} \left|\xi_i - \frac{1}{V} x(t_i; k_1, k_{-1}, k_2)\right|$$

Digression 2: Bromsulfalein test

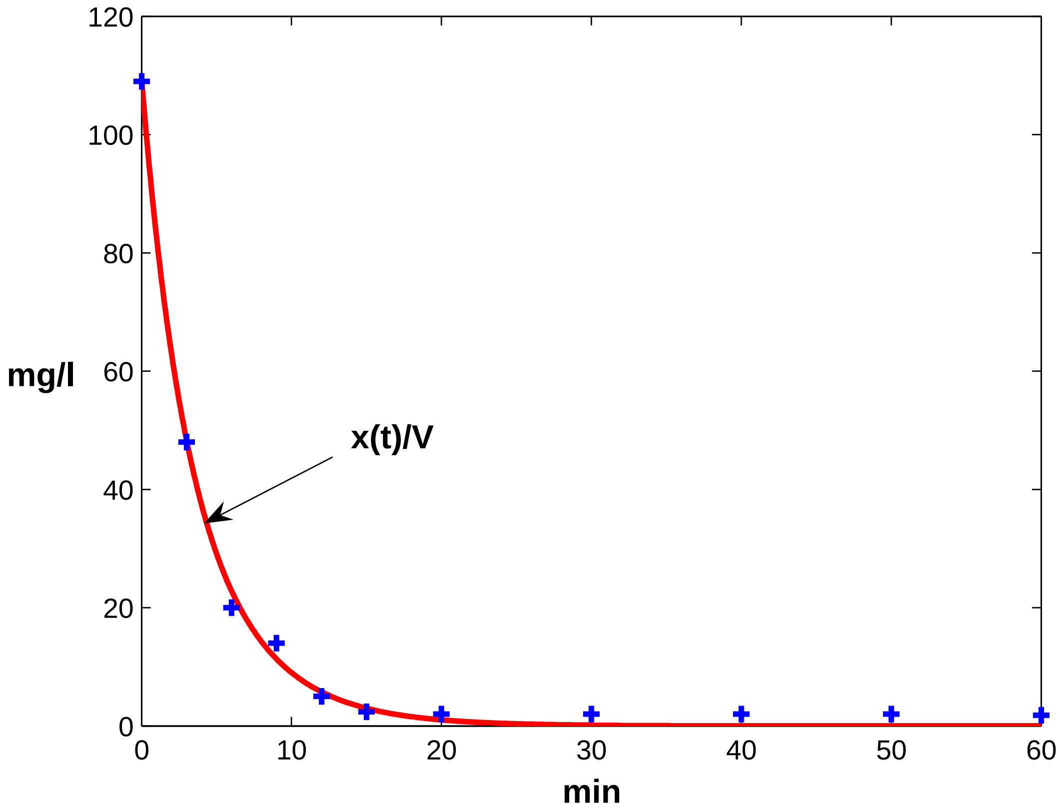
Cost functional J:

$$V = 5.4885\, l$$

$$k_1 = 0.2861\,\text{min}^{-1}$$

$$k_{-1} = 0.0350\,\text{min}^{-1}$$

$$k_2 = 0.3166\,\text{min}^{-1}$$



Digression 2: Bromsulfalein test

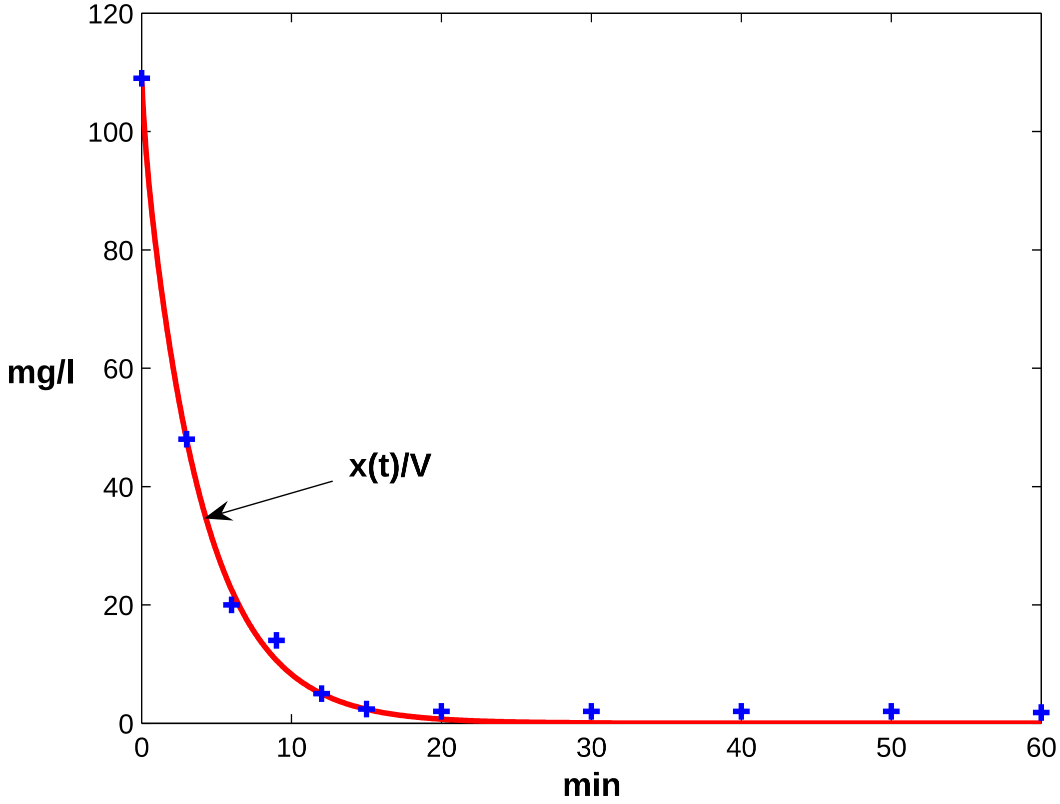
Cost functional $\tilde{J}$:

$$V = 5.5046\, l$$

$$k_1 = 0.5021\,\text{min}^{-1}$$

$$k_{-1} = 1.8297\,\text{min}^{-1}$$

$$k_2 = 2.0852\,\text{min}^{-1}$$



Digression 2: Bromsulfalein test

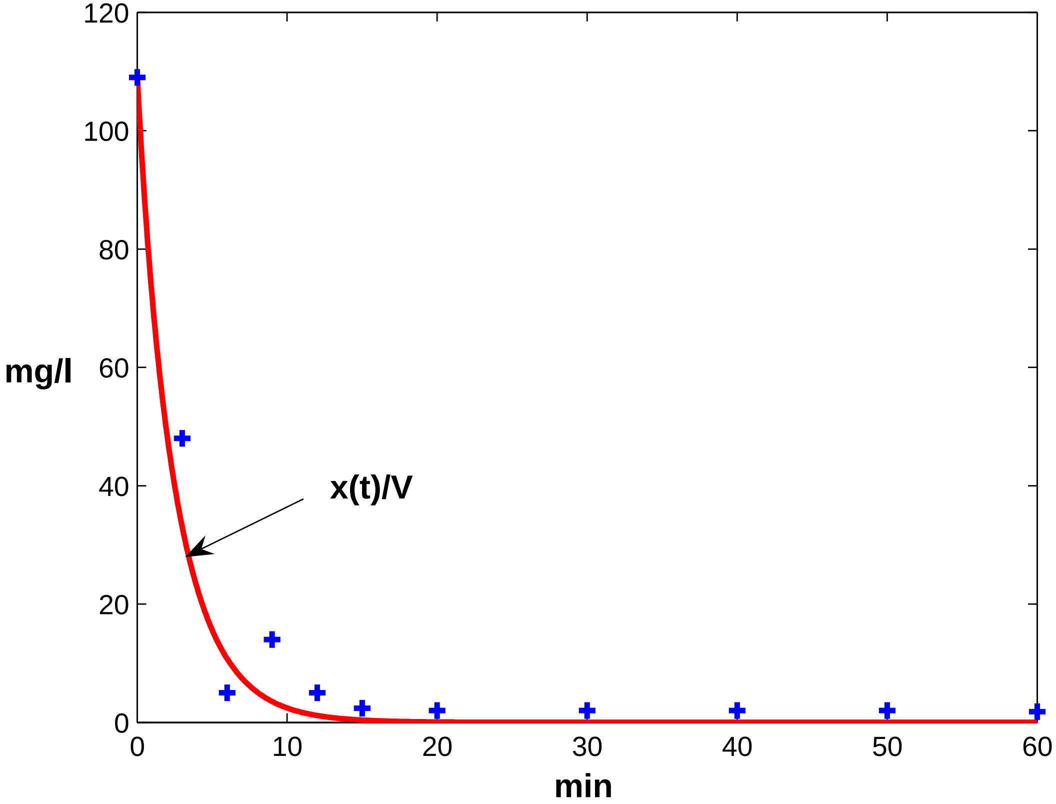
Cost functional J and one outlier:

