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An extension of QSIM with qualitative curvature

Abul Hossain [a], Kumar S. Ray [b,*]

[a] Department of Mathematics, Bengal Engineering College, Deemed University, P.O. Botanic garden, Howrah 711 103, W.B., India

[b] Electronics and Communication Sciences Unit, Indian Statistical Institute, 203, B.T. Road, Calcutta 700 035, India

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Abstract

The aim of this work is to extend the existing method of QSIM with qualitative curvature. We consider a new definition of the reasonable function by introducing the concept of the point of inflection. We generate the new tables for P-transitions and I-transitions and ultimately justify the need of the new definition of the reasonable function. We demonstrate that the new definition of the reasonable function produces qualitatively accurate curvature profile of the response which is absent in the existing QSIM. © 1997 Elsevier Science B.V.

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1. Introduction

In recent years qualitative reasoning about physical systems has become an important area in Artificial Intelligence. Although there are several types of qualitative reasoning [2,6,9], the key role is played by qualitative simulation (QSIM [9]): predictions of the possible behaviors consistent with incomplete knowledge of the structure of physical system. In QSIM [9] Kuipers introduces a constraint satisfaction algorithm which represents the qualitative state of a time-varying real variable $x(t)$ in terms of the qualitative magnitude (ordinal relations with a set of landmark values) and the sign of its derivative, $[x'(t)]$. In particular, the qualitative state in QSIM ignores the sign of the second derivative, $[x''(t)]$.

* Corresponding author. Email: ksray@isical.ernet.in.

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The aim of this paper is to extend QSIM where the qualitative state consists of qualitative magnitudes, $[x'(t)]$ and $[x''(t)]$. As a result of this extension we can obtain the information of direction of bulge and the additional landmark values represented at the points of inflection. Thus, a more enriched quality of qualitative description is obtained. The extended version of QSIM is called QSIM2. Now in the following paragraph we discuss the organization of the rest of the paper.

In Section 2 we describe the basic tools needed for QSIM2. Section 3 deals with the new P-transition and I-transition tables necessary for QSIM2. In Section 3.1 we describe the new landmark values using the transition tables of Section 3. In Section 4 we talk about some new constraints and sign algebra. Section 5 discusses qualitative function constraints and Section 5.1 discusses constraint consistency. In Section 6 we talk about global interpretations and global filters and in Section 6.1 we discuss infinity and asymptotic approach. In Section 7 we discuss the algorithm QSIM2 with one demo example. The basic steps of the algorithm QSIM2 are same as those of QSIM; but the input and output parameters of QSIM2 are different from QSIM and at every step QSIM2 evaluates some new features of the physical system for which the simulation is performed. Section 8 talks about the complexity of QSIM2. Section 9 discusses the detection of actual behaviors. In Section 10 we talk about the coarse state descriptions. In Section 11 the mixing tank problem is considered. Section 12 deals with the critical appreciation on QSIM and QSIM2 algorithms. In Section 13 we draw the conclusion.

2. Tools for QSIM2

In the following, for the extension of the existing QSIM with qualitative curvature we propose some new definitions for reasonable function, landmark value, distinguished time point, qualitative state, J-point, etc.

Definition 1. For $[a,b] \subseteq \mathbb{R}^*$, define $f : [a,b] \to \mathbb{R}^*$,[1] where $\mathbb{R}^*$ is the extended real number line, to be a *reasonable function of type* 2 or RFT2 if

(1) f and f' are continuous on $[a,b]$,
(2) f'' exists and is continuous on (a, b),
(3) the sign of $f''(t)$ changes only finitely many times in any bounded interval,
(4) $\lim_{t\to a^+} f''(t)$ and $\lim_{t\to b^-} f''(t)$ exist in $\mathbb{R}^*$ and define $f''(a)$, and $f''(b)$ respectively.

Reasonable function in [9] is defined here as a *reasonable function of type* 1 or RFT1.

Let the set of all RFT1s and RFT2s in $[a,b]$ be denoted by $\mathrm{R}_1[a,b]$ and $\mathrm{R}_2[a,b]$ respectively.

Definition 2. t' is said to be a *J-point of a function* f if there exists a number $\delta > 0$ such that

[1] For a list of symbols used, see Appendix A.

$$f''(t)\begin{cases} =0 & \text{in } [t', t'+\delta), \\ \neq 0 & \text{in } (t'-\delta, t'), \end{cases} \quad \text{or} \quad f''(t)\begin{cases} =0 & \text{in } (t'-\delta, t'], \\ \neq 0 & \text{in } (t', t'+\delta), \end{cases}$$

holds true where f'' exists in a δ-neighbourhood of t'.

Definition 3. Every $f \in \mathrm{R}_2[a,b]$ has associated with it a finite set of *landmark values* (LVs). The landmark values include $f(a)$, $f(b)$, the basic set $\{-\infty, 0, +\infty\}$ and the value of f at each of its critical points, inflection points, and J-points and may include any number of additional values. The set of all LVs of f will be denoted by $\mathrm{L}_2[f,a,b]$.
Similarly, if $f \in \mathrm{R}_1[a,b]$, then the set of all LVs of f will be denoted by $\mathrm{L}_1[f,a,b]$.

Definition 4. Let $f \in \mathrm{R}_2[a,b]$, and let $\mathrm{D}_2[f,a,b]$ be the set of all boundary elements of the set $\{t \in [a,b] \mid f(t) = x \text{ where } x \text{ is an LV of } f\}$. Then each $t \in \mathrm{D}_2[f,a,b]$ is said to be a *distinguished time point* or DTP. Two consecutive distinguished points will be denoted by CDTP.
Similarly, we can define $\mathrm{D}_1[f,a,b]$ as a set of all DTPs of $f \in \mathrm{R}_1[a,b]$.

It is obvious from the definition that

$$\mathrm{R}_2[a,b] \subseteq \mathrm{R}_1[a,b],$$
$$\mathrm{L}_2[f,a,b] \subseteq \mathrm{L}_1[f,a,b],$$
$$\mathrm{D}_1[f,a,b] \subseteq \mathrm{D}_2[f,a,b].$$

Definition 5. Let $l_1 < l_2 < \cdots < l_k$ be the LVs of $f \in \mathrm{R}_2[a,b]$. For any $t \in [a,b]$, $\mathrm{QS}(f,t)$, the qualitative state of f at t, is a triple $\langle \text{qval}, \text{qdir}, \text{db} \rangle$ where

$$(1) \quad \text{qval} := \begin{cases} l_j & \text{if } f(t) = l_j, \text{ an LV}, \\ (l_j, l_{j+1}) & \text{if } f(t) \in (l_j, l_{j+1}), \end{cases}$$

$$(2) \quad \text{qdir} := \begin{cases} + & \text{if } f'(t) > 0, \\ 0 & \text{if } f'(t) = 0, \\ - & \text{if } f'(t) < 0, \end{cases}$$

$$(3) \quad \text{db} := \begin{cases} + & \text{if } f''(t) > 0, \\ 0 & \text{if } f''(t) = 0, \\ - & \text{if } f''(t) < 0. \end{cases}$$

Example 6. Here we illustrate Definition 5 with the help of the following example represented by Fig. 1.

$$\mathrm{QS}(\text{water-temp}, \text{now}, \text{how}) := \langle (32°\mathrm{F}, 212°\mathrm{F}), +, - \rangle.$$

Kuipers [9] defines a pair (p,q) of LVs to be the corresponding values (CVs) of the physical parameters f and g if there exists a $t' \in [a,b]$ such that $f(t') = p$ and $g(t') = q$. Here, we have introduced inflection points as additional LVs.

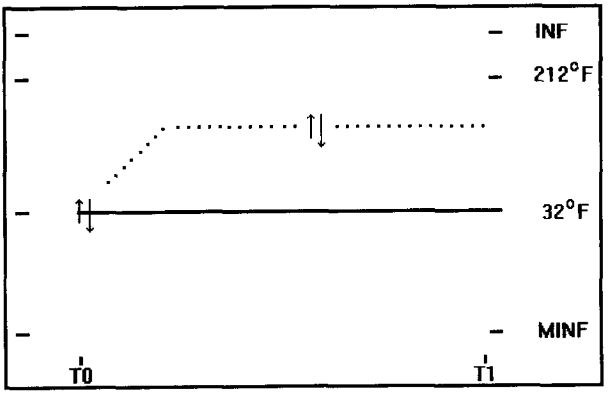


Fig. 1. Representation of QS using QSIM2. Small and big arrows represent the qualitative direction and the direction of bulge respectively.

Definition 7. We define the CVs (p, q) to be corresponding values of type one (CVT1) if both LVs are critical points and corresponding values of type two (CVT2) if both LVs are inflection points. Otherwise we we say that the corresponding values are of type 3 (that is, CVT3), which essentially retains the definition given as Definition 4.1 in [9].

With respect to our extended version of QSIM we state the following results which support the statement of Proposition 2.5 of [9] which is Proposition 24 in the present text.

Proposition 8. *If there are two consecutive time points $t', t'' \in \mathrm{D}_2[f, a, b]$ such that $t' < t''$ and $f(t') = f(t'')$, then there exists an LV l such that $f(t) = l \; \forall t \in [t', t'']$.*

Proof. Since $t' \in \mathrm{D}_2[f, a, b]$, we have from the definition, $f(t') \in \mathrm{L}_2[f, a, b]$ and, say, $f(t') = l$. So $f(t') = f(t'') = l$.

First we prove that $f'(t) \equiv 0$ in (t', t'').

Suppose not, then there is a $p \in (t', t'')$ such that $f'(p) \neq 0$, in particular, say, $f'(p) > 0$. Since $f'(t)$ is continuous, there exists a number $\delta > 0$ such that $f'(t) > 0$ $\forall t \in (p - \delta, p + \delta)$.

Thus, $f(t)$ is increasing in $(p - \delta, p + \delta)$ where $(p - \delta, p + \delta) \subset (t', t'') \subset [t', t'']$.

Existence of such a p implies that $f(t)$ is non-constant in $[t', t'']$. Therefore, by Rolle's Theorem, there exists a point $c \in (t', t'')$ such that $f'(c) = 0$. This implies that there exists a DTP of f between t' and t'' which contradicts our hypothesis that t' and t'' are CDTP.

Therefore, no such p can exist in (t', t''). Hence

$$f'(t) \equiv 0 \text{ in } (t', t''). \tag{1}$$

Let q be any point in (t',t''). We can apply the Mean Value Theorem on $[t',q]$. Now,

$$
\begin{aligned}
& f(q)-f(t')=(q-t')f'(h) \quad \text{for some } h\in(t',q).\\
& \quad\Rightarrow\quad f(q)-f(t')=0 \quad \text{by (1)}\\
& \quad\Rightarrow\quad f(t')=f(q)=f(t'')=l \quad \text{for any } q\in(t',t'')\\
& \quad\Rightarrow\quad f(t)=l \quad \forall t\in[t',t'']. \qquad \square
\end{aligned}
$$

Corollary 9. *If $f(t) = l$ in $[t',t'']$ where t' and t'' are CDTP, then $f'(t) \equiv 0$ in $[t',t'']$.*

Proof. Since $f(t) = l$ in $[t',t'']$, we have that $f'(t) \equiv 0$ in (t',t''). From the continuity of f', we get that $f'(t') = f'(t'') = 0$. Therefore, $f'(t) \equiv 0$ in $[t',t'']$. □

Proposition 10. *For any $f \in \mathrm{R}_2[a,b]$ and any $p \in (a,b)$ such that $f'(p) \neq 0$ and $f''(p) = 0$, either*

(a) *$(p, f(p))$ is a point of inflection, or*

(b) *there is a largest closed interval $[g,h] \subseteq [a,b]$ containing p in which $f''(t) \equiv 0$.*

Proof. Since $f \in \mathrm{R}_2[a,b]$, $f''(t)$ exists and is continuous in (a,b). Therefore for any point $p \in (a,b)$, either $f''(p) = 0$, or $f''(p) \neq 0$ holds true. For $f''(p) = 0$, since $f'(p) \neq 0$, the following cases are possible:

(a) $(p, f(p))$ is a point of inflection,

(b) (i) $(p, f(p))$ is a J-point and

(ii) there is an open interval containing p in which $f''(t) = 0$.

In case (b)(i), we collect all the semi-open intervals (from the Definition 2 it follows that the closed end point is p) for which $f''(t) = 0$ and taking the union of such semi-open intervals yields the largest semi-open interval, say, $(t',p]$, in which $f''(t) \equiv 0$. From this and the continuity of $f''(t)$, we get that $f''(t') = 0$. Therefore, $f''(t) = 0\ \forall t \in [t',p]$, which is the required largest interval. In case (b)(ii), in the same way, we can get the largest closed interval in which $f''(t)$ is identically zero. □

Proposition 11. *For the closed interval $[g,h]$ in Proposition 10, the following cases hold true:*

(a) *h is either a J-point, or $h = b$, and*

(b) *g is either a J-point, or $g = a$.*

Proof. (a) Now $p \in [g,h]$, then either $p = h$ or $p \in [g,h)$. For $p = h$, $(p, f(p))$ is a J-point. (From the proof of Proposition 10(b)(i).)

Next, let $p \in [g,h)$. Now, $[g,h] \subseteq [a,b]$. Then either $h = b$, or $h \neq b$. If $h \neq b$, then there is a positive number $\delta \leqslant b - h$ such that $f''(t) \neq 0$ in $(h, h+\delta)$, because $[g,h]$ is the largest interval in which $f''(t) \equiv 0$. Therefore, from the definition of J-point, it follows that h is a J-point.

