Optimal Control of High-Throughput-Screening Systems in a Dioid Framework

Jörg Raisch[1,2] and Thomas Brunsch[1,3]

[1]Fachgebiet Regelungssysteme, TU Berlin

[2]Fachgruppe System- und Regelungstheorie
Max-Planck-Institut für Dynamik komplexer technischer Systeme

[3] LARIS, Université d'Angers

. . . joint work with Laurent Hardouin (Université d'Angers)
and Thomas Haenel (CyBio AG). . .

Outline

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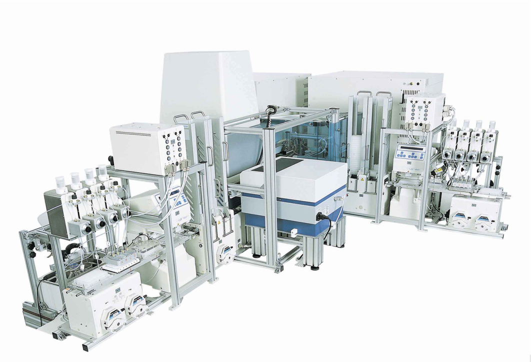
What is High-Throughput-Screening?

- Purpose of HTS: analyse large number of substances
- HTS plant: fully automated system with various resources (e.g., pipettors, incubators, readers, transportation devices)
- Typical mode of operation:
  - Aggregate (up to 1536) substances on microplates
  - Possibly need auxiliary plates to convey reactants etc
  - Batch: physical entity (one or several plates) needed for analysis



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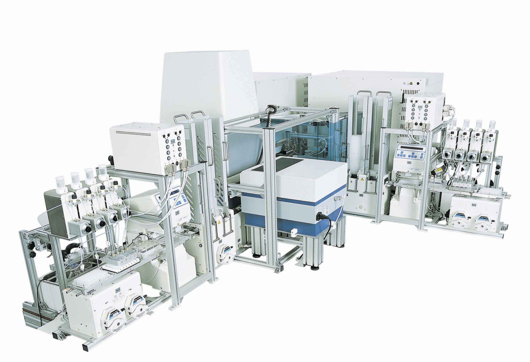

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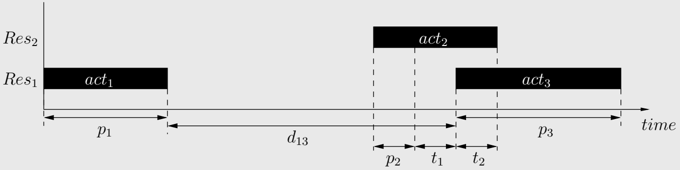
Requirements

User Provided Requirements:

. . . pertain to the single batch . . .

- Sequence of activities on available resources
- Minimal (sometimes also max.) times for (inter) activity durations
- Toy example:



Global Requirements:

- Identical time scheme for all batches!
- Subject to above constraints: maximise throughput!

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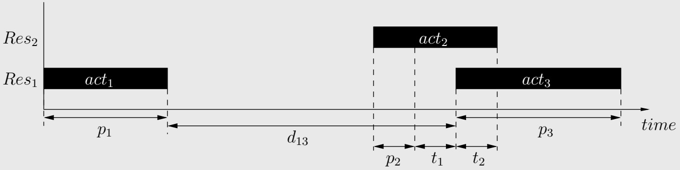

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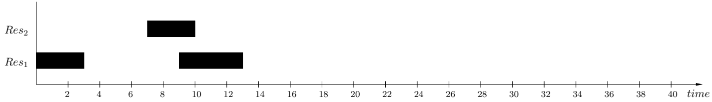
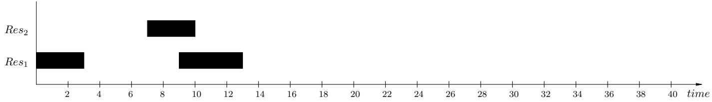
Scheduling Problem