$$V = 5.4897\, l$$

$$k_1 = 0.4427\, \text{min}^{-1}$$

$$k_{-1} = 0.1273\, \text{min}^{-1}$$

$$k_2 = 1.0444\, \text{min}^{-1}$$



Digression 2: Bromsulfalein test

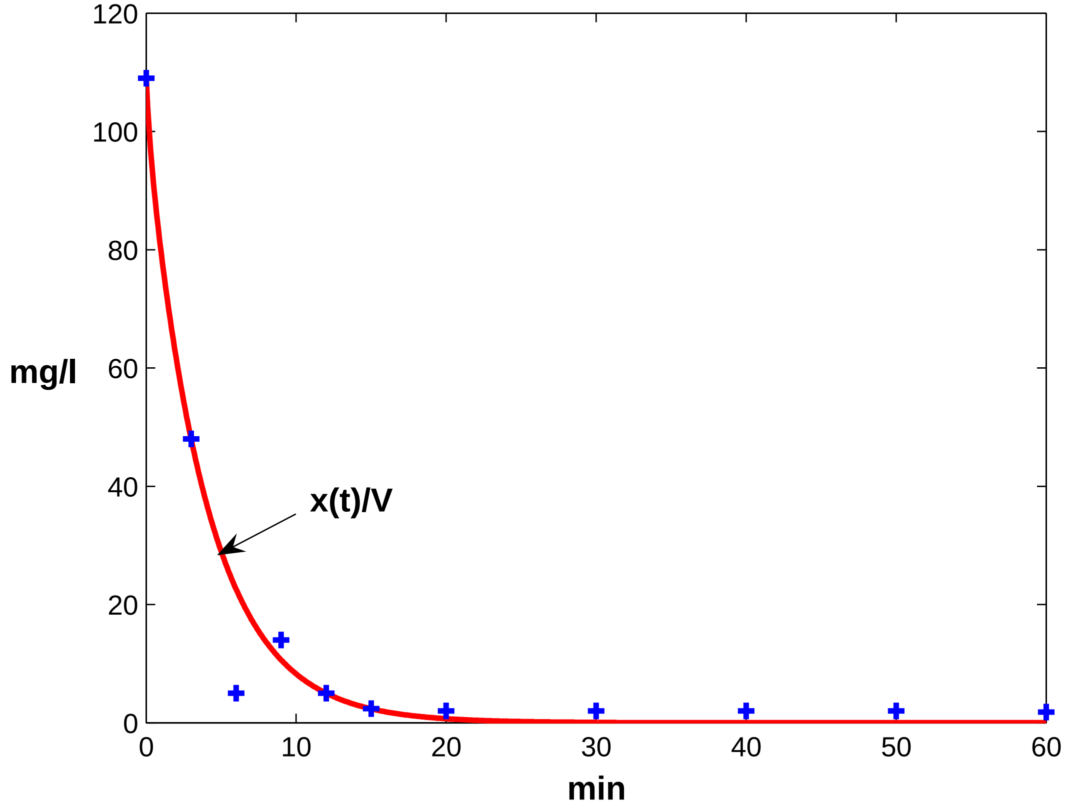
Cost functional $\tilde{J}$ and one outlier:

$$V = 5.5046\,l$$

$$k_1 = 0.4944\,\text{min}^{-1}$$

$$k_{-1} = 1.7460\,\text{min}^{-1}$$

$$k_2 = 2.0560\,\text{min}^{-1}$$



Digression 2: Bromsulfalein test

J	Case 1	Case 2	
	5.4885	5.4897	V
	0.2861	0.4427	k_1
	0.0350	0.1273	k_{-1}
	0.3166	1.0444	k_2

$\tilde{J}$	Case 1	Case 2	
	5.5046	5.5046	V
	0.5021	0.5046	k_1
	1.8297	1.7460	k_{-1}
	2.0852	2.0560	k_2

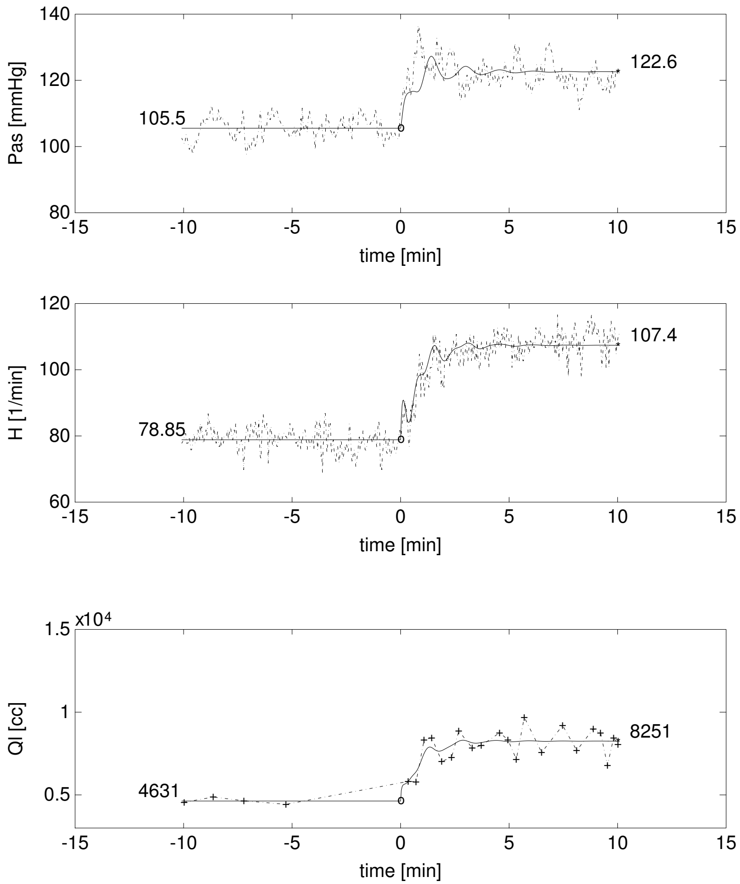
Digression 2: Bromsulfalein test

J	Case 1	Case 2	
	5.4885	5.4897	V
	0.2861	0.4427	k_1
	0.0350	0.1273	k_{-1}
	0.3166	1.0444	k_2

$\tilde{J}$	Case 1	Case 2	
	5.5046	5.5046	V
	0.5021	0.5046	k_1
	1.8297	1.7460	k_{-1}
	2.0852	2.0560	k_2

$\Longrightarrow$ L^1-cost functional less sensitive against outliers !!

Results



Measurements (dot-dashed) for P_{as}, H, Q_ℓ and model-output (solid).

Basic Concepts in the Methodology of Mathematical Modeling

Lecture 4: Receding Horizon Control (RHC)

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RHC

Model equations:

$$\begin{aligned} \dot{x}(t) &= \mathcal{F}(x(t), q) + Bu(t), \quad t \geq 0 \\ x(0) &= x^{\text{rest}}. \end{aligned} \tag{1}$$

($x = \text{col}\, P_{\text{as}}, P_{\text{vs}}, P_{\text{ap}}, P_{\text{vp}}, S_{\ell}, S_{\text{r}}, R_{\text{s}}, H),$
$B = \text{col}\,(1, 0, \ldots, 0)$)

Find $u(\cdot)$ such that $\lim_{t\to\infty} x(t) = x^{\text{exer}}$.

RHC

Minimize $J(x,u)$ over all $u \in L^2(t_b,t_e;\mathbb{R})$,

$$J(x,u) = \int_{t_b}^{t_e} \big((P_{\text{as}}(t) - P_{\text{as}}^{\text{exer}})^2 + \kappa_c^2 u(t)^2 \big)\, dt$$

$$+ \frac{\alpha_c}{2} (P_{\text{as}}(t_e) - P_{\text{as}}^{\text{exer}})^2,$$

where $x = x(\cdot; u)$ solves (1).