In a similar way we can prove (b). □

Proposition 12. *Let $a < t' < t'' < b$ be two CDTPs of $f \in R_2[a,b]$ such that $f(t') \neq f(t'')$. Then f cannot have extreme values at t' and t''. Moreover, if $t' = a$, $t'' = b$, and the function is strictly increasing or decreasing over $[a,b]$, then its extreme values are at t' and t''.*

Proof. For the first part of the proposition, if possible let f have extreme values at t' and t'' simultaneously, then

$$f'(t') = f'(t'') = 0.$$

Since $f'(t') = f'(t'')$, we have, by Rolle's Theorem, that there exists a point $c \in (t', t'')$ such that $f''(c) = 0$. By Propositions 10 and 11, we have either

(a) $(c, f(c))$ is a point of inflection, or
(b) there exists a closed interval $[g,h] \subseteq [a,b]$ containing c for which $f''(t) = 0$ $\forall t \in [g,h]$.

Now, in case (a), c is a DTP of f which contradicts the hypothesis. In case (b), if $g \in (t', t'')$, then by definition g is also a J-point and correspondingly contradicts the hypothesis. So, $g \in [a, t']$. Similarly we can show that $h \in [t'', b]$.

Therefore,

$$[t', t''] \subseteq [g,h] \subseteq [a,b].$$

Now, $f''(t) = 0$ in $[g,h]$. So, $f'(t) = l$, a constant, in $[g,h]$. Since $f'(t') = 0$ for $t' \in [g,h]$, we find that $l = 0$, i.e., $f'(t) = 0$ in $[g,h]$. Thus, $f(t) = l'$, a constant, in $[g,h]$. Thus, $f(t') = f(t'') = l'$ which contradicts the hypothesis.

The second part of the proposition follows obviously. □

Proposition 13. *If a DTP t' is both a critical point and a J-point, then there exists a $\delta > 0$ such that either*

(i) $f'(t) = f''(t) = 0 \; \forall t \in [t', t'+\delta)$ *and* $f'(t) \neq 0 \neq f''(t) \; \forall t \in (t'-\delta, t')$, *or*
(ii) $f'(t) = f''(t) = 0 \; \forall t \in (t'-\delta, t']$ *and* $f'(t) \neq 0 \neq f''(t) \; \forall t \in (t', t'+\delta)$ *holds true.*

Proof. For the proof see Appendix B. □

Proposition 14. *If Proposition* 13(i) *holds then for next DTP t'', $f'(t) = f''(t) = 0$ $\forall t \in [t', t'']$ holds.*

We are dealing with CDTP and the behavior of the physical parameters between them. Here we assume that LVs associated with them are different. In Proposition 12 we have proved that these two DTPs cannot both be critical points. We now explore possible characteristic features of CDTP. There are five possible cases for a particular DTP:

(i) Critical point (C),
(ii) Inflection point (I),
(iii) J-point (J),
(iv) Critical and J-point (CJ),
(v) Critical and inflection point (CI).

For any CDTP t', t'' of f, by (I) $\wedge$ (CJ), we mean that t' is an inflection point, and t'' a critical point and a J-point or vice versa. Here we list all valid assignments for the CDTP:

(1) (C) $\wedge$ (I);	(2) (C) $\wedge$ (J);	(3) (I) $\wedge$ (J);
(4) (I) $\wedge$ (CJ);	(5) (I) $\wedge$ (CI);	(6) (J) $\wedge$(CJ);
(7) (J) $\wedge$(CI);	(8) (I) $\wedge$ (I);	(9) (J) $\wedge$ (J).

We exclude some cases, because they are prohibited by Proposition 12.

For any pair in the above we shall prove that the qualitative state remains constant throughout the open interval composed of those DTPs, i.e. if t' and t'' are two CDTP of $f \in \mathrm{R}_2[a,b]$, then $\mathrm{QS}(f,p) = \mathrm{QS}(f,q)$ for any $p, q \in (t', t'')$. The proof will be completed if we prove that one of the following five possible cases holds for two CDTP $t' < t''$ of a function $f \in R_2[a,b]$:

($\bar{\mathrm{a}}$) $f''(t) \equiv 0 \ \forall t \in [t', t'']$,

($\bar{\mathrm{b}}$) $f''(t) > 0,\ f'(t) > 0 \ \forall t \in (t', t'')$,

($\bar{\mathrm{c}}$) $f''(t) > 0,\ f'(t) < 0 \ \forall t \in (t', t'')$,

($\bar{\mathrm{d}}$) $f''(t) < 0,\ f'(t) > 0 \ \forall t \in (t', t'')$,

($\bar{\mathrm{e}}$) $f''(t) < 0,\ f'(t) < 0 \ \forall t \in (t', t'')$.

In this section we assume the fact that $t' < t''$ and t', t'' are CDTP. We now introduce a useful notation about DTP to give a compact and amenable statement form of propositions whenever required. These are the characteristic features of t' and t'' of $f \in \mathrm{R}_2[a,b]$ and denoted by $\mathrm{CF}_f[t', t'']$.

Now, $\mathrm{CF}_f[t', t''] = [(\mathrm{I}), (\mathrm{J})]$ implies that t', and t'' are an inflection point and a J-point of f respectively.

Here $\mathrm{CF}_f[t', t''] = [(\mathrm{I}) \leftrightarrow (\mathrm{J})]$ implies that either t' and t'' are a J-point and an inflection point of f respectively or t' and t'' are an inflection point and a J-point of f respectively.

In the following propositions, it is understood that $\mathrm{CF}_f[t', t'']$ and $\mathrm{CF}[t', t'']$ are equivalent.

The proofs of Propositions 15–24 are given in Appendix B.

Proposition 15.

$$\mathrm{CF}[t', t''] = [(\mathrm{I}), (\mathrm{I})] \ \Rightarrow\ (\bar{\mathrm{b}}) \ \dot{\vee}\ (\bar{\mathrm{c}}) \ \dot{\vee}\ (\bar{\mathrm{d}}) \ \dot{\vee}\ (\bar{\mathrm{e}}).$$

Proposition 16.

(i) $\mathrm{CF}[t', t''] = [(\mathrm{C}), (\mathrm{I})] \ \Rightarrow\ (\bar{\mathrm{b}}) \ \dot{\vee}\ (\bar{\mathrm{e}})$,

(ii) $\mathrm{CF}[t', t''] = [(\mathrm{I}), (\mathrm{C})] \ \Rightarrow\ (\bar{\mathrm{c}}) \ \dot{\vee}\ (\bar{\mathrm{d}})$.

Proposition 17.

$$\mathrm{CF}[t', t''] = [(\mathrm{J}), (\mathrm{J})] \ \Rightarrow\ (\bar{\mathrm{a}}) \ \dot{\vee}\ (\bar{\mathrm{b}}) \ \dot{\vee}\ (\bar{\mathrm{c}}) \ \dot{\vee}\ (\bar{\mathrm{d}}).$$

Proposition 18.

(i) $\mathrm{CF}[t',t''] = [(\mathrm{C}),(\mathrm{J})] \Rightarrow (\bar{\mathrm{b}}) \dot{\vee} (\bar{\mathrm{e}})$,

(ii) $\mathrm{CF}[t',t''] = [(\mathrm{J}),(\mathrm{C}] \Rightarrow (\bar{\mathrm{c}}) \dot{\vee} (\bar{\mathrm{d}})$.

Proposition 19.

$\mathrm{CF}[t',t''] = [(\mathrm{I}) \leftrightarrow (\mathrm{J})] \Rightarrow (\bar{\mathrm{b}}) \dot{\vee} (\bar{\mathrm{c}}) \dot{\vee} (\bar{\mathrm{d}}) \dot{\vee} (\bar{\mathrm{e}})$.

Proposition 20.

(i) $\mathrm{CF}[t',t''] = [(\mathrm{I}),(\mathrm{CJ})] \Rightarrow (\bar{\mathrm{c}}) \dot{\vee} (\bar{\mathrm{d}})$,

(ii) $\mathrm{CF}[t',t''] = [(\mathrm{CJ}),(\mathrm{I})] \Rightarrow (\bar{\mathrm{b}}) \dot{\vee} (\bar{\mathrm{e}})$.

Proposition 21.

(i) $\mathrm{CF}[t',t''] = [(\mathrm{I}),(\mathrm{CI})] \Rightarrow (\bar{\mathrm{c}}) \dot{\vee} (\bar{\mathrm{d}})$,

(ii) $\mathrm{CF}[t',t''] = [(\mathrm{CI}),(\mathrm{I})] \Rightarrow (\bar{\mathrm{b}}) \dot{\vee} (\bar{\mathrm{e}})$.

Proposition 22.

(i) $\mathrm{CF}[t',t''] = [(\mathrm{J}),(\mathrm{CJ})] \Rightarrow (\bar{\mathrm{b}}) \dot{\vee} (\bar{\mathrm{e}})$,

(ii) $\mathrm{CF}[t',t''] = [(\mathrm{CJ}),(\mathrm{J})] \Rightarrow (\bar{\mathrm{c}}) \dot{\vee} (\bar{\mathrm{d}})$.

Proposition 23.

(i) $\mathrm{CF}[t',t''] = [(\mathrm{J}),(\mathrm{CI})] \Rightarrow (\bar{\mathrm{c}}) \dot{\vee} (\bar{\mathrm{d}})$,

(ii) $\mathrm{CF}[t',t''] = [(\mathrm{CI}),(\mathrm{J})] \Rightarrow (\bar{\mathrm{b}}) \dot{\vee} (\bar{\mathrm{e}})$.

Proposition 24. *If t' and t'' are two CDTP of any $f \in \mathrm{R}_2[a,b]$, then $\mathrm{QS}(f,p) = \mathrm{QS}(f,q)$ where $p,q \in (t',t'')$.*

Now we shall give the definition of qualitative state in the interval determined by CDTP. By Proposition 24, we find the qualitative state between CDTP is constant.

Definition 25. Let t' and t'' be CDTP. The *qualitative state* of f within the CDTP, $\mathrm{QS}(f,t',t'')$, is defined to be $\mathrm{QS}(f,t)$ for any $t \in (t',t'')$.

We see that qualitative state on a DTP, or between CDTP is the same as given in [9]. We also use here the same definition of qualitative behavior of f on $[a,b]$.

Similarly we use the same definition of system of functions (RFT2) on $[a,b]$ and its qualitative behavior as described by Kuipers [9].

3. State transitions

Using the basic tools of Section 2, in Tables 1 and 2 we extend the P-transitions and I-transitions of [9]. These extensions are needed for QSIM2.

Table 1
P-transitions

Name	$QS(f, t_i)$	$\Rightarrow$	$QS(f, t_i, t_{i+1})$
P-1	$\langle l_j, 0, 0\rangle$	$\Rightarrow$	$\langle l_j, 0, 0\rangle$
P-2	$\langle l_j, 0, 0\rangle$	$\Rightarrow$	$\langle (l_j, l_{j+1}), +, +\rangle$
P-3	$\langle l_j, 0, 0\rangle$	$\Rightarrow$	$\langle (l_{j-1}, l_j), -, -\rangle$
P-4	$\langle l_j, 0, +\rangle$	$\Rightarrow$	$\langle (l_j, l_{j+1}), +, +\rangle$
P-5	$\langle l_j, 0, -\rangle$	$\Rightarrow$	$\langle (l_{j-1}, l_j), -, -\rangle$
P-6	$\langle l_j, +, +\rangle$	$\Rightarrow$	$\langle (l_j, l_{j+1}), +, +\rangle$
P-7	$\langle l_j, +, 0\rangle$	$\Rightarrow$	$\langle (l_j, l_{j+1}), +, +\rangle$
P-8	$\langle l_j, +, 0\rangle$	$\Rightarrow$	$\langle (l_j, l_{j+1}), +, 0\rangle$
P-9	$\langle l_j, +, 0\rangle$	$\Rightarrow$	$\langle (l_j, l_{j+1}), +, -\rangle$
P-10	$\langle l_j, +, -\rangle$	$\Rightarrow$	$\langle (l_j, l_{j+1}), +, -\rangle$
P-11	$\langle (l_j, l_{j+1}), +, +\rangle$	$\Rightarrow$	$\langle (l_j, l_{j+1}), +, +\rangle$
P-12	$\langle (l_j, l_{j+1}), +, 0\rangle$	$\Rightarrow$	$\langle (l_j, l_{j+1}), +, 0\rangle$
P-13	$\langle (l_j, l_{j+1}), +, -\rangle$	$\Rightarrow$	$\langle (l_j, l_{j+1}), +, -\rangle$
P-14	$\langle l_j, -, -\rangle$	$\Rightarrow$	$\langle (l_{j-1}, l_j), -, -\rangle$
P-15	$\langle l_j, -, 0\rangle$	$\Rightarrow$	$\langle (l_{j-1}, l_j), -, +\rangle$
P-16	$\langle l_j, -, 0\rangle$	$\Rightarrow$	$\langle (l_{j-1}, l_j), -, 0\rangle$
P-17	$\langle l_j, -, 0\rangle$	$\Rightarrow$	$\langle (l_{j-1}, l_j), -, -\rangle$
P-18	$\langle l_j, -, +\rangle$	$\Rightarrow$	$\langle (l_{j-1}, l_j), -, +\rangle$
P-19	$\langle (l_{j-1}, l_j), -, +\rangle$	$\Rightarrow$	$\langle (l_{j-1}, l_j), -, +\rangle$
P-20	$\langle (l_{j-1}, l_j), -, 0\rangle$	$\Rightarrow$	$\langle (l_{j-1}, l_j), -, 0\rangle$
P-21	$\langle (l_{j-1}, l_j), -, -\rangle$	$\Rightarrow$	$\langle (l_{j-1}, l_j), -, -\rangle$

3.1. Discovering new LVs

We consider critical points and inflection points as LVs. When we discover new LVs both types of points may appear. Suppose $QS(f, t_i, t_{i+1}) = \langle (l_j, l_{j+1}), +, -\rangle$ where $l_1 < l_2 < \cdots < l_k$ is only a partial set of LVs of f. Then the transitions

$$QS(f, t_{i+1}) = \langle l^*, +, 0\rangle,$$
$$QS(f, t_{i+1}) = \langle l^*, 0, -\rangle$$

will be possible only when a newly discovered LV $l^* \in (l_j, l_{j+1})$, i.e., $l_j < l^* < l_{j+1}$ where l^* represents a newly discovered inflection point in the first case and a critical point in the second case. Therefore, a new landmark value is inserted in the partial set of LVs without violating its order. Taking other possible cases, we summarize these facts in the following proposition.