- This amounts to an optimal scheduling (activity resource allocation) problem
- Solved in first project stage [Mayer & R 2004, Mayer et al. 2008]
  - Formulate problem as an MINLP
  - Can transform MINLP into MILP (by approp. change of variables)
- Solution for our toy problem:
  - naive approach: “stacking” minimal-time single batches click below



  - optimal solution: click below



The Need for Feedback

- Scheduling solution obtained off-line $\rightsquigarrow$ cannot cope with unforeseen disturbances
- disturbances come in form of delays

Specifications:

- Recover optimal schedule while guaranteeing max. throughput
- If solution is non-unique: minimise number of batches with different time scheme (“waste batches”)

Mechanism of interaction:

- Control input: change starting times of activities
- Measurements: time of occurrence of all events (including start and finish times for all activities)

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User defined single batch requirements

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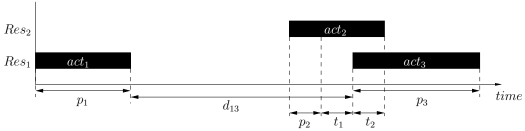

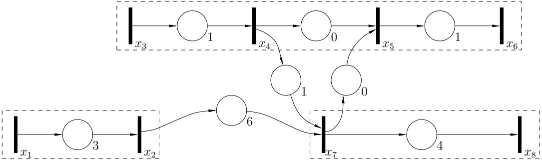

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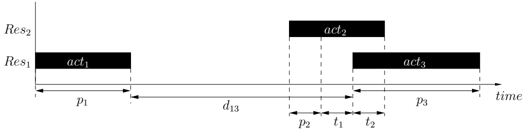

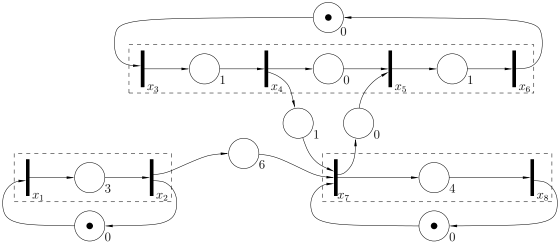

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Nesting of batches in optimal schedule

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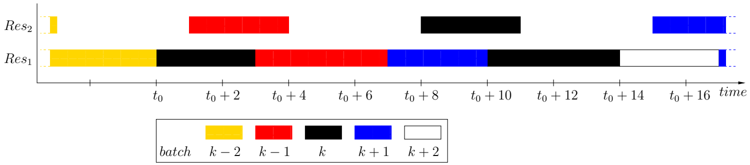

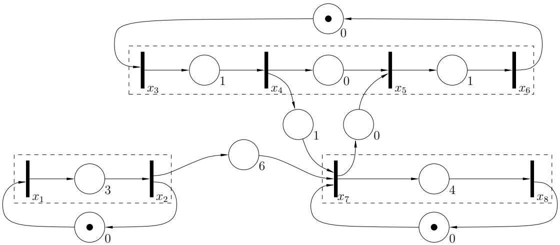

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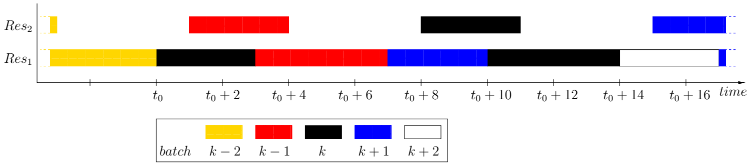