Problem of constraint optimization:

Minimize $J(x,u)$ subject to

$\dot{x}(t) = \mathcal{F}(x(t), q) + Bu(t), \quad t_b \le t \le t_e,$

$x(t_b) = x^{\text{rest}}.$

RHC

Introduce Lagrange multipliers:

$$
\begin{aligned}
\boldsymbol{L}(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{\lambda_1}, \boldsymbol{\lambda_2}) = \boldsymbol{J}(\boldsymbol{x}, \boldsymbol{u}) \\
&+ \int_{t_b}^{t_e} \left(\dot{\boldsymbol{x}}(t) - \boldsymbol{\mathcal{F}}(\boldsymbol{x}(t), \boldsymbol{q}) + \boldsymbol{B}\boldsymbol{u}(t)\right)^{\mathsf{T}} \boldsymbol{\lambda_1}(t)\, dt \\
&+ \left(\boldsymbol{x}(t_b) - \boldsymbol{x}^{\text{exer}}\right)^{\mathsf{T}} \boldsymbol{\lambda_2}
\end{aligned}
$$

RHC

First order necessary conditions:

a) State equations:

$$\dot{x}(t) = \mathcal{F}(x(t), q) + Bu(t), \quad t_b \leq t \leq t_e$$
$$x(t_b) = x^{\text{rest}}.$$

b) Adjoint equations:

$$\dot{\lambda}_1(t) + \mathcal{F}_x(x(t), q)^{\mathsf{T}}\lambda_1(t) - 2Q(x(t) - x^{\text{exer}}) = 0, \ t_b \leq t \leq t_e,$$
$$\lambda_1(t_e) = -\alpha_c Q(x(t_e) - x^{\text{exer}}),$$
$$\lambda_2 = \lambda_1(t_b),$$

where $Q = \text{diag}\,(1, 0, \ldots, 0)$.

RHC

c) Optimality condition:

$$2\kappa_c^2 u(t) = B^\top \lambda_1(t), \quad t_b \le t \le t_e,$$

Gradient of the reduced costs:

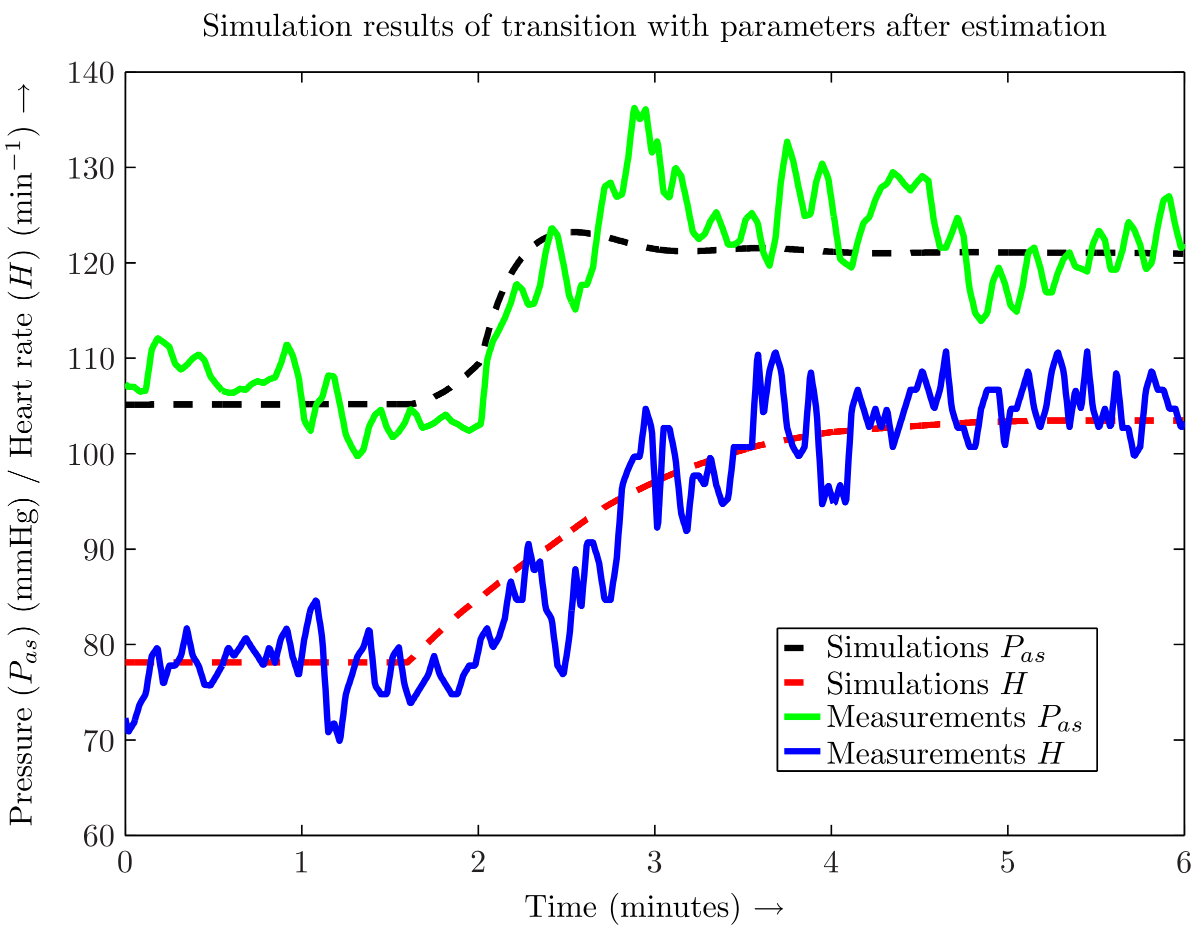
$$\nabla_u J(x(\cdot,u),u)(\cdot) = 2\kappa_c^2 u - B^\top \lambda_1, \quad t_b \le t \le t_e.$$

(Note that $\nabla_u J(x(\cdot,u),u)$ is in $\mathcal{L}(L^2(t_b,t_e;\mathbb{R}),\mathbb{R})$ and can be represented by an L^2-function)

$t_e = t_b + \Delta T$, $t_c = t_b + \rho\Delta T$, $\rho \in (0,1)$

Start with $t_b = 0$. Next t_b is given by $t_c = \rho\Delta T$, etc.

RHC – Example



Simulation results of transition with parameters after estimation
Pressure (P_{as}) (mmHg) / Heart rate (H) (min^{-1}) →
Time (minutes) →
140
130
120
110
100
90
80
70
60
0
1
2
3
4
5
6
Simulations P_{as}
Simulations H
Measurements P_{as}
Measurements H

Basic Concepts in the Methodology of Mathematical Modeling

Lecture 5: Generalized Sensitivities

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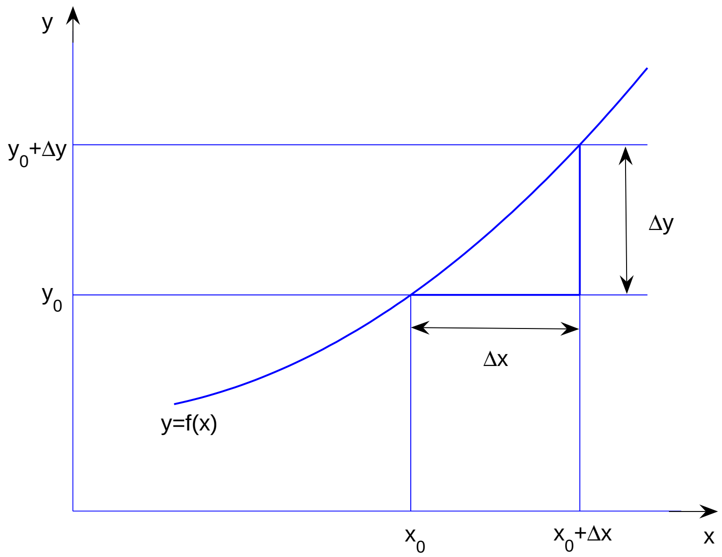
Classical sensitivities