Proposition 26. *Suppose $l_1 < l_2 < \cdots < l_k$ are all known LVs of an RFT2 f, which may have other LVs as yet unknown. Then the transitions shown in Table 3 are possible. The total ordering of the LVs remains unchanged.*

Table 2
I-transitions

Name	$QS(f, t_i, t_{i+1})$	$\Rightarrow$	$QS(f, t_{i+1})$
I-1	$\langle l_j, 0, 0\rangle$	$\Rightarrow$	$\langle (l_j, 0, 0\rangle$
I-2	$\langle (l_j, l_{j+1}), +, +\rangle$	$\Rightarrow$	$\langle l_{j+1}, +, 0\rangle$
I-3	$\langle (l_j, l_{j+1}), +, +\rangle$	$\Rightarrow$	$\langle l_{j+1}, +, +\rangle$
I-4	$\langle (l_j, l_{j+1}), +, +\rangle$	$\Rightarrow$	$\langle (l_j, l_{j+1}), +, +\rangle$
I-5	$\langle (l_j, l_{j+1}), +, +\rangle$	$\Rightarrow$	$\langle l^*, +, 0\rangle$ [a]
I-6	$\langle (l_j, l_{j+1}), +, 0\rangle$	$\Rightarrow$	$\langle l_{j+1}, +, 0\rangle$
I-7	$\langle (l_j, l_{j+1}), +, 0\rangle$	$\Rightarrow$	$\langle (l_j, l_{j+1}), +, 0\rangle$
I-8	$\langle (l_j, l_{j+1}), +, -\rangle$	$\Rightarrow$	$\langle l_{j+1}, +, 0\rangle$
I-9	$\langle (l_j, l_{j+1}), +, -\rangle$	$\Rightarrow$	$\langle l_{j+1}, 0, -\rangle$
I-10	$\langle (l_j, l_{j+1}), +, -\rangle$	$\Rightarrow$	$\langle l_{j+1}, +, -\rangle$
I-11	$\langle (l_j, l_{j+1}), +, -\rangle$	$\Rightarrow$	$\langle (l_j, l_{j+1}), +, -\rangle$
I-12	$\langle (l_j, l_{j+1}), +, -\rangle$	$\Rightarrow$	$\langle l^*, +, 0\rangle$
I-13	$\langle (l_j, l_{j+1}), +, -\rangle$	$\Rightarrow$	$\langle l^*, 0, -\rangle$
I-14	$\langle (l_j, l_{j+1}), +, -\rangle$	$\Rightarrow$	$\langle l^*, 0, 0\rangle$
I-15	$\langle (l_{j-1}, l_j), -, +\rangle$	$\Rightarrow$	$\langle l_{j-1}, 0, +\rangle$
I-16	$\langle (l_{j-1}, l_j), -, +\rangle$	$\Rightarrow$	$\langle l_{j-1}, -, 0\rangle$
I-17	$\langle (l_{j-1}, l_j), -, +\rangle$	$\Rightarrow$	$\langle l_{j-1}, -, +\rangle$
I-18	$\langle (l_{j-1}, l_j), -, +\rangle$	$\Rightarrow$	$\langle (l_{j-1}, l_j), -, +\rangle$
I-19	$\langle (l_{j-1}, l_j), -, +\rangle$	$\Rightarrow$	$\langle l^*, -, 0\rangle$
I-20	$\langle (l_{j-1}, l_j), -, +\rangle$	$\Rightarrow$	$\langle l^*, 0, +\rangle$
I-21	$\langle (l_{j-1}, l_j), -, +\rangle$	$\Rightarrow$	$\langle l^*, 0, 0\rangle$
I-22	$\langle (l_{j-1}, l_j), -, 0\rangle$	$\Rightarrow$	$\langle l_{j-1}, -, 0\rangle$
I-23	$\langle (l_{j-1}, l_j), -, 0\rangle$	$\Rightarrow$	$\langle (l_{j-1}, l_j), -, 0\rangle$
I-24	$\langle (l_{j-1}, l_j), -, -\rangle$	$\Rightarrow$	$\langle l_{j-1}, -, -\rangle$
I-25	$\langle (l_{j-1}, l_j), -, -\rangle$	$\Rightarrow$	$\langle l_{j-1}, -, 0\rangle$
I-26	$\langle (l_{j-1}, l_j), -, -\rangle$	$\Rightarrow$	$\langle (l_{j-1}, l_j), -, -\rangle$
I-27	$\langle (l_{j-1}, l_j), -, -\rangle$	$\Rightarrow$	$\langle l^*, -, 0\rangle$

[a] Here * denotes the newly generated landmark value.

Table 3
The set of possible transitions

Name	$QS(f, t_i, t_{i+1})$	$\Rightarrow$	$QS(f, t_{i+1})$
I-5	$\langle (l_j, l_{j+1}), +, +\rangle$	$\Rightarrow$	$\langle l^*, +, 0\rangle$
I-12	$\langle (l_j, l_{j+1}), +, -\rangle$	$\Rightarrow$	$\langle l^*, +, 0\rangle$
I-13	$\langle (l_j, l_{j+1}), +, -\rangle$	$\Rightarrow$	$\langle l^*, 0, -\rangle$
I-14	$\langle (l_j, l_{j+1}), +, -\rangle$	$\Rightarrow$	$\langle l^*, 0, 0\rangle$
I-19	$\langle (l_{j-1}, l_j), -, +\rangle$	$\Rightarrow$	$\langle l^*, -, 0\rangle$
I-20	$\langle (l_{j-1}, l_j), -, +\rangle$	$\Rightarrow$	$\langle l^*, 0, +\rangle$
I-21	$\langle (l_{j-1}, l_j), -, +\rangle$	$\Rightarrow$	$\langle l^*, 0, 0\rangle$
I-27	$\langle (l_{j-1}, l_j), -, -\rangle$	$\Rightarrow$	$\langle l^*, -, 0\rangle$

Note that all the P-transitions and I-transitions except the set of transitions represented by Table 3 are satisfied by Propositions 8–24 of Section 2.

4. Some new constraints and sign algebra

In this section, we introduce two important constraints which together generalize the DERIV constraint. These new constraints are DERIV^+ and DERIV^-. In the following section we formally define them.

Definition 27. $\mathrm{DERIV}^+(f,g)$ is a two-place predicate on $\mathrm{R}_2[a,b]$ which holds true *iff* $f'(t) = mg(t)$ $\forall t \in [a,b]$ where $m > 0$.

$\mathrm{DERIV}^-(f,g)$ is defined in the same way except that $m < 0$.

Note: For $m = 1$, we have $f'(t) = g(t)$ $\forall t \in [a,b]$ and thus $\mathrm{DERIV}(f,g)$. So, $\mathrm{DERIV}^+(f,g)$ implies $\mathrm{DERIV}(f,g)$ when $m = 1$. Clearly, $\mathrm{DERIV}(f,g)$ implies $\mathrm{DERIV}^+(f,g)$.

Now we discuss the concept of sign algebra. We represent below the addition operation $\oplus$ and multiplication operation $\odot$ on the set of signs by the following tables:

$\oplus$	$+$	0	$-$
$+$	$+$	$+$	?
0	$+$	0	$-$
$-$	?	$-$	$-$

$\odot$	$+$	0	$-$
$+$	$+$	0	$-$
0	0	0	0
$-$	$-$	0	$+$

We find that $+\oplus-$ or $-\oplus+$ cannot be uniquely evaluated. In such case "?" represents any one of the symbols $+$, 0 or $-$. We denote the sign operator by "[ ]" which denotes the sign of the quantity. Thus,

$$[a] = \begin{cases} + & \text{if } a > 0, \\ 0 & \text{if } a = 0, \\ - & \text{if } a < 0, \end{cases}$$

i.e., $[\ ] : Q \to \{+,0,-\}$ where Q is the quantity space.

Addition is not preserved under the sign operator, because ambiguities arise when we add two opposite signs, since $+\oplus-$ or $-\oplus+$ may yield any one of the signs in $\{+,0,-\}$.

So in general, $[A+B] \neq [A] \oplus [B]$ for all A, B belonging to the quantity space. We can illustrate this fact by considering the following example:

$$[7+(-5)] = [2] = + \quad \text{and} \quad [7] \oplus [(-5)] = + \oplus - = ?.$$

So,

$$[7+(-5)] \neq [7] \oplus [(-5)].$$

When we can evaluate $[A] \oplus [B]$ uniquely, this will be the value of $[A+B]$, i.e., in this case

$$[A+B] = [A] \oplus [B] \tag{2}$$

holds true.

This is possible only when the two arguments are of the same sign, or one is zero. We need to evaluate $[A+B]$ by its arguments, i.e., by $[A]$ and $[B]$. Therefore, we always resort to (2) whenever it is needed.

5. Qualitative function constraints

There are two types of monotonic function constraints described by Kuipers in his early paper on qualitative simulation [9]. These monotonic function constraints are M^+ and M^-.

Here we introduce some additional monotonic function constraints such as L^+, L^-, M^{++}, M^{+-}, M^{-+} and M^{--}.

Definition 28. L^+ is a two-place predicate on RFT2. $\mathrm{L}^+(f,g)$ is true *iff* there exists a monotonic function

$$H : g[a,b] \to f[a,b]$$

such that $H'(x) > 0$ and $H''(x) = 0$ for all x in the interior of the domain of definition.

L^- is defined in the same way where we require $H'(x) < 0$ instead of $H'(x) > 0$.

From the definition it follows that

$$\mathrm{L}^+(f,g) \Leftrightarrow \mathrm{L}^+(g,f) \quad \text{and} \quad \mathrm{L}^-(f,g) \Leftrightarrow \mathrm{L}^-(g,f).$$

Proposition 29. *Let $f, g \in \mathrm{R}_2[a,b]$.*

(i) *If $\mathrm{L}^+(f,g)$ holds then $[f''(t)] = [g''(t)]$ is true.*
(ii) *If $\mathrm{L}^-(f,g)$ holds then $[f''(t)] = -[g''(t)]$ is true.*

Proof. Since $\mathrm{L}^+(f,g)$ or $\mathrm{L}^-(f,g)$ holds, there exists a linear monotonic function

$$H : f[a,b] \to g[a,b]$$

such that $f(t) = H(g(t))$. So, $f'(t) = H'(g(t)) \cdot g'(t)$ and

$$f''(t) = H''(g(t)) \cdot (g'(t))^2 + H'(g(t)) \cdot g''(t) = H'(g(t)) \cdot g''(t)$$

(for $H''(g(t)) \equiv 0$). So,

$$[f''(t)] = [H'(g(t)) \cdot g''(t)] = [H'(g(t))] \odot [g''(t)].$$

In case (i), $H'(g(t)) > 0$, i.e., $[H'(g(t))] = +$. Therefore, $[f''(t)] = [g''(t)]$. In case (ii), $H'(g(t)) < 0$, i.e., $[H'(g(t))] = -$. Therefore, $[f''(t)] = -[g''(t)]$. $\square$

Proposition 30. *Let $f, g \in \mathrm{R}_2[a,b]$ be such that $\mathrm{L}^-(f,g)$. Then for all $t \in (a,b)$,*

$$\begin{aligned} f''(t) > 0 &\quad \textit{iff} \quad g''(t) < 0, \\ f''(t) = 0 &\quad \textit{iff} \quad g''(t) = 0, \\ f''(t) < 0 &\quad \textit{iff} \quad g''(t) > 0. \end{aligned}$$

Proof. The proof can be established as in the above. □

In the sequel we introduce the following propositions which may be applied in the filtering process.

Proposition 31. *Let $\mathrm{M}^+(x,y)$ be true. Then $[x'(t_i)] = 0$ implies that $[y''(t_i)] = [x''(t_i)]$ where t_i is a DTP.*

Proof. Since $\mathrm{M}^+(x,y)$, there is a monotonic increasing function f such that $y = f(x)$. Now, since $y'' = f''(x)(x')^2 + f'(x)x''$, the proposition follows from the equation

$$y''(t_i) = f''(x(t_i))(x'(t_i))^2 + f'(x(t_i))x''(t_i). \qquad \square$$

Proposition 32. *Let $\mathrm{M}^-(x,y)$ be true. Then $[x'(t_i)] = 0$ implies that $[y''(t_i)] = -[x''(t_i)]$ where t_i is a DTP.*

Proof. The proof of this proposition can be established as in the above. □

Now we discuss the monotonic function constraints, viz., M^{++}, M^{+-}, M^{-+} and M^{--}. These are classes of monotonic functions obtained by partitioning M^+ and M^-. We shall define these constraints and deduce some properties of it which are given below.

Definition 33. M^{++} is a two-place predicate on RFT2. $\mathrm{M}^{++}(f,g)$ holds true *iff* there exists a monotonic function

$$H : f[a,b] \to g[a,b]$$

such that $H'(x) > 0$ and $H''(x) > 0$ hold for all x in the interior of the domain of definition.

M^{+-} can be defined similarly by taking $H''(x) < 0$ instead of $H''(x) > 0$.

M^{++} is the set of all increasing functions of concave-up shapes while M^{+-} is the set of all increasing functions of concave-down shapes.

Similarly we can define M^{-+} and M^{--} constraints which are the classes of all monotonic decreasing functions with concave-up and concave-down shapes respectively.

Now we stipulate the following results.