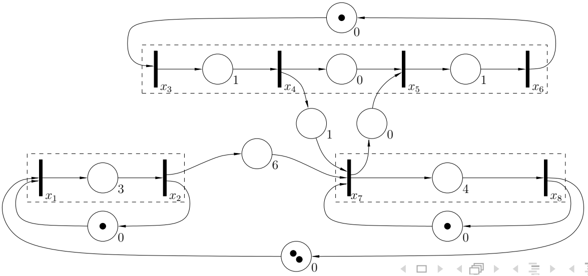

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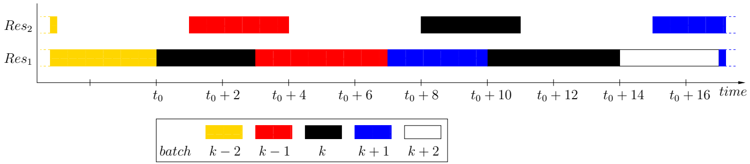

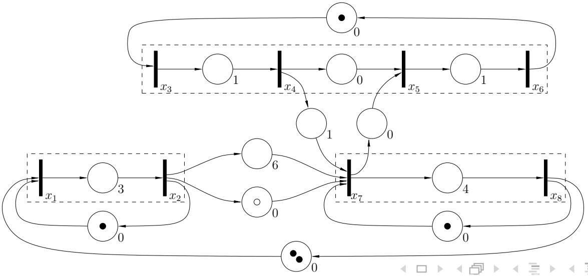

TEG Model

- Model is a Timed Event Graph (TEG)
- Provides information on event times

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$$x_7(k) \quad \ldots \quad \text{time when activity 3 in batch } k \text{ starts}$$
$$x_7(k) \geq \max\{x_4(k)+1, x_2(k)+6, x_2(k+1), x_8(k-1)\}$$

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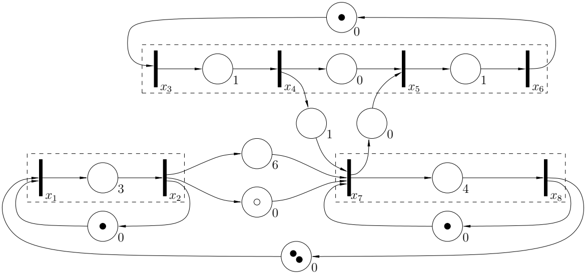

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TEG Model Ctd.

- In general:

$$x_i(k) \ \geq \max_{j,l}\{b_{ijl}x_j(k-l)+a_{ijl}\},$$
$$b_{ijl} \in \{0,1\}, \ \ a_{ijl} \in \mathbb{R}^+ \ \ (\text{resp. } \mathbb{Z}^+), \ \ i=1,\ldots n$$

- Note that l also ranges over negative integers
- Looks awful (nonlinear implicit high-order difference relation)
- Will look much nicer (linear!) in suitable dioid algebras

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Dioids

A dioid (or idempotent semiring) is an algebraic structure containing two binary operations $\oplus$ ("addition") and $\otimes$ ("multiplication") defined on a set $\mathcal{D}$, such that

- $\oplus$ is associative and commutative
- $\oplus$ is idempotent, i.e., $a \oplus a = a \; \forall a \in \mathcal{D}$
- $\otimes$ is associative
- $\otimes$ is distributive w.r.t. $\oplus$
- zero element ε, i.e., $a \oplus \varepsilon = a \; \forall a \in \mathcal{D}$
- unit element e, i.e., $a \otimes e = e \otimes a = a \; \forall a \in \mathcal{D}$
- ε is absorbing for $\otimes$, i.e., $\varepsilon \otimes a = a \otimes \varepsilon = \varepsilon \; \forall a \in \mathcal{D}$

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Examples of Dioids

Max-Plus Algebra:

$(\max, +)$-algebra defined on $\mathbb{Z} \cup \{-\infty\}$ (resp. $\mathbb{R} \cup \{-\infty\}$):

- Addition: $a \oplus b := \max(a, b)$
- Multiplication: $a \otimes b := a + b$
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E.g., [Cuninghame-Green 1979, Baccelli et al. 1992]