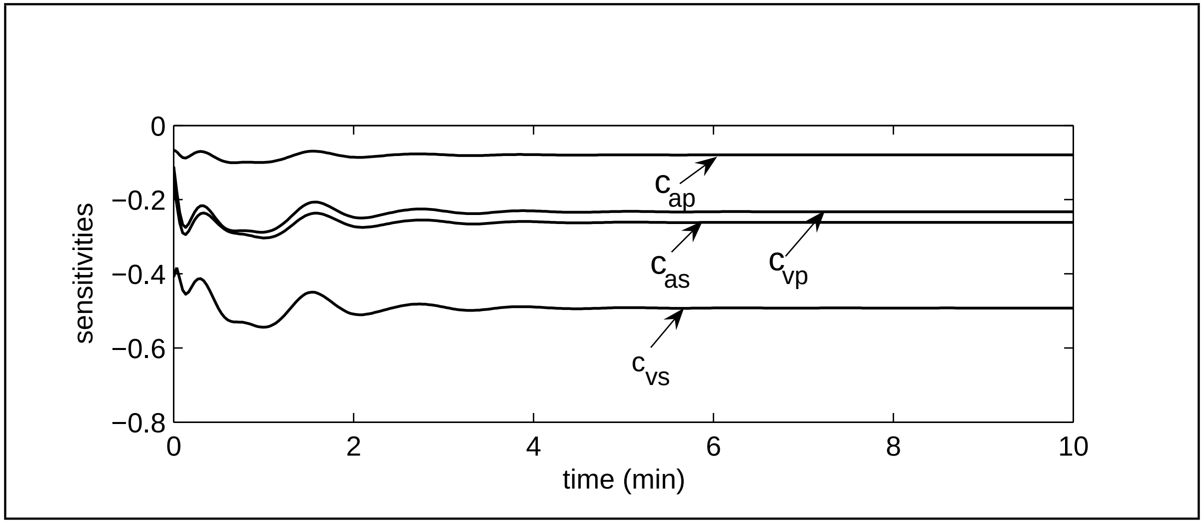


Relative errors:
$\Delta x/x_0$ and $\Delta y/y_0$

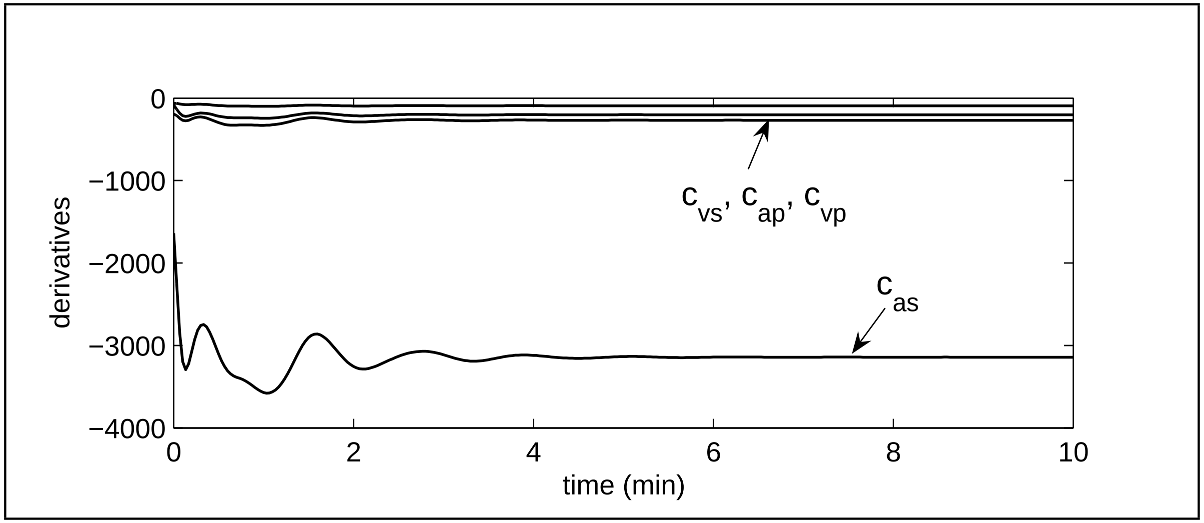
Sensitivity of y with respect to x at x_0:

$$\sigma_{y,x}(x_0) = \lim_{\Delta x \to 0} \frac{\Delta y/y_0}{\Delta x/x_0} = \frac{x_0}{y_0}\, y'(x_0).$$

Classical sensitivities



Sensitivities of P_{as}



Derivatives of P_{as}

Generalized sensitivities

Sensitivity:
Measure for the dependence of outputs or states on parameters.

Generalized sensitivity:
Sensitivity of the parameter estimates with respect to variations in the measurements.

Generalized sensitivities

Single output system: $y(t) = f(t, \theta)$, $0 \leq t \leq T$,

$\theta = \left(\theta_1, \ldots, \theta_p\right)^{\mathsf{T}}$ . . . model parameters
ξ_k . . . measurements for $y(t_k), 0 \leq t_1 < \cdots < t_M \leq T$

$$\xi_k = z(t_k) + e_k, \quad k = 1, \ldots, M,$$

$z(t)$ . . . 'true' output of the system
e_k . . . measurement noise for ξ_k

Generalized sensitivities

Assumptions on e_k:

(i) e_k has zero mean, $k = 1, \dots, M$.

(ii) The e_k's are identically distributed.

(iii) The variance σ_k^2 of e_k is not dependent on θ.

Generalized sensitivities

Basic assumption:

$$\exists \theta_0 : \quad z(t_k) = f(t_k, \theta_0),\ k = 1, \ldots, M.$$

Output least squares formulation ($\xi = (\xi_1, \ldots, \xi_M)$):

$$\hat{\theta}_0 = \mathrm{argmin}_\theta\, J(\xi, \theta),$$

$$J(\xi, \theta) = \sum_{k=1}^{M} \frac{1}{\sigma_k^2} \big(\xi_k - f(t_k, \theta)\big)^2$$

Generalized sensitivities

Assumptions:

a) Unique local identifiability at θ_0.

$$\forall \theta_1 \in \mathcal{U}(\theta_0) \exists ! \hat{\theta}_1 : \hat{\theta}_1 = \operatorname{argmin}_\theta J(\ldots f(t_k, \theta_1) + e_k \ldots, \theta)$$

Note: We consider $\xi \sim \xi(\theta_0)$, because $\xi = F(\theta_0) + e$!!

b) Estimates are unbiased, i.e., $E(\hat{\theta}_0) = \theta_0$.

$\Longrightarrow$

$$\nabla_\theta J(\xi, \hat{\theta}_0) = 0, \quad \nabla_{\theta\theta} J > 0.$$

Generalized sensitivities

Quantity of interest: $\dfrac{\partial \hat{\theta}}{\partial \theta}$

$$\frac{\partial \hat{\theta}(\theta)}{\partial \theta} = -\big(\nabla_{\theta\theta} J(\xi(\theta), \hat{\theta}(\theta))\big)^{-1} \nabla_{\xi\theta} J(\xi(\theta), \hat{\theta}(\theta)) \frac{\partial F(\theta)}{\partial \theta}$$

$$F(\theta) = \big(f(t_1, \theta), \ldots, f(t_M, \theta)\big)$$

Generalized sensitivities

$\Longrightarrow$ (taking expected values)

$$\frac{\partial \hat{\theta}(\theta)}{\partial \theta} = \sum_{k=1}^{M} \frac{1}{\sigma_k^2} \left(\Big(\sum_{j=1}^{M} \frac{1}{\sigma_j^2} \big(\nabla_\theta f(t_j, \theta)\big)^{\mathsf{T}} \nabla_\theta f(t_j, \theta) \Big)^{-1} \times \big(\nabla_\theta f(t_k, \theta)\big)^{\mathsf{T}} \right) \nabla_\theta f(t_k, \theta) \equiv I.$$

Estimate $\hat{\theta}_j$ for $(\theta_0)_j$ is independent from the estimate $\hat{\theta}_k$ for $(\theta_0)_k$, $k \neq j$

Generalized sensitivities

Modification: All deviations $\xi_k - f(t_k, \theta)$, $k = 1, \ldots, M$, still enter the cost functional, but we only have access to the measurements $\xi_1, \ldots, \xi_{k_0}$, $1 \leq k_0 \leq M$.