Proposition 34. *Let $x(t)$ and $y(t)$ belong to the set RFT2 and let $F(x(t)) = y(t)$ where F is a strictly monotonic (either increasing or decreasing) function. Let $G = F^{-1}$ and $x'(t) \neq 0$ in some neighbourhood of some point t_i. Then $G'(F(x)) = 1/F'$ and $G''(F(x)) = F''/(F')^3$ hold true in that neighbourhood of t_i.*

Proof. The proof is given in Appendix B. □

From the above proposition we have the following corollary.

Corollary 35.

$$\begin{aligned} \mathrm{M}^{++}(x,y) &\Leftrightarrow \mathrm{M}^{+-}(y,x), \\ \mathrm{M}^{-+}(x,y) &\Leftrightarrow \mathrm{M}^{-+}(y,x), \\ \mathrm{M}^{--}(x,y) &\Leftrightarrow \mathrm{M}^{--}(y,x) \end{aligned}$$

Proposition 36. *If $\mathrm{M}^{++}(x,y)$ holds true, then*

$$\begin{aligned} [x''(t)] = + &\Rightarrow [y''(t)] = +, \\ [x''(t)] = 0 &\Rightarrow [y''(t)] = +, \\ [y''(t)] = 0 &\Rightarrow [x''(t)] = -, \\ [y''(t)] = - &\Rightarrow [x''(t)] = -. \end{aligned}$$

Proof. Since M^{++} holds true, there exists an $f \in \mathrm{M}^{++}$ such that $y(t) = f(x(t))$. Taking the second derivative we obtain

$$y''(t) = f'(x(t)) \cdot x''(t) + f''(x(t)) \cdot (x'(t))^2$$

from which the proposition follows. □

Proposition 37. *If $\mathrm{M}^{+-}(x,y)$ holds true, then*

$$\begin{aligned} [x''(t)] = - &\Rightarrow [y''(t)] = -, \\ [x''(t)] = 0 &\Rightarrow [y''(t)] = -, \\ [y''(t)] = + &\Rightarrow [x''(t)] = +, \\ [y''(t)] = 0 &\Rightarrow [x''(t)] = +. \end{aligned}$$

Proposition 38. *If $\mathrm{M}^{--}(x,y)$ holds true, then*

$$\begin{aligned} [x''(t)] = + &\Rightarrow [y''(t)] = -, \\ [x''(t)] = 0 &\Rightarrow [y''(t)] = -. \end{aligned}$$

Note that since $\mathrm{M}^{--}(x,y) \Rightarrow \mathrm{M}^{--}(y,x)$, we have

$$\begin{aligned} [y''(t)] = + &\Rightarrow [x''(t)] = -, \\ [y''(t)] = 0 &\Rightarrow [x''(t)] = -. \end{aligned}$$

Proposition 39. *If* $\mathrm{M}^{-+}(x,y)$ *holds true, then*

$$[x''(t)] = - \Rightarrow [y''(t)] = +,$$
$$[x''(t)] = 0 \Rightarrow [y''(t)] = +.$$

5.1. Constraint consistency

Kuipers [9] gave detailed rules and an application perspective for constraint consistency. For consistency in our setting, we exploit his results for each type of constraint which tests a tuple for qualitative state transition. There are three types of tests namely consistency of the qualitative magnitudes, consistency of the directions of change and of the direction of bulge.

5.1.1. Qualitative magnitude consistency

We shall now discuss the qualitative magnitude consistency (QMC) aspect. The propositions discussed for the ADD and MULT constraints in Appendix B in Kuipers' work [9] remain unaltered in our setting for any sign of direction of bulge. Slight modifications are needed at the time we use M^+ and M^- constraints in our environment. Hence we state the propositions for M^+ in the following. The proofs of the following propositions are the same as in Kuipers' work. We shall also state analogous propositions for the L^+ constraint for the same purpose.

Proposition 40. *Suppose* $\mathrm{M}^+(f,g)$ *with* $\mathrm{CVT1}(p,q)$, *and*

$$\mathrm{QS}(f,t_1,t_2) = \langle (p,p'),-,?\rangle, \qquad \mathrm{QS}(g,t_1,t_2) = \langle (q,q'),-,?\rangle,$$

where "?" denotes any sign in $\{+,0,-\}$, *then one of the following possibilities must be true at* t_2:

(1) $f(t_2) = p$ *and* $g(t_2) = q$,
(2) $f(t_2) > p$ *and* $g(t_2) > q$.

Proposition 41. *Suppose* $\mathrm{M}^+(f,g)$ *with* $\mathrm{CVT1}(p,q)$, *and*

$$\mathrm{QS}(f,t_1,t_2) = \langle (p,p'),-,?\rangle, \qquad \mathrm{QS}(g,t_1,t_2) = \langle (q'',q'),-,?\rangle,$$

where $q'' \neq q$, *then one of the following two possibilities must be true at* t_2:

(1) $f(t_2) > p$ *and* $g(t_2) = q''$,
(2) $f(t_2) > p$ *and* $g(t_2) > q''$.

We shall state below the analogous propositions for the L^+ constraint.

Proposition 42. *Let* $\mathrm{L}^+(f,g)$ *with* $\mathrm{CVT2}(p,q)$, *and*

$$\mathrm{QS}(f,t_1,t_2) = \langle (p,p'),-,+\rangle, \qquad \mathrm{QS}(g,t_1,t_2) = \langle (q,q'),-,+\rangle.$$

Then one of the following two possibilities must be true at t_2:

(1) $f(t_2) = p$ *and* $g(t_2) = q$,
(2) $f(t_2) > p$ *and* $g(t_2) > q$.

Proof. The proof is analogous to that of Proposition 34. □

Proposition 43. *Let* $\mathrm{L}^+(f,g)$ *with* $\mathrm{CVT2}(p,q)$, *and*

$$\mathrm{QS}(f,t_1,t_2) = \langle (p,p'),-,+\rangle, \qquad \mathrm{QS}(g,t_1,t_2) = \langle (q'',q'),-,+\rangle,$$

where $q'' \neq q$, *then one of the following two possibilities must be true at* t_2:
(1) $f(t_2) > p$ *and* $g(t_2) = q''$,
(2) $f(t_2) > p$ *and* $g(t_2) > q''$.

Proof. The proof is analogous to that of Proposition 36. □

It is pertinent to mention that similar propositions hold whether the constraint is either M^+ or M^- or L^+ or L^-, or whether the corresponding limits are approached from above, below or one from each side. Direction of change consistency is well presented by Kuipers [9]. We absorb that and in the following we introduce the direction of bulge consistency for the ADD constraint and MULT constraint.

5.1.2. Direction of bulge consistency

The following tables represent the valid direction of change and direction of bulge for ADD and MULT constraints. The tables below summarize the combination of direction of change and direction of bulge constraints. In these tables the upper left-most corner[2] represents the operation we consider and lower right-most corner represents that quantity for which the evaluation is performed.

- ADD(f,g,h): Here $h = f + g$. So, $h' = f' + g'$ and $h'' = f'' + g''$. Therefore,

$$[h'] = [f' + g'] = [f'] \oplus [g'],$$
$$[h''] = [f'' + g''] = [f''] \oplus [g''],$$

(1)

Sd1 $[g']$ / $[f']$	+	0	−
+	+	+	?
0	+	0	−
−	?	−	−
			$[h']$

[2] Key: Sd1—first derivative, Sd2—second derivative.

(2)

Sd2 $[f'']$ \ $[g'']$	+	0	−
+	+	+	?
0	+	0	−
−	?	−	−

$[h'']$

(B) MULT(f, g, h): The combination of the sign of magnitude, direction of change and direction of bulge that satisfy the MULT constraint are given below. Direction of change consistency that satisfies the MULT constraint depends on the sign of f, g, h and direction of bulge consistency depends on the sign of f, g, h, f', g' and h'.

(1)

$\odot$ $[f]$ \ $[g]$	+	0	−
+	+	0	−
0	0	0	0
−	−	0	+

$[h]$

Now,

$$\begin{aligned} \text{MULT}(f, g, h) &\Rightarrow h = fg \\ &\Rightarrow h' = f'g + fg' \\ &\Rightarrow h'' = f''g + 2f'g' + fg''. \end{aligned}$$

So,

$$\begin{aligned} [h] &= [fg] = [f][g], \\ [h'] &= [f'g + fg'] = [f'g] \oplus [fg'] \\ &= [f'] \odot [g] \oplus [f] \odot [g'] \\ [h''] &= [f''g + 2f'g' + fg''] \\ &= [f''g] \oplus [2f'g'] \oplus [fg''] \\ &= [f''] \odot [g] \oplus [f'] \odot [g'] \oplus [f] \odot [g'']. \end{aligned}$$

(2) If $[f] = [g] = +$.

Sd1, $[f']$ \ $[g']$	+	0	−
+	+	+	?
0	+	0	−
−	?	−	−

$[h']$

(2i) If $[f'] = [g'] = 0$.

Sd2, $[f'']$ \ $[g'']$	+	0	−
+	+	+	?
0	+	0	−
−	?	−	−

$[h'']$

(2ii) If $[f'] = [g'] = +$, or $[f'] = [g'] = -$.

Sd2, $[f'']$ \ $[g'']$	+	0	−
+	+	+	?
0	+	+	?
−	?	?	?

$[h'']$

(2iii) If $[f'] = +$, $[g'] = -$, or $[f'] = -$, $[g'] = +$.

Sd2 $[f'']$ \ $[g'']$	+	0	−
+	?	?	?
0	?	−	−
−	?	−	−

$[h'']$

(3) If $[f] = [g] = -$.

Sd1 $[f']$ \ $[g']$	+	0	−
+	−	−	?
0	−	0	+
−	?	+	+

$[h']$

(3i) If $[f'] = 0$, or $[g'] = 0$.

Sd2 $[f'']$ \ $[g'']$	+	0	−
+	−	−	?
0	−	0	+
−	?	+	+

$[h'']$

(3ii) If $[f'] = [g'] = +$, or $[f'] = [g'] = -$.

Sd2 $[f'']$ \ $[g'']$	+	0	−
+	?	?	?
0	?	+	+
−	?	+	+

$[h'']$

(3iii) If $[f'] = +$, $[g'] = -$, or $[f'] = -$, $[g'] = +$.

Sd2 $[f'']$ \ $[g'']$	+	0	−
+	−	−	?
0	−	−	?
−	?	?	?

$[h'']$

(4) If $[f] = +$, $[g] = -$.

Sd1 $[f']$ \ $[g']$	+	0	−
+	?	−	−
0	+	0	−
−	+	+	?

$[h']$

(4i) If $[f'] = 0$, or $[g'] = 0$.

Sd2: $[f'']$ \ $[g'']$	+	0	−
+	?	−	−
0	+	0	−
−	+	+	?

$[h'']$

(4ii) If $[f'] = [g'] = +$, or $[f'] = [g'] = -$.

Sd2: $[f'']$ \ $[g'']$	+	0	−
+	?	?	?
0	+	+	?
−	+	+	?

$[h'']$

(4iii) If $[f'] = +$, $[g'] = -$, or $[f'] = -$, $[g'] = +$.

Sd2: $[f'']$ \ $[g'']$	+	0	−
+	?	−	−
0	?	−	−
−	?	?	?

$[h'']$

(5) If $[f] = -$, $[g] = +$. The tables for (5), (5i), (5ii) and (5iii) can be evaluated by transposing tables for (4), (4i), (4ii) and (4iii), respectively.

(6) If $[f] = +$, $[g] = 0$.

Sd1 $[f']$ \ $[g']$	+	0	−
+	+	0	−
0	+	0	−
−	+	0	−

$[h']$

(6i) If $[f'] = 0$, or $[g'] = 0$.

Sd2 $[f'']$ \ $[g'']$	+	0	−
+	+	0	−
0	+	0	−
−	+	0	−

$[h'']$

(6ii) If $[f'] = [g'] = +$, or $[f'] = [g'] = -$.

Sd2 $[f'']$ \ $[g'']$	+	0	−
+	+	+	?
0	+	+	?
−	+	+	?

$[h'']$

(6iii) If $[f'] = +$, $[g'] = -$, or $[f'] = -$, $[g'] = +$.

Sd2 $[f'']$ \ $[g'']$	+	0	−
+	?	−	−
0	?	−	−
−	?	−	−

$[h'']$

(7) If $[f] = 0$, $[g] = +$. The tables for (7), (7i), (7ii) and (7iii) can be evaluated by transposing tables for (6), (6i), (6ii) and (6iii), respectively.

(8) If $[f] = -$, $[g] = 0$.

Sd1 $[f']$ \ $[g']$	+	0	−
+	−	0	+
0	−	0	+
−	−	0	+

$[h']$

(8i) If $[f'] = 0$, or $[g'] = 0$.

Sd2 $[f'']$ \ $[g'']$	+	0	−
+	−	0	+
0	−	0	+
−	−	0	+

$[h'']$

(8ii) If $[f'] = [g'] = +$, or $[f'] = [g'] = -$.

Sd2 $[f'']$ \ $[g'']$	$+$	0	$-$
$+$	?	$+$	$+$
0	?	$+$	$+$
$-$	?	$+$	$+$

$[h'']$

(8iii) If $[f'] = +$, $[g'] = -$, or $[f'] = -$, $[g'] = +$.

Sd2 $[f'']$ \ $[g'']$	$+$	0	$-$
$+$	$-$	$-$	?
0	$-$	$-$	?
$-$	$-$	$-$	?

$[h'']$

(9) If $[f] = -$, $[g] = 0$. The tables for (9), (9i), (9ii) and (9iii) can be evaluated by transposing tables for (8), (8i), (8ii) and (8iii) respectively.

(10) If $[f] = [g] = 0$.