Matrix Operations in Dioids

Dioid operations can be easily generalised to the matrix case: for $A, B \in \mathcal{D}^{n\times m}$ and $C \in \mathcal{D}^{m\times l}$, we have:

$$\text{addition: } [A \oplus B]_{ij} = [A]_{ij} \oplus [B]_{ij}$$

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Example (Max-Plus Algebra):

$$\begin{pmatrix} 1 & 3 \\ 4 & 2 \end{pmatrix} \oplus \begin{pmatrix} 4 & 1 \\ 7 & 6 \end{pmatrix} = \begin{pmatrix} 4 & 3 \\ 7 & 6 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 3 \\ 4 & 2 \end{pmatrix} \otimes \begin{pmatrix} 2 \\ 3 \end{pmatrix} = \begin{pmatrix} (1 \otimes 2) \oplus (3 \otimes 3) \\ (4 \otimes 2) \oplus (2 \otimes 3) \end{pmatrix} = \begin{pmatrix} 6 \\ 6 \end{pmatrix}$$

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Note: the symbol $\otimes$ is often omitted ...

Natural Order on Dioids

Dioids are endowed with a natural order:

$$a \oplus b = a \Leftrightarrow a \succeq b$$

Examples

- Scalars in the (max, $+$)-algebra are totally ordered:

$$\text{e.g., } 4 \oplus 8 = \max(4, 8) = 8 \Leftrightarrow 8 \succeq 4$$

- Scalars in the (min, $+$)-algebra are totally ordered:

$$\text{e.g., } 4 \oplus 8 = \min(4, 8) = 4 \Leftrightarrow 4 \succeq 8$$

- Matrices in the (max, $+$)-algebra are partially ordered:

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Complete Dioids

A dioid $(\mathcal{D}, \oplus, \otimes)$ is complete if

- it is closed for infinite sums, i.e., $\top := \bigoplus_{a\in\mathcal{D}} \in \mathcal{D}$ (the "top" element)
- $\otimes$ distributes over infinite sums

Remark: can define Kleene star operator on complete dioids:

$$a^* := \bigoplus_{i\in\mathbb{N}_0} a^i \in \mathcal{D}, \quad \text{with } a^0 := e \text{ and } a^k := a^{k-1}a$$

Useful: least solution of $x = ax \oplus b$ is a^*b

Examples:

- (max, +)-algebra becomes a complete dioid if $\mathcal{D} = \mathbb{Z} \cup \{-\infty, +\infty\}$, with $\top = +\infty$
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A 2-Dimensional Dioid

$\mathbb{B}[\![\gamma, \delta]\!]$ ... the set of formal power series $s = \bigoplus_{k,t} s(k,t)\gamma^k\delta^t$ with

- coefficients from the Boolean dioid ($\oplus$ is OR, $\otimes$ is AND)
- exponents in $\overline{\mathbb{Z}} = \mathbb{Z} \cup \{-\infty, +\infty\}$

$\mathbb{B}[\![\gamma, \delta]\!]$ is equipped with the usual rules for addition and multiplication:

$$s = s_1 \oplus s_2 \quad \ldots \quad s(k,t) = s_1(k,t) \oplus s_2(k,t)$$

$$s = s_1 \otimes s_2 \quad \ldots \quad s(k,t) = \bigoplus_{k_1+k_2=k,\, t_1+t_2=t} s_1(k_1,t_1) \otimes s_2(k_2,t_2)$$

Example and Visualisation

$$s_1 = \gamma^1\delta^1 \oplus \gamma^3\delta^2$$

$$s_2 = \gamma^4\delta^4$$

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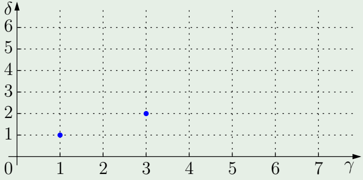

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A 2-Dimensional Dioid

$\mathbb{B}[\![\gamma,\delta]\!]$ . . . the set of formal power series $s = \bigoplus_{k,t} s(k,t)\gamma^k\delta^t$ with