$\Longrightarrow$

$$\frac{\partial \hat{\theta}}{\partial \theta} = \Big(\sum_{j=1}^{M} \frac{1}{\sigma_j^2} \big(\nabla_\theta f(t_j, \theta)\big)^{\mathsf{T}} \nabla_\theta f(t_j, \theta)\Big)^{-1}$$

$$\times \sum_{k=1}^{k_0} \frac{1}{\sigma_k^2} \nabla_\theta f(t_k, \theta)\big)^{\mathsf{T}} \nabla_\theta f(t_k, \theta).$$

Generalized sensitivities

Generalized sensitivity for parameter θ_i:

$$g_i(t_{k_0}) = \sum_{k=1}^{k_0} \frac{1}{\sigma_k^2} \Bigg(\Bigg(\overbrace{\sum_{j=1}^{M} \frac{1}{\sigma_j^2} \big(\nabla_\theta f(t_j,\theta)\big)^{\mathsf{T}} \nabla_\theta f(t_j,\theta)}^{\mathcal{M} :=} \Bigg)^{-1} \big(\nabla_\theta f(t_k,\theta)\big)^{\mathsf{T}} \Bigg)_i \big(\nabla_\theta f(t_k,\theta)\big)_i.$$

Note that

$$\text{rank}\, \big(\nabla_\theta f(t_j,\theta)\big)^{\mathsf{T}} \nabla_\theta f(t_j,\theta) = 1, \quad \text{but} \quad \mathcal{M} \in \mathbb{R}^{p \times p}$$

Incremental gen. sensitivities

Incremental generalized sensitivity functions:

$$g_{\mathsf{inc},i}(t_{k_0}) = g_i(t_{k_0}) - g_i(t_{k_0-1}), \quad k_0 = 1, \dots, M.$$

Explicit representation:

$$g_{\mathsf{inc},i}(t_{k_0}) = \frac{1}{\sigma_{k_0}^2}\Big(\mathcal{M}^{-1}\big(\nabla_\theta f(t_{k_0}, \theta)\big)^{\mathsf{T}}\Big)_i \big(\nabla_\theta f(t_{k_0}, \theta)\big)_i,$$
$$k_0 = 1, \dots, M, \ i = 1, \dots, p.$$

Interpretation

Fisher information matrix:

$$\mathcal{J}(\theta) = \sum_{k=1}^{M} \frac{1}{\sigma_k^2} \big(\nabla_\theta f(t_k, \theta)\big)^{\mathsf{T}} \nabla_\theta f(t_k, \theta) \eta_k$$

η_k . . . weight for measurement ξ_k at time t_k ($= 1$ in our case)
Information index: $\ln\big(\det \mathcal{J}(\theta)\big)$
$\frac{\partial}{\partial \eta_k} ln(\det \mathcal{J}(\theta))$ . . . information on the parameters θ provided by the measurement ξ_k.

Interpretation

$$\boxed{\frac{\partial}{\partial \eta_k} \ln(\det \mathcal{J}(\theta)) = \sum_{i=1}^{p} g_{i,\text{inc}}(t_k) \geq 0}$$

$\Longrightarrow \qquad k \to \sum_{i=1} g_i(t_k)$ is increasing

Identification procedure is efficient, i.e.,

$$\text{Cov}\,\hat{\theta} = \mathcal{J}(\hat{\theta})^{-1} = \mathcal{M}^{-1} \qquad \text{(Cramer-Rao bound)}$$

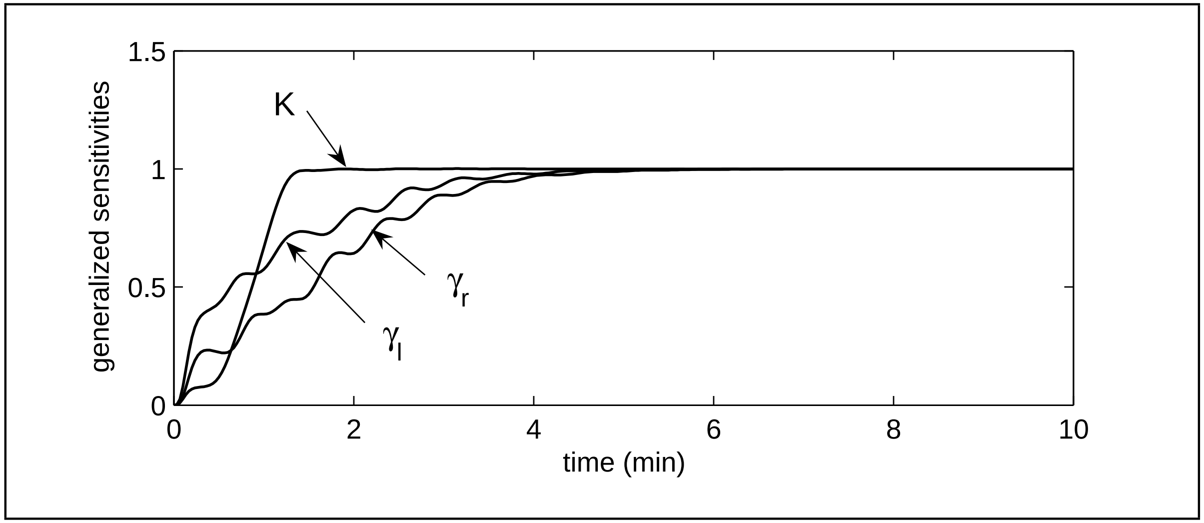
Interpretation

a) Information provided by the measurements for given parameters uncorrelated$\Longrightarrow$generalized sensitivity functions for these parameters monotonically increasing

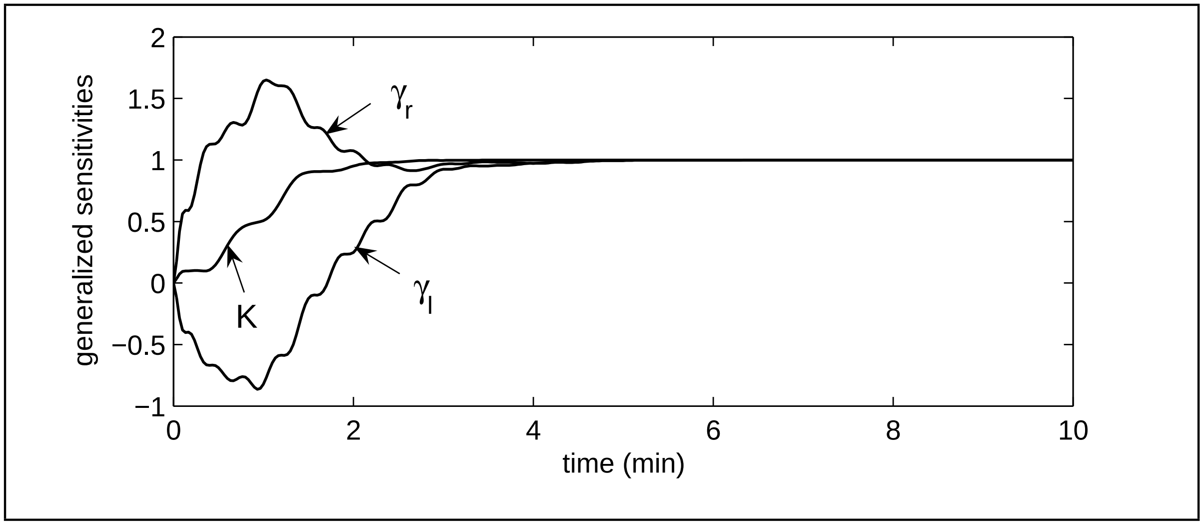
b) In case of a) measurements in that time interval, where the generalized sensitivity function of a parameter has most of its increase from 0 to 1, are the measurements which carry most of the information on that parameter.

c) Is the information on given parameters rather strongly correlated$\Longrightarrow$oscillations of the generalized sensitivity functions