Sd1 $[f']$ \ $[g']$	$+$	0	$-$
$+$	0	0	0
0	0	0	0
$-$	0	0	0

$[h']$

(10i) If $[f'] = 0$, or $[g'] = 0$.

Sd2 $[f'']$ \ $[g'']$	+	0	−
+	0	0	0
0	0	0	0
−	0	0	0

$[h'']$

(10ii) If $[f'] = [g'] = +$, or $[f'] = [g'] = -$.

Sd2 $[f'']$ \ $[g'']$	+	0	−
+	+	+	+
0	+	+	+
−	+	+	+

$[h'']$

(10iii) If $[f'] = +$, $[g'] = -$, or $[f'] = -$, $[g'] = +$.

Sd2 $[f'']$ \ $[g'']$	+	0	−
+	−	−	−
0	−	−	−
−	−	−	−

$[h'']$

The corresponding tables for M^+, M^-, L^+ and L^- can be constructed.

6. Global interpretations and global filters

The definition of global interpretation is the same as in [9], i.e. a global interpretation is an assignment of a transition to each function in the system and it serves the same purpose as posed by Kuipers. So generating global interpretations has a similar applicability in our setting.

Global filters also have similar applicability. Global filters such as "No change", "Cycle" and "Divergence" are equally applicable in our framework with the same significance. In this respect the "No change" filter which is the transition set {I-1, I-4, I-7} in [9] will be {I-1, I-4, I-11, I-18, I-23, I-26} in our setting.

Thus, from the above results the QSIM algorithm of [9] is modified to the pure QSIM2 algorithm. Additional heuristic filters such as "Quiescence" and "No divergence" [9] may be used in any particular application.

6.1. *Infinity and asymptotic approach*

For the fulfillment of our setting, the infinity and asymptotic approach of [9] requires two additional corollaries of Propositions A.6 and A.7 of [9].

Corollary 44. *Let* $f[a,\infty] \to \mathbb{R}^*$ *be an RFT2. If the limit of* $f(t)$ *as* $t \to \infty$ *is finite, then* $\lim_{t\to\infty} f''(t) = 0$.

Corollary 45. *Let* $f[a,b] \to \mathbb{R}^*$ *be an RFT2, and* $\lim_{t\to b} f(t) = \infty$, *where b is finite, then* $\lim_{t\to b} f''(t) = \infty$.

Through the discussions of earlier sections the theoretical formulation of QSIM2 is completed.

7. Qualitative simulation

This section describes the qualitative simulation algorithm, i.e. QSIM2.

7.1. *Input and output*

(1) A set $\{f_1, f_2, \ldots, f_m\}$ of symbols representing the functions in the system.
(2) A set of constraints that are applied to the following function symbols: $M^+(f,g)$, $M^-(f,g)$, $L^+(f,g)$, $L^-(f,g)$, $M^{++}(f,g)$, $M^{+-}(f,g)$, $M^{-+}(f,g)$, $M^{--}(f,g)$, ADD(f,g,h), MULT(f,g,h), MINUS(f,g), DERIV(f,g), DERIV$^+(f,g)$, or DERIV$^-(f,g)$. Each constraint may have associated corresponding values for its functions.
(3) Each function is associated with a totally ordered set of symbols representing landmark values; each function has at least the basic set of landmarks $\{-\infty, 0, +\infty\}$.

(4) Each function may have upper and lower range limits, which are landmark values beyond which the current set of constraints no longer apply. A range limit may be associated with a new operating region which has its own constraints and range limits.

(5) An initial time point symbol, t_0, and qualitative values for each of the f_i at t_0 are given.

The result of the qualitative simulations is one or more qualitative behavior descriptions for the function symbols given. Each qualitative behavior description consists of the following:

(1) A sequence $\{t_0, t_1, \ldots, t_n\}$ of symbols represents the distinguished time points of the system's behavior.

(2) Each function f_i has a totally ordered set of landmark values, possibly extending the original given set.

(3) Each function has at each DTP, or interval between CDTP, a qualitative state description expressed in terms of the landmark values of that function.

7.2. *The algorithm QSIM2*

The steps involved in the algorithm QSIM2 are the same as in QSIM [9]. Only Table 1 of step 2 of QSIM [9] will be replaced by the new P-transitions and I-transitions (see Tables 1 and 2 of Section 3 of the present paper). Apart from the difference in transitions table, at each step QSIM2 evaluates some new features which are introduced due to its extension from QSIM [9] and which are discussed in Sections 4–6.

7.3. *Demonstration example*

To illustrate the power of QSIM2 we consider the ball system of [9].

We demonstrate here one cycle of the QSIM2 algorithm on the Ball system [9]. This simple system consists of a ball thrown upward under constant gravity. The corresponding QDEs for the system are:

$$\mathrm{DERIV}(Y, V), \quad \mathrm{DERIV}(V, A), \quad A(t) = g < 0.$$

We consider here the second state where the ball is approaching the maximum height (as yet undiscovered) with the initial states as shown in Table 4. These states show that the QSIM2 algorithm needs richer state descriptions than QSIM. I-transitions take place, because the current states show their states in the time interval (t_0, t_1). Possible state transitions for each function are derived from Table 2 (see Tables 5–7). Here the possibility $Y(t_1) = \infty$ is excluded for simplicity. (However this possibility would be excluded by the methods given in Appendix A.2 of [9].)

In the step transition tuples are formed for each constraint. Apply consistency filtering. The mark "c" (in Table 8) shows the eliminated tuple for constraint consistency filtering. Here for example the tuple (I-11, I-22) is inconsistent for

$$+ = \left[\frac{\mathrm{d}Y}{\mathrm{d}t}\right] \neq [V] = 0.$$

Table 4
List of initial states

$QS(Y, t_0, t_1)$	=	$\langle(0,\infty),+,-\rangle$
$QS(V, t_0, t_1)$	=	$\langle(0,\infty),-,0\rangle$
$QS(A, t_0, t_1)$	=	$\langle g,0,0\rangle$

Table 5
Possible state transitions derived from Table 2

Name	$QS(Y, t_0, t_1)$	$\Rightarrow$	$QS(Y, t_1)$
I-11	$\langle(0,\infty),+,-\rangle$	$\Rightarrow$	$\langle(0,\infty),+,-\rangle$
I-12	$\langle(0,\infty),+,-\rangle$	$\Rightarrow$	$\langle Y_1^*,+,0\rangle$
I-13	$\langle(0,\infty),+,-\rangle$	$\Rightarrow$	$\langle Y_{max},0,-\rangle$
I-14	$\langle(0,\infty),+,-\rangle$	$\Rightarrow$	$\langle Y_2^*,0,0\rangle$

Table 6
Possible state transitions derived from Table 2

Name	$QS(V, t_0, t_1)$	$\Rightarrow$	$QS(V, t_1)$
I-22	$\langle(0,\infty),-,0\rangle$	$\Rightarrow$	$\langle 0,-,0\rangle$
I-23	$\langle(0,\infty),-,0\rangle$	$\Rightarrow$	$\langle(0,\infty),-,0\rangle$

Table 7
Possible state transition derived from Table 2

Name	$QS(A, t_0, t_1)$	$\Rightarrow$	$QS(A, t_1)$
I-1	$\langle g,0,0\rangle$	$\Rightarrow$	$\langle g,0,0\rangle$

Table 8
List of formed transition tuples

DERIV(Y, V)	DERIV(V, A)
(I-11, I-22)c	(I-22, I-1)
(I-11, I-23)	(I-23, I-1)
(I-12, I-22)c	
(I-12, I-23)c	
(I-13, I-22)	
(I-13, I-23)c	
(I-14, I-22)c	
(I-14, I-23)c	

Table 9
List of global interpretations

Y	V	A
I-11	I-23	I-1
I-13	I-22	I-1

Table 10
List of successor states

$QS(Y, t_1)$	=	$\langle Y_{max}, 0, - \rangle$
$QS(V, t_1)$	=	$\langle (0, -, 0 \rangle$
$QS(A, t_1)$	=	$\langle g, 0, 0 \rangle$

The remaining tuples form the two global interpretations shown in Table 9.

Between these interpretations the first interpretation is identical to the predecessor qualitative state descriptions. Therefore, application of change of the "No change" filter yields the unique successor qualitative state descriptions (i.e. the second interpretation) at the time point t_1. The successor states are shown in Table 10.

Y_{max} is the newly discovered landmark value. QSIM2 outputs are shown in Fig. 2. The ball system, as described by the QDEs, shows three physical parameters, viz., height (Y), velocity (V) and acceleration (A). Since here acceleration is constant, a simple analysis reveals that velocity is linear and height is parabolic in nature. These features are explicit in the QSIM2 outputs as shown in Fig. 2; but are not explicit in the corresponding QSIM outputs (Fig. 5 of [9]).

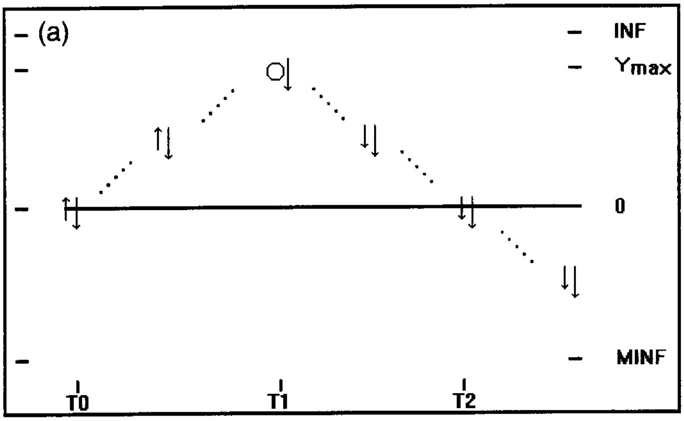
8. Complexity of QSIM2

Now we analyze the algorithmic complexity of QSIM2. Obviously, the time and space required to execute algorithm QSIM2 with the same input as [9] are more than those of the QSIM algorithm. This is the result of taking a larger fixed length transition table for P-transitions and I-transitions that allow the curvature profile in addition to the predicted behavior.

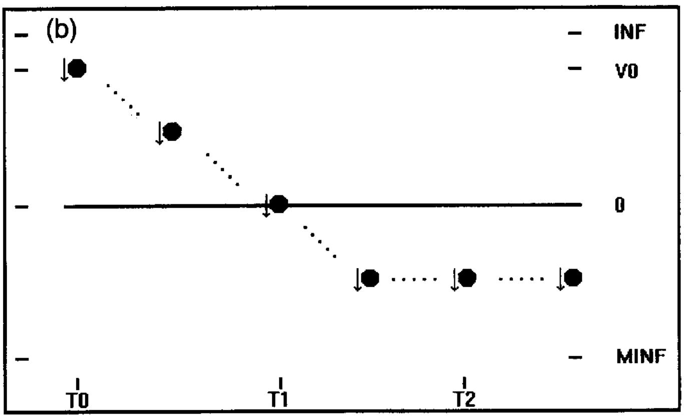
Let a system have p parameters, c constraints and let the largest behavior be of length t (t is then, on average, log of the total number of qualitative states [9]).

A constraint cannot have more than three parameters, so $p = O(c)$. Here also a set of transitions is assigned to each parameter from a fixed length table as in [9] and not more than 7 transitions are assigned to each parameter; these require 7^p transitions. Although it actually needs $7p$ transitions requiring $O(p)$ time.

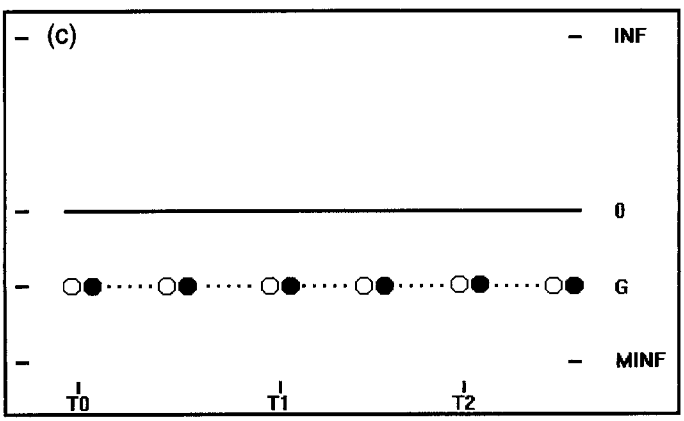
A constraint can have almost 7^3 transition tuples. Filtering a tuple against direction of change tables [9] takes constant time and the number of CVT1 grows linearly with the length t of the behavior. This requires $O(ct)$ time. Therefore, constraint filtering requires the sum of the times due to the direction of change and to the direction of bulge, both of which require $O(ct)$ time.



QSIM2: Height



QSIM2: Velocity



QSIM2: Accelleration

Here, as in [9], Waltz filtering takes $O(c)$ time and the remaining parts of the product space, which is in general small, form the global interpretation.

The global filter which checks previous identical states requires $O(pt)$ time.

Thus, the QSIM2 algorithm is exponential in the worst case.

9. Detection of actual behaviors

In this section we show that all actual behaviors of a mechanism are predicted by its qualitative simulation, i.e., QSIM2. To demonstrate the above claim, we borrow from Kuipers' [9] one definition and some theorems which are proved in our framework.

Definition 46 (Kuipers [9]). Let u be an RFT2 where $u : [a,b] \to \mathbb{R}$ and let a qualitative behavior description of the function symbol h be

$$\mathrm{QS}(h,t_0), \mathrm{QS}(h,t_0,t_1), \ldots, \mathrm{QS}(h,t_{n-1},t_n), \mathrm{QS}(h,t_n)$$

with DTPs $\{t_0,t_1,\ldots,t_n\}$ and landmarks $\{l_1,l_2,\ldots,l_k\}$. We say that u satisfies the behavioral description if there is an order-preserving mapping

$$m : \{t_0,t_1,\ldots,t_n\} \xrightarrow{\text{into}} \{l_1,l_2,\ldots,l_k\}$$

with $m(t_0) = a$ and $m(t_n) = b$, and an order-preserving mapping m of $\{l_1,l_2,\ldots,l_k\}$ into $\mathbb{R}$, such that for all DTPs t_i, $\mathrm{QS}(u,m(t_i))$ matches $\mathrm{QS}(h,t_i)$ and $\mathrm{QS}(u,m(t_i),m(t_{i+1}))$ matches $\mathrm{QS}(h,t_i,t_{i+1})$.