- coefficients from the Boolean dioid ($\oplus$ is OR, $\otimes$ is AND)
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$\mathbb{B}[\![\gamma,\delta]\!]$ is equipped with the usual rules for addition and multiplication:

$$s = s_1 \oplus s_2 \quad \dots \quad s(k,t) = s_1(k,t) \oplus s_2(k,t)$$

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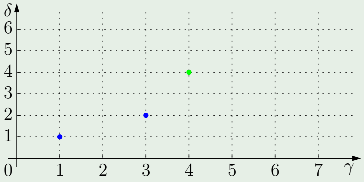
Example and Visualisation



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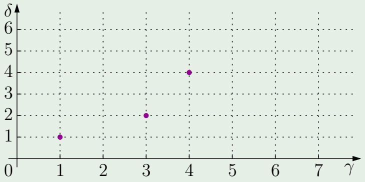

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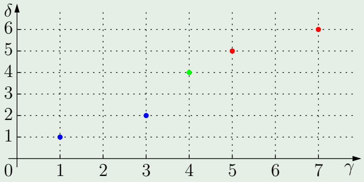

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- Want the following interpretation for a monomial $\gamma^k \delta^t$:
  - *k*th occurrence of event is at time *t* at the earliest
  - equivalently: at time *t*, event has occurred at most *k* times
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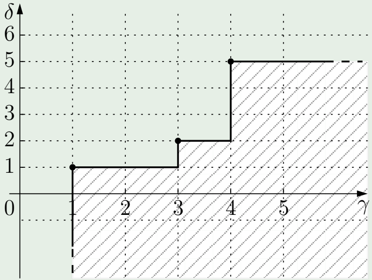

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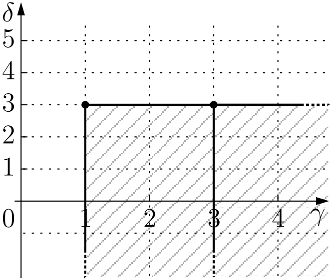

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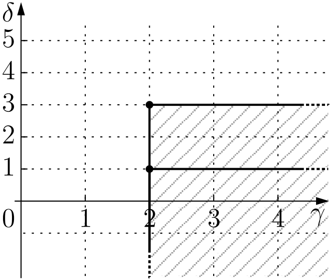

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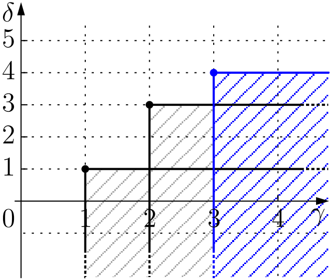

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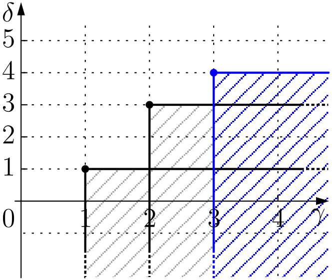

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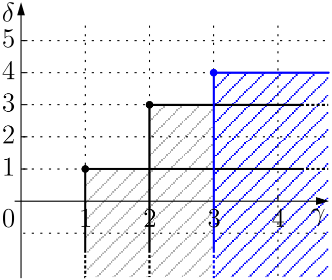