Examples

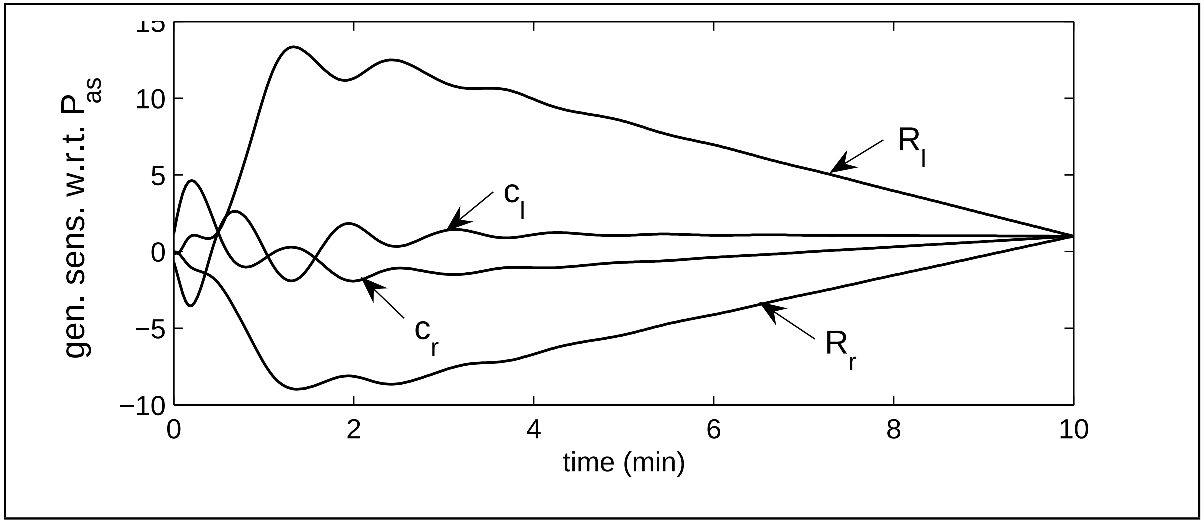


P_{as}

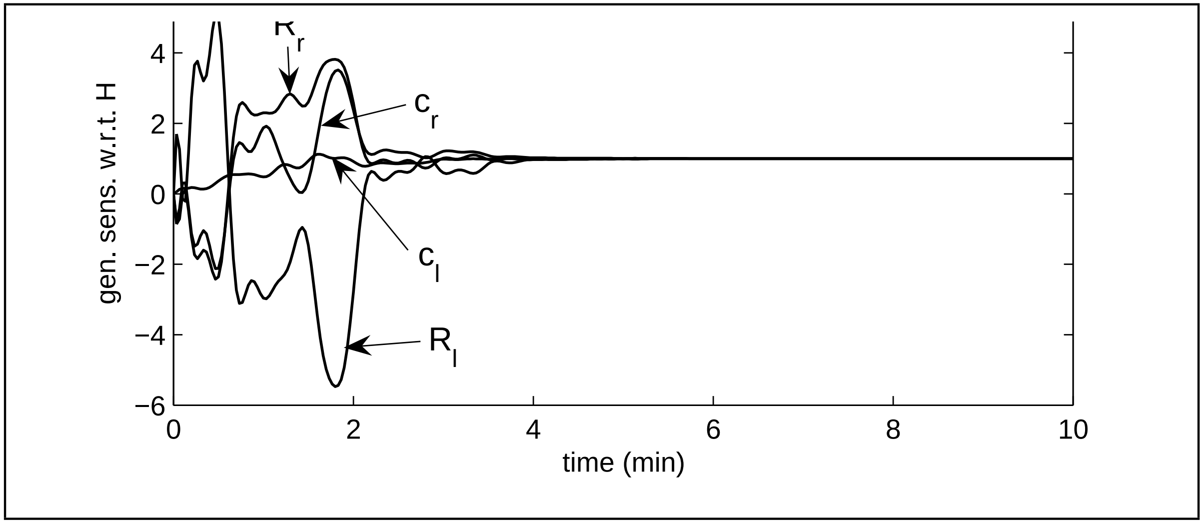


H

Examples

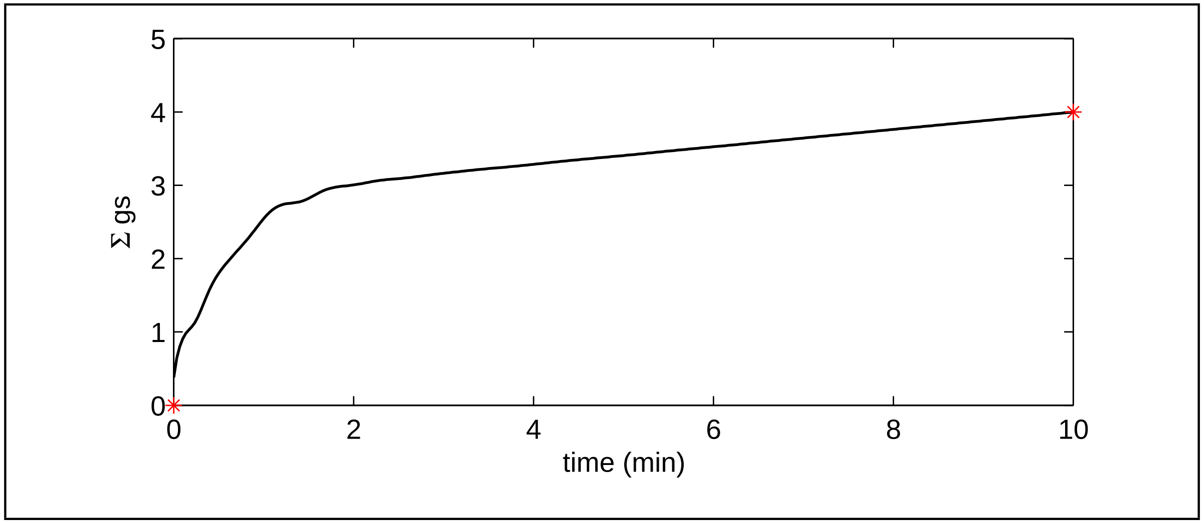


P_{as}



H

Examples



Sum of generealized sensitivities for P_{as}

Basic Concepts in the Methodology of Mathematical Modeling

Lecture 6: The Basic Model and Time Series

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The basic model

$$c_{\text{as}}\dot{P}_{\text{as}} = Q_\ell - F_{\text{s}},$$

$$c_{\text{vs}}\dot{P}_{\text{vs}} = F_{\text{s}} - Q_{\text{r}},$$

$$c_{\text{ap}}\dot{P}_{\text{ap}} = Q_{\text{r}} - F_{\text{p}},$$

$$\boxed{\dot{x}(t) = \mathcal{F}(x(t), q) + Bu(t)}$$

$$c_{\text{vp}}\dot{P}_{\text{vp}} = F_{\text{p}} - Q_\ell,$$

$$\ddot{S}_\ell + \gamma_\ell \dot{S}_\ell + \alpha_\ell S_\ell = \beta_\ell H,$$

$$\ddot{S}_{\text{r}} r + \gamma_{\text{r}} \dot{S}_{\text{r}} + \alpha_{\text{r}} S_{\text{r}} = \beta_{\text{r}} H,$$

$$\dot{R}_{\text{s}} = \frac{1}{K}\Big(A_{\text{pesk}}\big(F_{\text{s}} C_{\text{a},\text{O}_2} - M\big) - (P_{\text{as}} - P_{\text{vs}})\Big),$$

$$\dot{H} = u(t)$$

LQR control

$$u(t) = K(x(t) - x^{\text{exer}}), \quad K = -B^{\mathsf{T}}X,$$

$$XA + A^{\mathsf{T}}X - XBB^{\mathsf{T}}X + C^{\mathsf{T}}C = 0,$$

where $A = (\partial\mathcal{F}/\partial)(x^{\text{exer}}, q)$, $B = \text{col}(0, \ldots, 1)$, $C = (q_{\text{as}}, 0, \ldots, 0)$.