Theorem 47 (Kuipers [9]). *Let*

$$F[u(t),u'(t),\ldots,u^n(t)] = 0 \tag{3}$$

be an ODE of order n, and let $\{u(t_0) = y_0, u'(t_0) = y_1, \ldots, u^n(t_0) = y_n\}$ be the initial conditions on the solution to (3). *Suppose that* (3) *and its initial conditions are satisfied by an RFT2 $u : [a,b] \to \mathbb{R}$. Let C be the set of functions and constraints derived from* (3) *by the method stated in* [9, Section 3.3], *and let,* $\mathrm{QS}(F,t_0)$ [9, p. 229] *be the qualitative state description derived from the given set of initial conditions. Let T be the tree of qualitative descriptions derived from C and* $\mathrm{QS}(F,t_0)$ *by the QSIM2 algorithm. Then the function u and the subexpression functions derived from it satisfy some behavioral description in T.*

Proof. We shall give the proof in the same manner as Kuipers has given in [9]. Here we have to show that any actual solution of (3) is not discarded by any filtering operations so that u and its derived function must satisfy some behavioral description in T.

Fig. 2. Predicted behaviors of the ball system. Key: The short arrows ↑ and ↓, the long arrows $\Big\uparrow$ and $\Big\downarrow$, the circle ⊃ and the disk • represent qualitative direction, direction of bulge, points for which the pertinent function has zero first derivative and zero second derivative respectively.

Due to qualitative abstraction of initial conditions u satisfies $\mathrm{QS}(F, t_0)$. Step 2 in QSIM2 generates all possible qualitative state transitions for the functions in C from a given qualitative state using the transition tables. Thus any change in the qualitative state of the system must be included in the possibilities generated. Step 3 of QSIM2 [3] filters out all combinations of transitions due to individual constraint inconsistency. Inconsistent sets of direction of change and direction of bulge are detected by comparison with the tables given in Section 5.1.2. The proper implications of sets of corresponding values are checked against Propositions B1–B3 and B9 of [9] and Propositions 40–43 in this paper. The pairwise consistency filtering of [9] is also applicable in our setting; this filtering of step 4 eliminates from consideration of transitions tuples which are inconsistent with all neighboring tuples and could not contribute to a global interpretation. Step 5 eliminates combination of tuples which do not make consistent assignments of state transitions to particular functions. Finally, the global filters do not eliminate possible behaviors of the system. So at each stage of the simulation, all possible successors to the current qualitative state lie in the space generated and no genuinely possible successor is eliminated. □

Theorem 48 (Kuipers [9]). *Let C be a set of function symbols and qualitative constraints, and let $\mathrm{QS}(F, t_0)$ be the initial qualitative state description. Let T be the tree of qualitative state descriptions derive from C and $\mathrm{QS}(F, t_0)$ by the pure QSIM2 algorithm. For some C and $\mathrm{QS}(F, t_0)$ there are behaviors in T which do not correspond to any solution $u : [a, b] \to \mathbb{R}$ to any differential equation and initial condition corresponding to C and $\mathrm{QS}(F, t_0)$.*

Proof. We shall give the proof as Kuipers did in [9]. Qualitative simulation on the model of the spring mass system (as given in [9]) using QSIM2 produces the same behaviors (see Fig. C.1 in Appendix C) as QSIM does (see Fig. 7 in [9, p. 320]), which shows that QSIM2 produces stable (behavior 1), decreasing (behavior 2) and increasing (behavior 3) oscillation; although only one behavior is correct which is stable oscillation. But no local inference rule is able to determine the actual solution which in this case is the stable oscillation. Therefore, the other two solutions are spurious solutions which are predicted by the QSIM2 algorithm. □

Theorems 47 and 48 lead to the following corollary.

Corollary 49 (Kuipers [9]). *If a set of constraints is consistent, and if QSIM2 predicts a single behavior, then that behavior represents the actual behavior of the mechanism.*

Qualitative simulation of the QDE model using QSIM2 may sometimes yield intractable branching. A solution to this problem can be obtained from the concepts given in [10]. But a detailed solution of such a problem along the lines of [10] has yet to be explored. In the following section for the completion of our work we briefly propose one method towards the solution of the above mentioned problem.

[3] Step 1 of QSIM2 means step 1 of QSIM, because we do not change the basic algorithm of qualitative simulation QSIM.

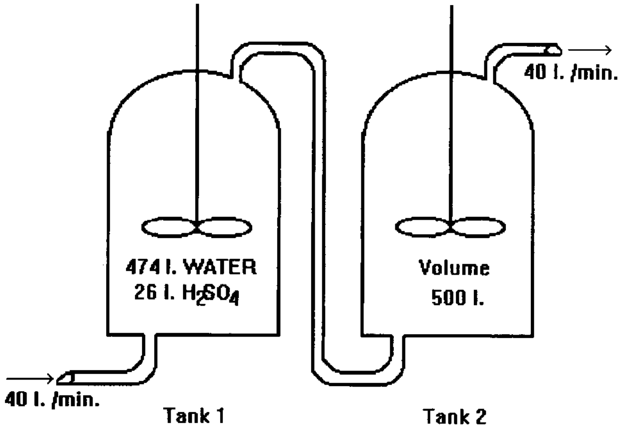


Fig. 3. Mixing tank example.

10. Coarse state descriptions

Kuipers et al. [10] have defined the term *chatter* to identify those variables in the QDE model which account for intractable branching. We shall use the same perspective in this paper; but here we depend on experimental results to identify chattering variables.

To circumvent this chattering aspects Kuipers et al. [10] have adopted two approaches:

- using HOD (higher order derivative) constraints; and
- ignoring qualitative direction.

The first approach is part of future work with respect to QSIM2. We adopt the second method with a different viewpoint. In this method, direction of bulge (db) is ignored for certain variables which are responsible for branching. Ignoring db yields the transition tables similar to those of Kuipers [9]. But these transition tables [9] will generate the loss of an important source of constraints. Hence, we use the original transition tables of QSIM2 and resort to a simple technique as stated below.

By ignoring db we adopt a method where qualitative value (qval) and qualitative directions are only taken into consideration leaving db ignored. We denote this method by *ign-db*. Although this gives partial state descriptions when we compare with QSIM2, it yields full information whenever we compare the result with the QSIM output (see Fig. 5 for X4 and X5.)

11. Mixing tank problem

Two tanks (see Fig. 3) having capacity of 500 liters each are interconnected by a pipe. Tank 1 contains 26 liters of sulfuric acid in fresh to give 500 liters of dilute acid. Assume that 40 liters/min. of fresh water enter tank 1 and that the mixture leaves tank 1 and enters tank 2, which initially contained 500 liters of fresh water. The dilute acid in

Table 11
List of initial states

$QS(x_1, t_0)$	=	$\langle 0.05, -, + \rangle$
$QS(x_2, t_0)$	=	$\langle 0, +, - \rangle$
$QS(x_3, t_0)$	=	$\langle -0.40, +, - \rangle$
$QS(x_4, t_0)$	=	$\langle 0.40, -, + \rangle$
$QS(x_5, t_0)$	=	$\langle 0.50, -, + \rangle$

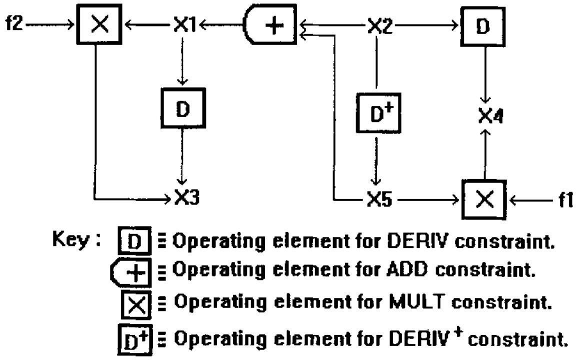


Fig. 4. Structure described by constraints.

tank 2 is assumed to have uniform density, and to leave tank 2 also at 40 liters/min. Find the qualitative behavior of the acid concentration over time.

Solution: We take two parameters x_1 and x_2 representing the concentration per unit in tank 1 and tank 2 respectively at any time t.

The dynamics are modeled by the following differential equation with initial conditions:

$$\dot{x}_1(t) = -0.08x_1(t),$$
$$\dot{x}_2(t) = 0.08x_1(t) - 0.08x_2(t),$$

where $t_0 = 0$, $x_1(t_0) = 0.05$, $x_2(t_0) = 0$.

Abstraction of parameters: Let $x_3 = \dot{x}_1$, $x_1 - x_2 = x_5$, so $x_1 = x_2 + x_5$, $x_4 = \dot{x}_2$, $x_4 = 0.08x_5 = f_1.x_5$ where $f_1 = 0.08$, $\dot{x}_2 = 0.08x_5$, $x_3 = -0.08x_1 = f_2.x_1$ where $f_2 = -0.08$.

Corresponding QDE model:

$$\text{DERIV}(x_1, x_3), \quad \text{DERIV}(x_2, x_4), \quad \text{ADD}(x_2, x_5, x_1),$$
$$\text{DERIV}^+(x_2, x_5), \quad \text{MULT}(f_1, x_5, x_4), \quad \text{MULT}(f_2, x_1, x_3).$$

and initial states as shown in Table 11.

Fig. 4 represents the structure described by the constraints. The simulation results using QSIM2 and the comparative study with that of QSIM are shown in Fig. 5. A comprehensive discussion on the simulation results are given in Section 12.

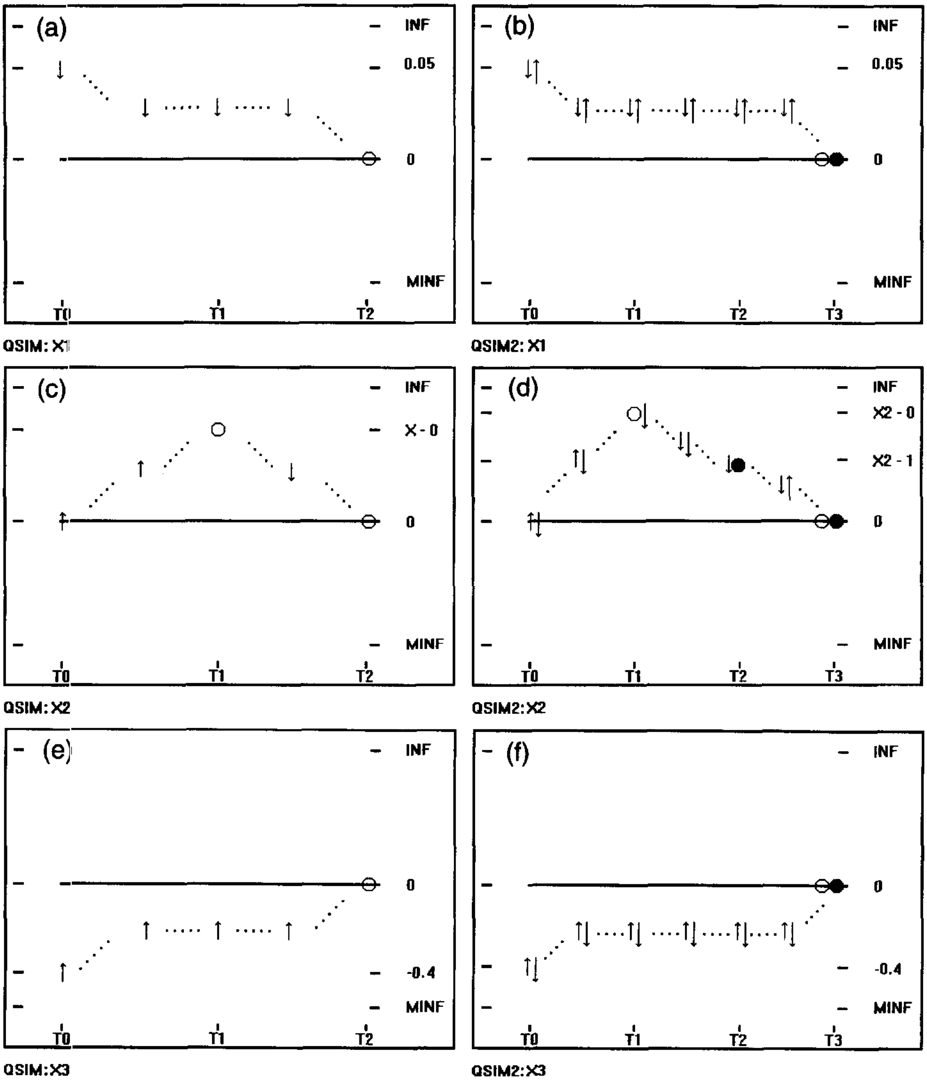


Fig. 5. QSIM and QSIM2 outpus for the mixing tank problem.

12. Critical appreciation

In this section we discuss the strengths and weaknesses of QSIM2 over QSIM.