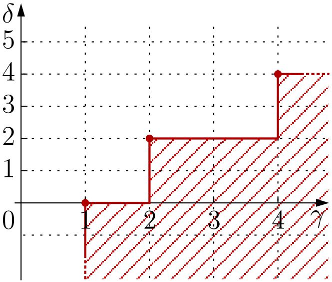

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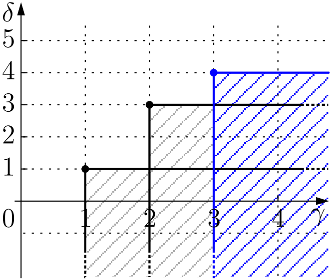
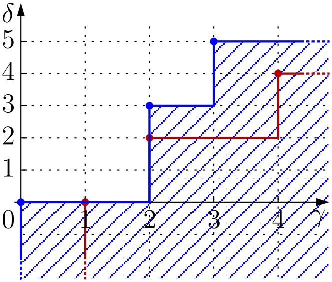
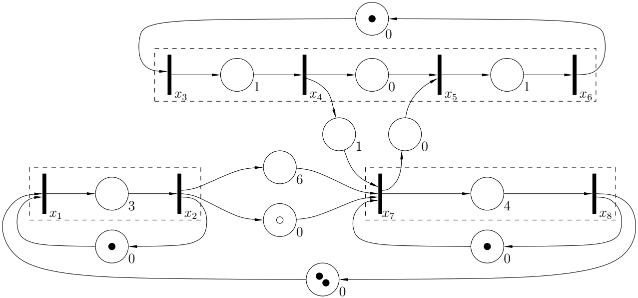




Outline

TEG Model in $\mathcal{M}_{in}^{ax}[\![\gamma,\delta]\!]$

Recall our toy example:



e.g., $x_7 = (\gamma^0\delta^6 \oplus \gamma^{-1}\delta^0)x_2 \oplus \gamma^0\delta^1 x_4 \oplus \gamma^1\delta^0 x_8$

In general:

$$x = Ax$$

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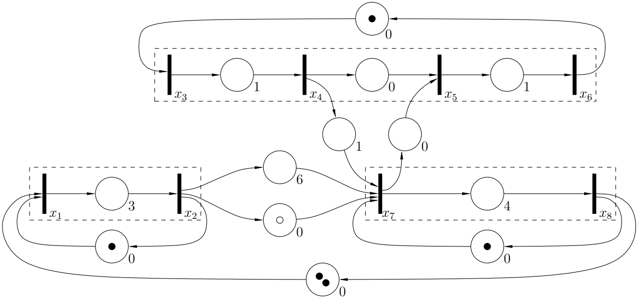

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Equipping the Model with Control and Outputs

Control

- Provides earliest possible times for start events of activities:

$$x = Ax \oplus Bu$$

- In our toy example: B an 8×3 matrix, with $B_{11}, B_{32}, B_{73} = e$
- Can observe everything $\rightsquigarrow$ state feedback: $u = Kx \oplus v$

Performance output

- Time for the "finish" event of the last activity: $y = Cx$
- In our toy example: $C = (\varepsilon, \varepsilon, \varepsilon, \varepsilon, \varepsilon, \varepsilon, \varepsilon, e)$

Closed loop

- Closed loop state equations: $x = (A \oplus BK)x \oplus Bv$
- ...with least solution $x = (A \oplus BK)^* Bv$
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Scalar Example for the Star Operator in $\mathcal{M}_{in}^{ax}[\![\gamma, \delta]\!]$

Recall: the least solution of $x = \underbrace{\left(\gamma^1\delta^2 \oplus \gamma^2\delta^6\right)}_{a} x \oplus e$ is $x = a^*$

Doing the calculations:

$$\underbrace{\left(\gamma^1\delta^2 \oplus \gamma^2\delta^6\right)^*}_{a^*} = \underbrace{\gamma^0\delta^0}_{e} \oplus \underbrace{\gamma^1\delta^2 \oplus \gamma^2\delta^6}_{a} \oplus \underbrace{\gamma^2\delta^4 \oplus \gamma^3\delta^8 \oplus \gamma^4\delta^{12}}_{a^2} \oplus \ldots$$

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gives a periodic series, where a basic pattern $(\gamma^0\delta^0 \oplus \gamma^1\delta^2)$ is repeated periodically with two events occurring every six time units

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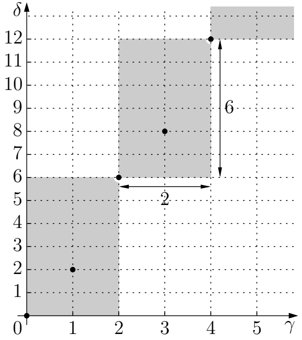