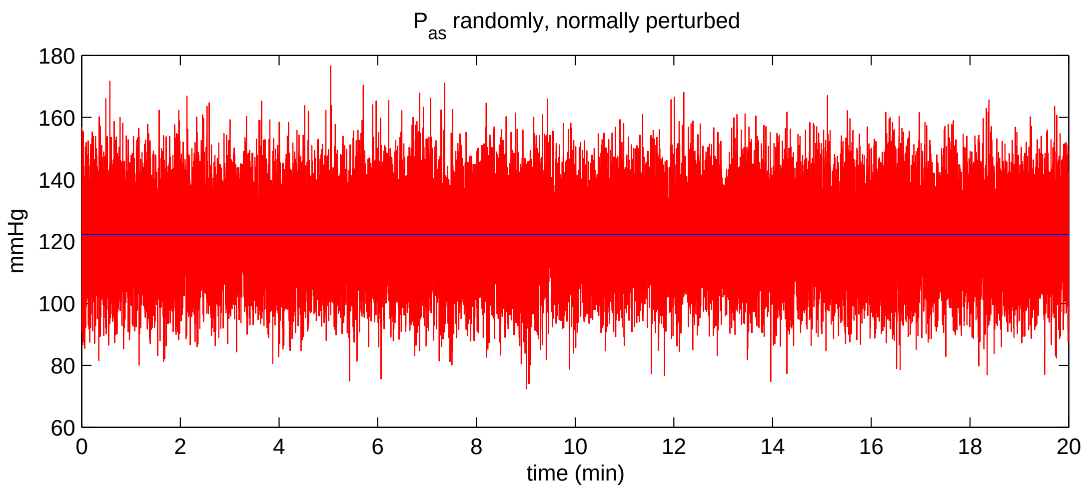
$$u(t) = k_1 P_{\text{as}} + k_2 P_{\text{vs}} + \cdots + k_{10} H.$$

Stochastic perturbations:

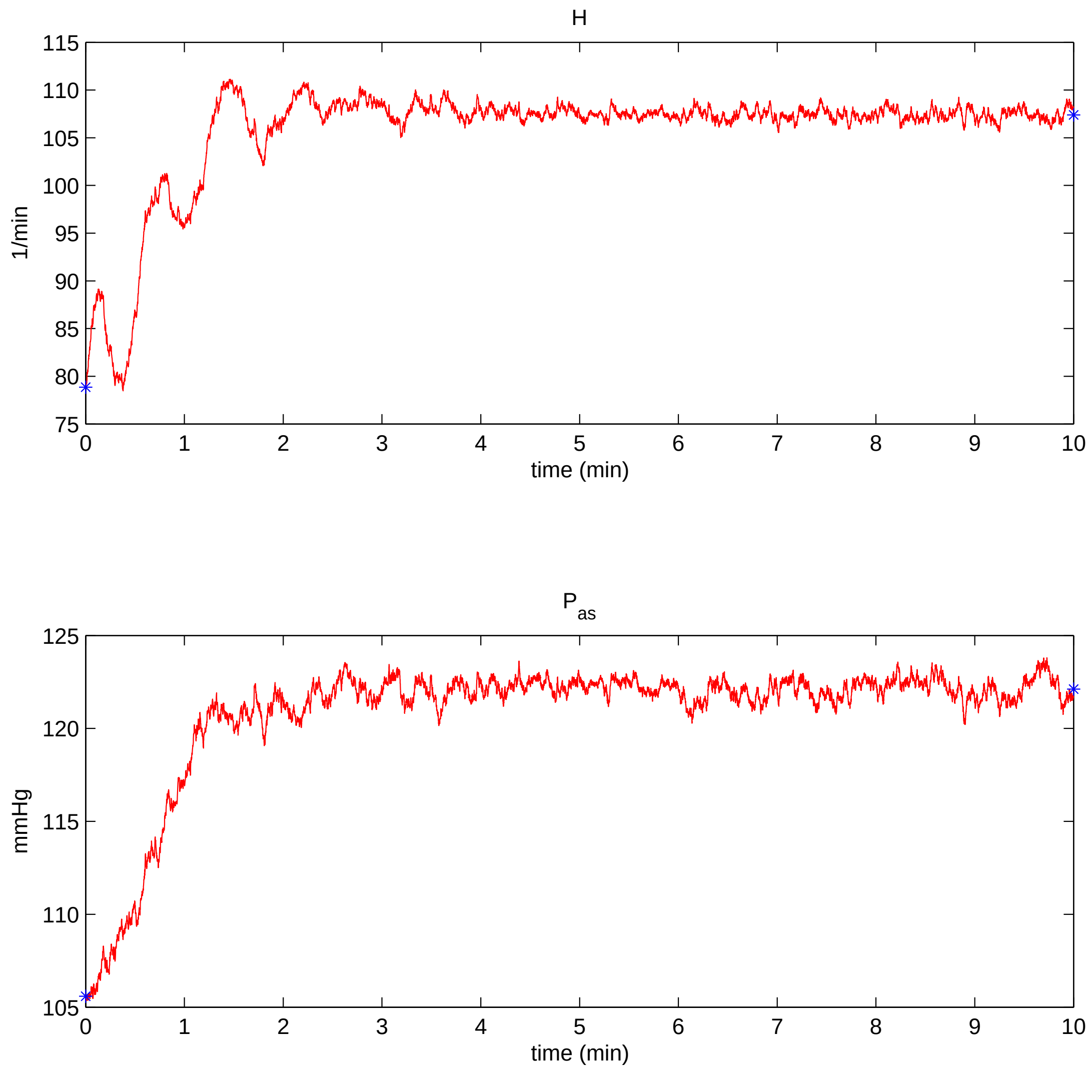
a) $u(t) = k_1\big(P_{\text{as}} + \mathcal{N}(t)\big) + \cdots + k_{10}H$