QSIM2 is the straightforward extension of QSIM incorporating the sign of second derivative (direction of bulge, i.e., db) in the state description of the parameters to capture the qualitatively important curvature profile, inflection point, etc., in the predicted trajectories of the qualitative model given by the qualitative differential equations (QDEs) and at the same time imposing a stronger constraint which can be used to

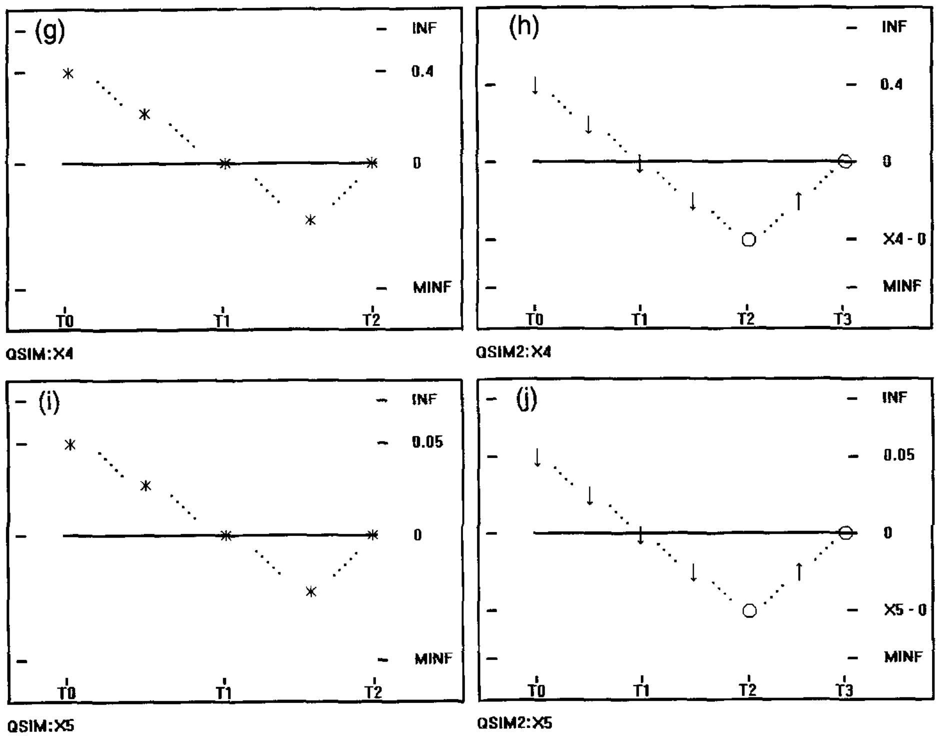


Fig. 5 — continued.

eliminate spurious behaviors produced during the qualitative simulation using QSIM2. QSIM2 always carries more information (in terms of direction of bulges, points of inflection) than QSIM. But there are situations where QSIM2 produces a higher number of predicted behaviors than QSIM. Further, the direction of bulges are constraining over the qualitative direction during qualitative simulation (using QSIM2); therefore *chatter* [10] may occur due to its direction of bulge description rather than its qualitative state description.

QSIM2 transition tables are much larger than those of QSIM. This causes enhanced computational cost of QSIM2 over QSIM. Note that the possible state transitions (P-transitions and I-transitions) of QSIM2 collapse to those of QSIM [9, p.300], if we ignore the direction of bulge.

Due to higher resolution in the state descriptions, QSIM2 has a possibility of producing more branches during the qualitative simulation. Moreover, QSIM2 requires second order derivative information of each parameter in the system to start with the qualitative simulation.

QSIM2 may produce intractable branching which may be curtailed by introducing higher order derivative constraints as proposed in [10]. But in the present paper this particular aspect has not been considered but will be treated as a separate research problem in future.

Coarser state descriptions (pertinent to QSIM2) as discussed in Section 10, in presence of *chatter* of certain variables will carry information which is equal to that of QSIM. For instance, with respect to Fig. 5, the qualitative description X4 is obtained by QSIM (ignoring qdir). Whereas the qualitative description X4 obtained by QSIM2 (ignoring db) contains information such as qualitative direction and landmark values which are equivalent to the usual QSIM description. A similar argument is true for "QSIM: X5" and "QSIM2: X5". Thus the qualitative descriptions of "QSIM2: X4" and "QSIM2: X5" are more enriched than those of "QSIM: X4" and "QSIM: X5".

Further the QSIM2 outputs for the parameters X1, X2 and X3 show the direction of bulges in addition to the qualitative directions. Moreover in "QSIM2: X2", we get the qualitatively important inflection point at the time point T2. In "QSIM2: X4" and "QSIM2: X5", we get the qualitative direction with landmark values at the time point T2 which manifests the more accurate trend of the behaviors of X4 and X5. Such accurate trend is absent in "QSIM: X4" and "QSIM: X5".

From the above discussion it is understood that QSIM2 provides more information at additional computational cost. Now the choice of the modeler depends on the actual application of the model. For instance, if we go for model (qualitative model) based analysis (qualitative analysis), synthesis and design (qualitative design [16,17]) of a decision maker/controller for a physical system/process we may need to have specific information about transient overshoot/undershoot, intermediate oscillations and steady state behavior of a parameter under a specific excitation/input. Under such circumstances, direction of bulge, inflection points, etc., are important information to be considered for design and, hence, QSIM2 will be the more desirable choice. But we should always remember that a detailed model (that may be qualitative or quantitative) of a process/system will always yield a complex design of a controller/decision maker, which may produce better precision in the ultimate response of the process or system but at high implementation cost. So, if really high precision is needed it is always worth paying the high cost. But there are many situations where high precision is not needed. Under such circumstances it is always advisable to go by the simple model (qualitative or quantitative) for low cost design of the decision maker/controller. Thus the cost-benefit tradeoff is guided by the design specifications of the application domain and a modeler should be careful before he/she takes a judicious judgment about the selection of a particular model.

13. Conclusion

Both the qualitative models, i.e. QSIM and QSIM2, try to find out and cancel the spurious behaviors so as to get the fewer and fewer numbers of trajectories. Since the actual behaviors are always included in the predicted trajectories (see Theorem 47), the reliability of the qualitative model is always ensured. Therefore the researchers in this field have an equal interest in finding various local and global filters.

QSIM frameworks require an abstraction relation which transforms ordinary differential equations to qualitative constraint equations. Because of this fact, Kuipers [10] adopted the semantic "QDE", abbreviation of qualitative differential equation, denoting

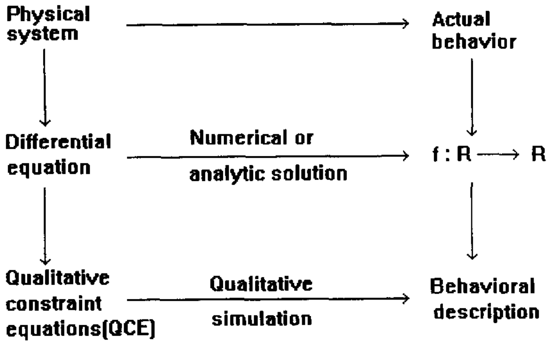


Fig. 6. Prediction by qualitative simulation and solution of differential equations are both abstractions of actual behaviors.

the qualitative constraint equations. Here a semantic dilemma arises because QDE is merely an abstraction of an ODE. But, for example, if there is any algebraic equation in addition to QDE, then the abstracted version of it lacks its full semantic exploration. We, therefore, prefer the semantic QCE (qualitative constraint equations) in place of QDE capturing the semantic caption of a larger class of equations.

The QSIM2 approach is a straightforward outgrowth of QSIM introduced by Kuipers. QSIM2 is different from the qualitative model of Kuipers et al. [10] in which they consider the HOD (Higher Order Derivative) constraints to reduce *chatter* ("intractable branching representing uninteresting or even spurious distinctions among qualitative behaviors" [10]) in the predicted behaviors and realize curvature perspective. We have considered the sign of the second derivatives throughout the process. Our approach has an advantage, beside its weaknesses (see Section 12), that it can discover inflection points as landmarks which are the important features of a curve. So QSIM2 can automatically extract the additional features such as curvature, inflection points, which manifest the exact pattern of the simulated behaviors.

It is also possible to implement directly the HOD constraint approach in our work which can further reduce chatter in the predicted behaviors.

Kuipers et al. [10] did not extend their analysis beyond the third order derivative. We can include the third order derivative in addition to qdir and db which yields larger tables for P-transitions and I-transitions and a pertinent analysis can be performed.

In the present paper we simply concentrate on the qualitative modeling aspect of a physical system. Design of a qualitative controller [13, 14] based on the analysis of such a qualitative model (i.e., QSIM and QSIM2) will be part of our future research work.

Acknowledgements

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Appendix A. List of symbols

$\mathbb{R}^*$	:=	Extended real number line.
RFT1	:=	Reasonable function of type 1.
RFT2	:=	Reasonable function of type 2.
$\mathrm{R}_1[a,b]$	:=	Set of all RFT1s in $[a,b]$.
$\mathrm{R}_2[a,b]$	:=	Set of all RFT2s in $[a,b]$.
LV	:=	Landmark value.
DTP	:=	Distinguished time point.
CDTP	:=	Consecutive DTPs.
$\mathrm{D}_1[f,a,b]$	:=	set of all DTPs of $f \in \mathrm{R}_1[a,b]$.
$\mathrm{D}_2[f,a,b]$	:=	set of all DTPs of $f \in \mathrm{R}_2[a,b]$.
$\mathrm{L}_1[f,a,b]$	:=	set of all LVs of $f \in \mathrm{R}_1[a,b]$
	:=	$\{f(t') \mid t' \in \mathrm{D}_1[f,a,b]\}$.
$\mathrm{L}_2[f,a,b]$	:=	set of all LVs of $f \in \mathrm{R}_2[a,b]$
	:=	$\{f(t') \mid t' \in \mathrm{D}_2[f,a,b]\}$.
qval	:=	Qualitative value.
qdir	:=	Qualitative direction.
db	:=	Direction of bulge.
$\mathrm{QS}(f,t)$	:=	Qualitative state of f at time point t.
$\mathrm{QS}(f,t',t'')$	:=	Qualitative state of f in open interval (t',t'').
(C)	:=	Critical point.
(I)	:=	Inflection point.
(J)	:=	J-point.
(CI)	:=	Critical and inflection point.
(CJ)	:=	Critical and J-point.
$\mathrm{CF}_f[t',t'']$	:=	Characteristic feature of f at t' and t'' respectively.
$\mathrm{CF}_f[t',t''] = [(\mathrm{I}),(\mathrm{J})]$	:=	t' and t'' are an inflection point and a J-point of f respectively.
$\mathrm{CF}_f[t',t''] = [(\mathrm{I}) \leftrightarrow (\mathrm{J})]$	:=	t' is an inflection point and t'' is a J-point of f and vice versa.
$\mathrm{B}_\delta(\uparrow p)$	:=	$(p, p+\delta)$.
$\mathrm{B}_\delta(\downarrow p)$	:=	$(p-\delta, p)$.
$\dot{\vee}$	:=	exclusive OR.
$\mathrm{B}_\delta^{f'>0}(\uparrow t')$	:=	$\{\mathrm{B}_\delta(\uparrow t') \mid f'(t) > 0\ \forall t \in \mathrm{B}_\delta(\uparrow t')\}$.
$\mathrm{B}_{\delta(\uparrow t')}^{f'>0}$	:=	$\sup_\delta \mathrm{B}_\delta^{f'>0}(\uparrow t')$.
$\mathrm{B}_\delta^{f''>0}(\uparrow t')$	:=	$\{\mathrm{B}_\delta(\uparrow t') \mid f''(t) > 0\ \forall t \in \mathrm{B}_\delta(\uparrow t')\}$.
$\mathrm{B}_{\delta(\uparrow t')}^{f''>0}$	:=	$\sup_\delta \mathrm{B}_\delta^{f''>0}(\uparrow t')$.
QSIM2	:=	Extension of QSIM with qualitative curvature.
$[x]$	:=	Sign of x which is either $+$ or 0 or $-$.
QMC	:=	Qualitative magnitude consistency.
CVs	:=	Corresponding values.

CVT1	:=	Corresponding values of type 1.
CVT2	:=	Corresponding values of type 2.
ODE	:=	Ordinary differential equation.
QDE	:=	Qualitative differential equation.
Sd1	:=	First derivative.
Sd2	:=	Second derivative.

Appendix B. Proofs

Proof of Proposition 13. Since t' is a J-point, there exists a $\delta > 0$ such that

$$\text{(a)} \quad f''(t) \begin{cases} = 0 & \text{in } [t', t' + \sigma), \\ \neq 0 & \text{in } (t' - \sigma, t'), \end{cases}$$

or

$$\text{(b)} \quad f''(t) \begin{cases} = 0 & \text{in } (t' - \sigma, t'], \\ \neq 0 & \text{in } (t', t' + \sigma). \end{cases}$$

We now consider case (a) only.

Since t' is a critical point, $f'(t') = 0$. Now since $f''(t) = 0\ \forall t \in [t', t' + \delta)$, we have $f'(t) = C$, a constant, $\forall t \in (t', t' + \delta)$. Let $\{x_n\}$ be any sequence in $(t', t' + \delta)$ which converges to t'. By continuity of f', we can write $\lim_{n\to\infty} f'(x_n) = f'(\lim_{n\to\infty} x_n)$. Therefore,

$$f'(t') = f'\big(\lim_{n\to\infty} x_n\big) = \lim_{n\to\infty} f'(x_n) = C.$$

Since $f'(x_n) = C\ \forall n$. Therefore, $C = f'(t') = 0$. $\square$

Proof of Proposition 15. Since $\mathrm{CF}[t', t''] = [(\mathrm{I}), (\mathrm{I})]$, we have $f''(t') = f''(t'') = 0$ and $f'(t) \neq 0$ in (t', t''). Now by the definition of inflection point there exists a $\delta > 0$ such that

$$f''(t) > 0 \quad \text{in } \mathrm{B}_\delta(\uparrow t'), \tag{B.1}$$

or

$$f''(t) < 0 \quad \text{in } \mathrm{B}_\delta(\uparrow t'), \tag{B.2}$$

where $\mathrm{B}_\delta(\uparrow p) = (p, p + \delta)$.