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- Recall aims of feedback:
  - recover optimal schedule while guaranteeing maximal throughput
  - use remaining degrees of freedom to minimise number of batches with different time scheme
- This is equivalent to starting all activities as late as possible while preserving maximal throughput (just-in-time policy)
- Formally: find greatest K such that

$$G_{\text{ref}} \succeq C(A \oplus BK)^* B$$

  with G_{ref} a given maximal throughput reference model
- Note:
  - "greatest" and "$\succeq$" are in the sense of the natural order in $\mathcal{M}_{in}^{ax}[\![\gamma, \delta]\!]$
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  - use remaining degrees of freedom to minimise number of batches with different time scheme
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- $a \otimes x = b$ and $x \otimes a = b$ generally don't have solutions
- Instead, look for greatest solution of

$$a \otimes x \preceq b \quad \text{and} \quad x \otimes a \preceq b$$

- These are called left and right residuals, $a \backslash\!\!\circ b$ and $b \,/\!\!\circ\, a$
- Can be extended to the matrix case: the greatest solutions of $A \otimes X \preceq B$ and $X \otimes A \preceq B$ are $A \backslash\!\!\circ B$ and $B \,/\!\!\circ\, A$, where

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  - Want greatest solution of $(\gamma^1\delta^2 \oplus \gamma^2\delta^3)x \preceq \gamma^3\delta^4$
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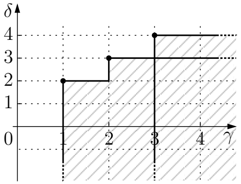

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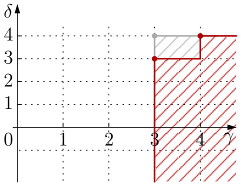
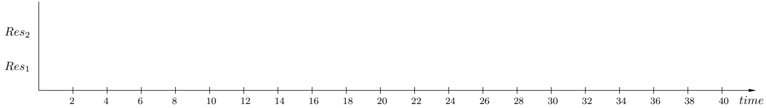


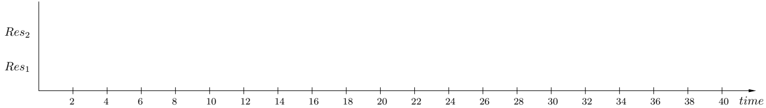
Putting the Pieces Together

- Recall: want greatest K s.t. $G_{\text{ref}} \succeq C(A \oplus BK)^* B$ with G_{ref} any maximal throughput reference model
- Choose $G_{\text{ref}} = CA^*B$
- Apply standard manipulations involving the star operator and residuation ([Lhommeau et al. 2005]) to obtain ([B et al. 2012a])

$$K_{\text{opt}} = (CA^*B) \backslash\!\!\circ\, CA^*B \,/\!\!\circ\, (A^*B)$$

- Need causal projection of K_{opt} ...
- Simulation of disturbance scenario: open loop (top), closed loop (bottom) – click below





Outline

Conclusions

- Addressed feedback synthesis problem for HTS systems
- Approach based on available optimal (off-line) schedule
- Model for feedback synthesis is a Timed Event Graph; time relations become linear & algebraic in the dioid $\mathcal{M}_{in}^{ax}[\![\gamma, \delta]\!]$
- Feedback recovers optimal schedule after delays; starts all activities a late as possible subject to maintaining maximal throughput ($\rightsquigarrow$ minimise number of “waste” batches)
- Have illustrated results for a toy example
- Approach successfully applied to full scale industrial problems, which may involve hundreds of activities on dozens of resources
- Approach can be extended to handle minimal and maximal time intervals ($\rightsquigarrow$ dual product, dual residuation ([B et al. 2012b]))

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- DAAD, for funding under the PROCOPE scheme
- You, for your patience

More Details

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