b) $u(t) = k_1 P_{\text{as}} + \cdots + k_{10}H + \mathcal{N}(t)$

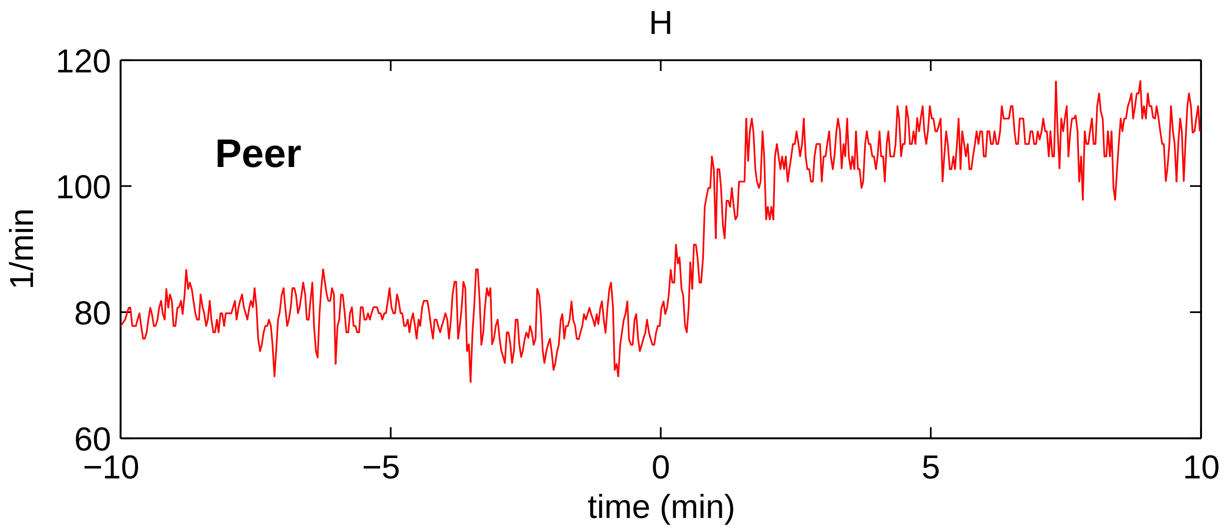
Perturbation of P_{as}



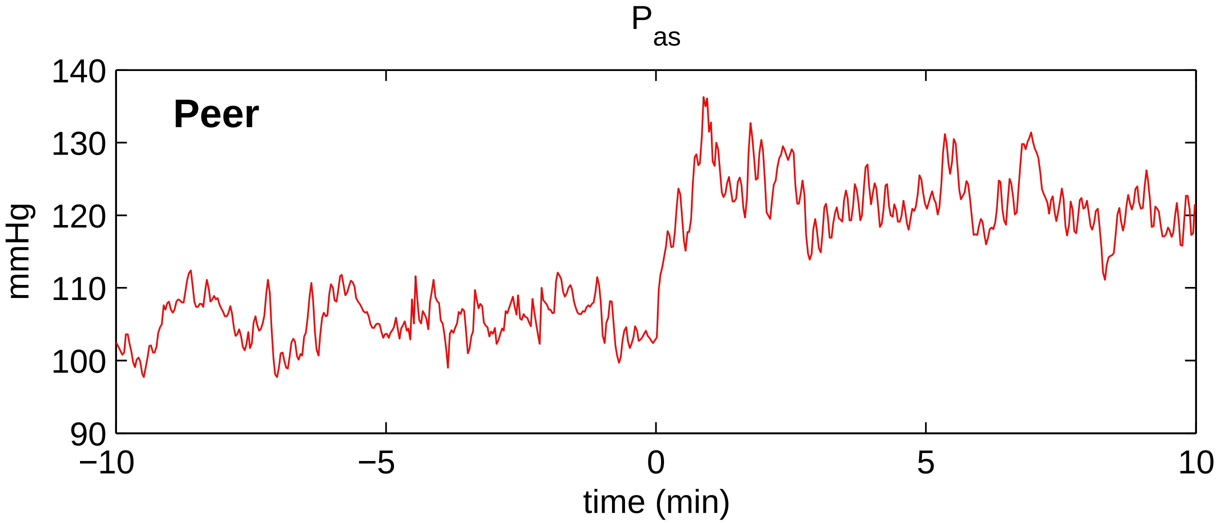
Outputs of the model



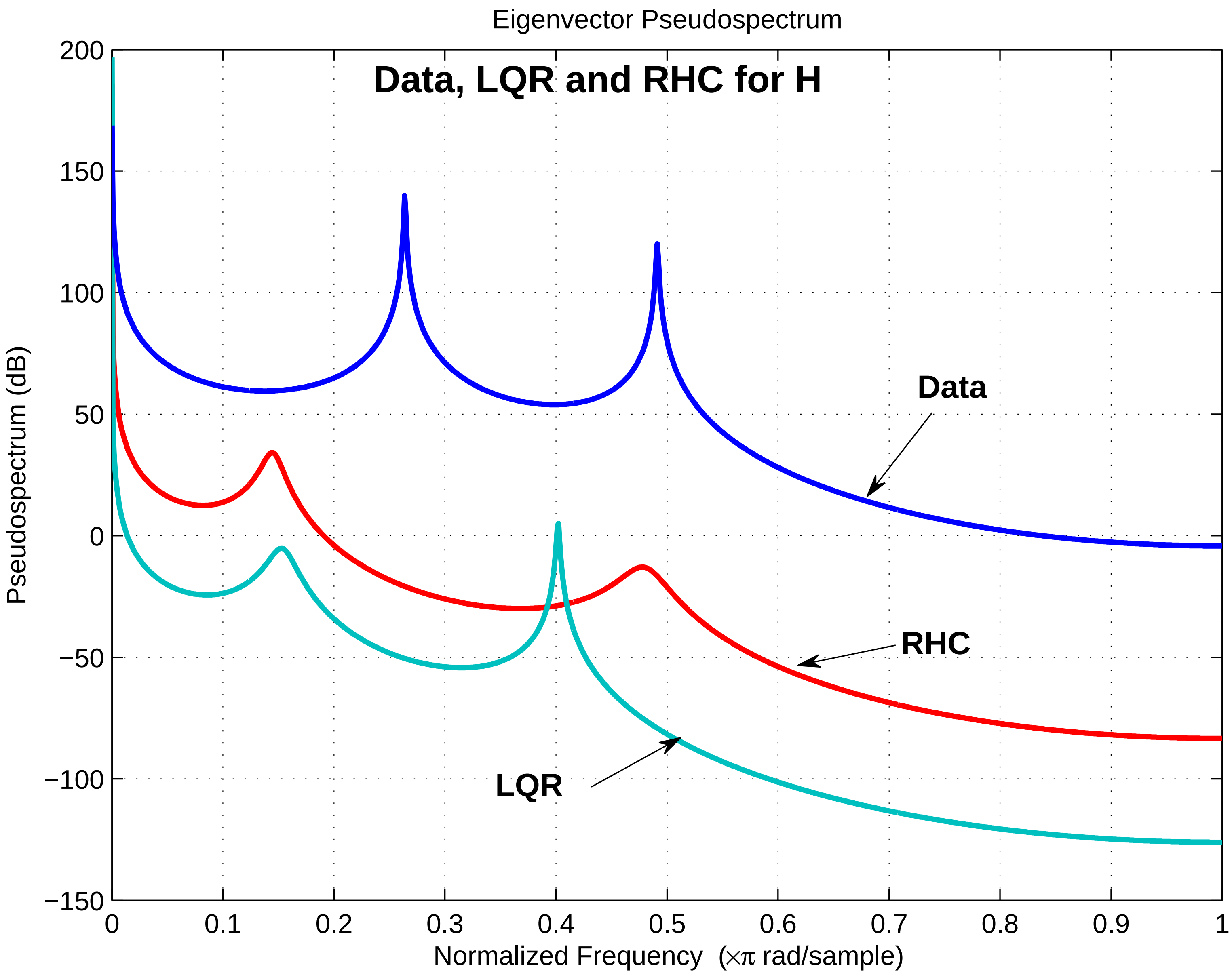
Data



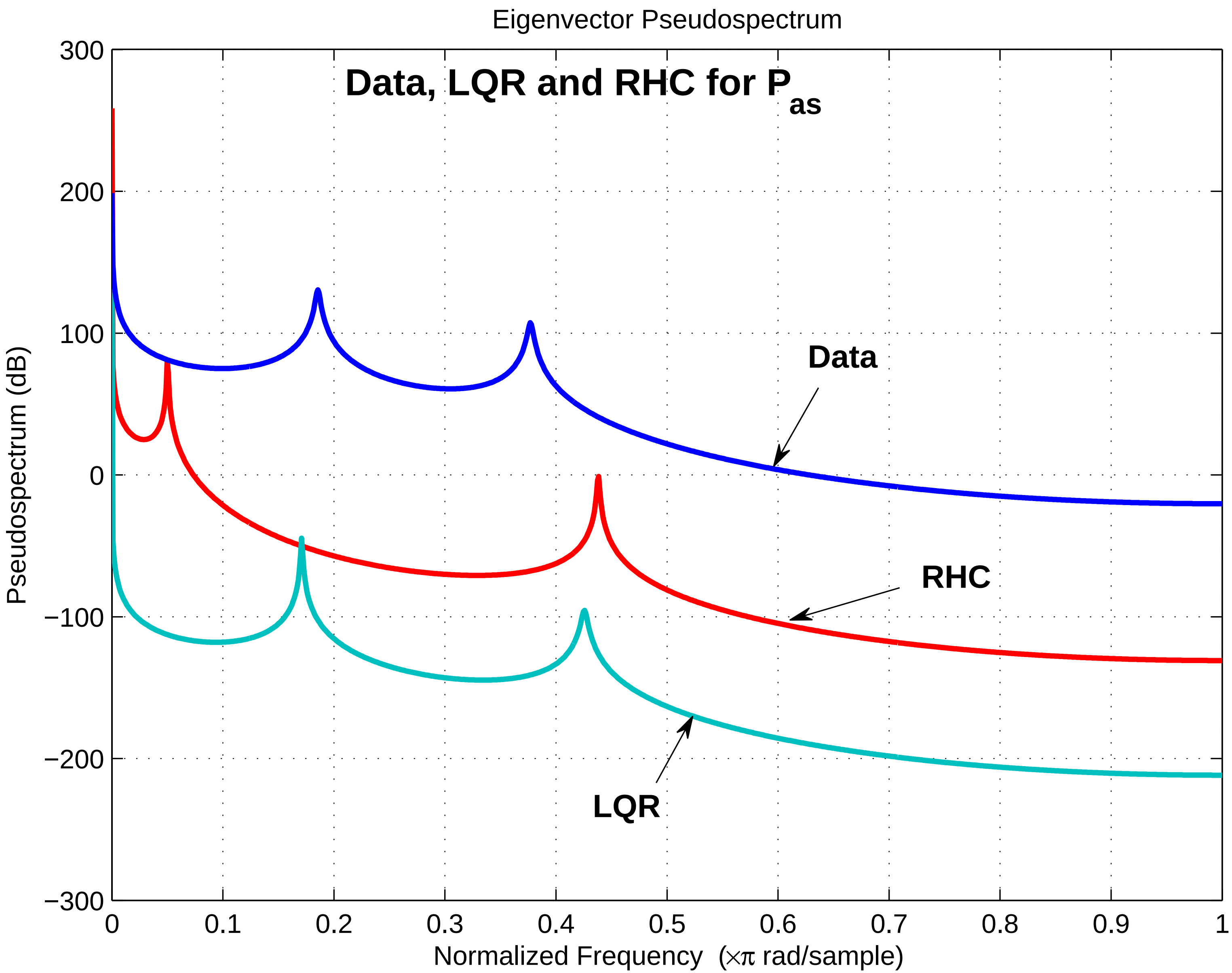
Data



Eigenvector pseudospectrum



Eigenvector pseudospectrum



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