Now we consider (B.1) and define

$$\mathrm{B}_\delta^{f''>0}(\uparrow t') = \{(t', t' + \delta) \text{ such that } f''(t) > 0 \text{ in } \mathrm{B}_\delta(\uparrow t')\}.$$

$\sup_\delta \mathrm{B}_\delta^{f''>0}(\uparrow t')$ exists because δ is bounded. In fact, $\delta < b - a$.

We define

$$\sup_\delta \mathrm{B}_\delta^{f''>0}(\uparrow t') = \mathrm{B}_{\delta(\uparrow t')}^{f''>0}.$$

So, $B_{\delta(\uparrow t')}^{f''>0} = B_{\delta(\uparrow t')}^{f''>0}(\uparrow t')$.

Clearly $f''(t' + \delta(\uparrow t')) \leqslant 0$. By the continuity of $f''(t)$, we conclude that $f''(t' + \delta(t')) = 0$. Therefore, $t' + \delta(t') = t''$.

Now $f'(t') > 0$, or $f'(t') < 0$, t' is an inflection point. Since $f'(t)$ is continuous, $f'(t)$ cannot change its sign without zero crossing. Therefore, $f'(t) > 0$ in (t', t''), or $f'(t) < 0$ in (t', t''). Since $f'(t) \neq 0$ in (t', t''), because t', t'' are CDTP, we get that

$(\bar{\mathrm{b}})$ $\quad f''(t) > 0,\ f'(t) > 0\ \forall t \in (t', t'')$

$(\bar{\mathrm{c}})$ $\quad f''(t) > 0,\ f'(t) < 0\ \forall t \in (t', t'')$.

Similarly considering (B.2), we shall get $(\bar{\mathrm{d}})$ and $(\bar{\mathrm{e}})$. □

Proof of Proposition 16. (i) Since $\mathrm{CF}[t', t''] = [(\mathrm{C}), (\mathrm{I})]$, we have $f'(t') = 0$, $f''(t'') = 0$ and $f'(t) \neq 0$ in (t', t''), $f''(t) \neq 0$ in (t', t''). Since t' is a critical point, there exists a $\delta > 0$ such that

$$f'(t) > 0 \quad \text{in } B_\delta(\uparrow t'), \tag{B.3}$$

or

$$f'(t) < 0 \quad \text{in } B_\delta(\uparrow t'). \tag{B.4}$$

Now first we consider the case (B.3). Let

$$B_\delta^{f'>0}(\uparrow t') = \{B_\delta(\uparrow t') \mid f'(t) > 0\ \forall t \in B_\delta(\uparrow t)\}.$$

$\sup_\delta B_\delta^{f'>0}(\uparrow t')$ exists because δ is bounded. Let

$$\sup_\delta B_\delta^{f'>0}(\uparrow t') = B_{\delta(\uparrow t')}^{f'>0}.$$

Now $t' - \delta(t') > t''$ because $f'(t'') \neq 0$ for t'' is simply an inflection point. Now, $f''(t') \neq 0$ (by hypothesis).

Therefore, either

$$f''(t') > 0, \tag{B.5}$$

or

$$f''(t') < 0. \tag{B.6}$$

Let $\Delta t' > 0$ be a small number such that

$$t' + \Delta t' \in B_{\delta(\uparrow t')}^{f'>0}. \tag{B.7}$$

By using Taylor's theorem it follows that

$$f(t' + \Delta t') = f(t') + \Delta t' \cdot f'(t') + \frac{(\Delta t')^2}{2!} \cdot f''(t' + \theta \cdot \Delta t'),$$

where $0 < \theta < 1$.

Therefore,

$$f(t' + \Delta t') - f(t') = \Delta t' \cdot f'(t') + \frac{(\Delta t')^2}{2!} \cdot f''(t' + \theta \cdot \Delta t').$$

Since f is increasing (by (B.7)) and $f'(t') = 0$, we have $f''(t' + \theta \cdot \Delta t') > 0$. So, $f''(t') > 0$ because if $f''(t') < 0$ then there is a point $\xi \in (t', t' + \theta \cdot \Delta t')$ so that $f''(\xi) = 0$ by the Intermediate Value Theorem which contradicts our hypothesis. By the same argument, we calculate that $f''(t) > 0$ in (t', t''). Therefore, (B.7) holds.

Similarly, in case (B.4), we can prove that $(\bar{\mathrm{e}})$ holds true.

(ii) Here $\mathrm{CF}[t', t''] = [(\mathrm{I}), (\mathrm{C})]$. Since $f'(t'') = 0$, there exists a $\mu > 0$ such that

$$f'(t) > 0 \quad \text{in } \mathrm{B}_\mu(\downarrow t''), \tag{B.8}$$

or

$$f'(t) < 0 \quad \text{in } \mathrm{B}_\mu(\downarrow t''), \tag{B.9}$$

where

$$\mathrm{B}_\delta(\downarrow p) = (p - \delta, p).$$

Now we consider the case (B.8). Let

$$\mathrm{B}_\mu^{f'>0}(\downarrow t'') = \{\mathrm{B}_\mu(\downarrow t'') \mid f'(t) > 0 \text{ in } \mathrm{B}_\mu(\downarrow t'')\}.$$

Let

$$\sup_\mu \mathrm{B}_\mu^{f'>0}(\downarrow t'') = \mathrm{B}_{\mu(\downarrow t'')}^{f'>0}. \tag{B.10}$$

For a small number $\Delta t'' > 0$, we use Taylor's theorem on $f(t'' - \Delta t'')$ and get

$$f(t'' - \Delta t'') = f(t'') - \Delta t'' \cdot f'(t'') + \frac{(-\Delta t'')^2}{2!} \cdot f''(t'' - \theta_1 \cdot \Delta t''),$$

where $0 < \theta_1 < 1$. Therefore,

$$f(t'' - \Delta t'') - f(t'') = \frac{(\Delta t'')^2}{2!} \cdot f''(t'' - \theta_1 \cdot \Delta t''), \tag{B.11}$$

where $0 < \theta_1 < 1$. Now from (B.10), the *left-hand side* of (B.11) is negative. Therefore, $f''(t'' - \theta_1 \cdot \Delta t'') < 0$.

By the same argument as the previous one, we have $f''(t'') < 0$ and accordingly we can find $f''(t) < 0\ \forall t \in (t', t'')$. Therefore we get $(\bar{\mathrm{d}})$.

Considering case (B.9), we shall find $(\bar{\mathrm{c}})$ similarly. □

Proof of Proposition 17. From Proposition 8, we get that if $f(t') = f(t'')$, then $f(t) = l$ in $[t', t'']$ for some $l \in L_2[a, b]$. Then $f'(t) \equiv 0$ in $[t', t'']$ by Corollary 9. This implies that $f''(t) = 0$ in (t', t''). Since t' and t'' are J-points, $f''(t') = f''(t'') = 0$.

Therefore, $f''(t) = 0$ in $[t', t'']$. Next, let $f(t') \neq f(t'')$. Now t' is a J-point, then by definition of J-point, there exists a $\delta > 0$ such that

$$\text{(a)} \quad f''(t) \begin{cases} = 0 & \text{in } [t', t' + \delta), \\ \neq 0 & \text{in } (t' - \delta, t'), \end{cases}$$

or

$$\text{(b)} \quad f''(t) \begin{cases} = 0 & \text{in } (t' - \delta, t'], \\ \neq 0 & \text{in } (t', t' + \delta). \end{cases}$$

First we consider the case (a) and we shall show that the case (b) cannot hold for the above hypothesis. For case (a), we define a set

$$\mathrm{A}_\delta^f(t') = \{[t', t' + \delta) \mid f''(t) = 0 \ \forall t \in [t', t' + \delta)\}.$$

Here $\delta > 0$ because, otherwise the interval $[t', t' + \delta)$ is meaningless.

Now, $\sup_\delta \mathrm{A}_\delta^f(t')$ exists because $\delta(b - t')$ is bounded. Say,

$$\sup_\delta \mathrm{A}_\delta^f(t') = \mathrm{A}_{\delta(t')}^f = [t', t' + \delta(t')).$$

Now, we shall show that $f''(t' + \delta(t')) = 0$, Let $\{x_n\}$ be any sequence in $[t', t' + \delta(t'))$ converging to $t' + \delta(t')$. Then by continuity of f'',

$$\lim_{n \to \infty} f''(x_n) = f''(\lim_{n \to \infty} x_n) = f''(t' + \delta(t')).$$

But $f''(x_n) = 0 \ \forall n$. Therefore, $\lim_{n \to \infty} f''(x_n) = 0$. So $f''(t' + \delta(t')) = C$. Therefore, $f''(t) = 0$ in $[t', t' + \delta(t')]$. Now, $\delta(t') \neq 0$, because there is another J-point $t'' > t'$. Therefore, there exists a $\sigma > 0$ such that $f''(t) \neq 0$ in $(t' + \delta(t'), t' + \delta(t') + \sigma)$. So, $t' + \delta(t')$ is the next J-point after t', since $t' < t''$ are CDTP. Therefore $t' + \delta(t') = t''$. So, $f''(t) \equiv 0$ in $[t', t'']$. Similarly if t'' is a J-point having a left semi-closed interval with right end point t'' in which $f''(t) = 0$ expanding the interval we reach t'. This proves the part $(\bar{\mathrm{a}})$.

Now remembering possible cases are that t' and t'' are J-points and f is identically zero in the left semi-open interval with closed end point t' and in the right semi-open interval with closed end point t'' respectively. Accordingly we can prove the proposition as we have done in the proof of Proposition 15. □

Proof of Proposition 18. The proof is the same as that of Proposition 16. □

Proof of Proposition 19. The proof is the same as that of Proposition 15. □

Proof of Proposition 24. The proof of Proposition 24 follows from Propositions 8–23.

Proof of Proposition 34. We have,

$$G(F(x(t))) = x(t).$$

Now,

$$\frac{\mathrm{d}}{\mathrm{d}t}G(F(x(t))) = \frac{\mathrm{d}}{\mathrm{d}t}x(t),$$

or

$$\frac{\mathrm{d}}{\mathrm{d}F}G(F(x(t)))\frac{\mathrm{d}F}{\mathrm{d}x}\cdot\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{\mathrm{d}x}{\mathrm{d}t}.$$

So,

$$\frac{\mathrm{d}}{\mathrm{d}F}[G(F(x(t)))]\frac{\mathrm{d}F}{\mathrm{d}x} = 1 \quad (\text{since } x'(t) \neq 0). \tag{B.12}$$

So,

$$G'(F(x(t))) = \frac{1}{F'}. \tag{B.13}$$

Again from (B.12), we have that $G'(F(x(t)))F' = 1$. So,

$$\frac{\mathrm{d}}{\mathrm{d}t}[G'(F(x(t)))F'] = 0,$$

or

$$\frac{\mathrm{d}}{\mathrm{d}F}[G'(F(x))]\frac{\mathrm{d}}{\mathrm{d}x}F\cdot\frac{\mathrm{d}x}{\mathrm{d}t}\cdot F' + G'(F(x))\frac{\mathrm{d}F'}{\mathrm{d}x}\cdot\frac{\mathrm{d}x}{\mathrm{d}t} = 0,$$

or

$$G''(F(x))(F')^2 + G'(F(x))F'' = 0 \quad (\text{since } x'(t) \neq 0),$$

or

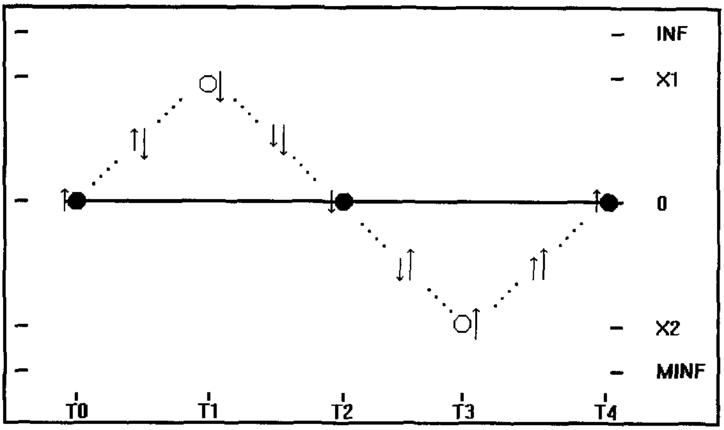
$$G''(F(x)) = -\frac{G'(F(x))F''}{(F')^2} = -\frac{F''}{(F')^3} \quad (\text{using (B.13)}). \qquad \square$$

Appendix C. Spring mass system

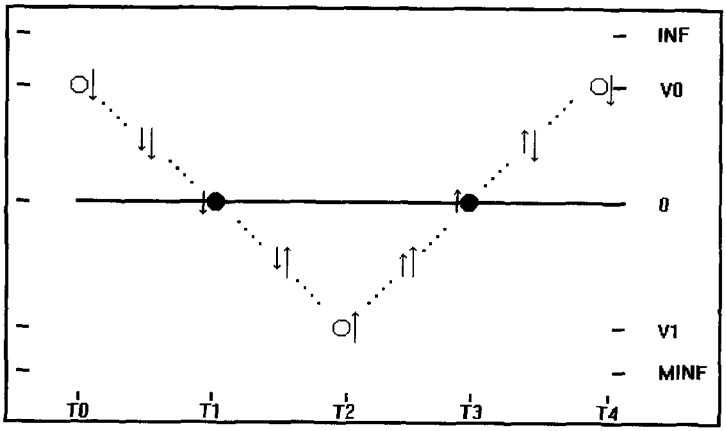
Here we consider an undamped oscillatory system [9, pp. 318] composed of a spring with a mass on it, oscillating on a frictionless surface and modeled by the QDEs:

$$\mathrm{DERIV}(X, V), \quad \mathrm{DERIV}(V, A), \quad \mathrm{L}^{-}(A, X)$$

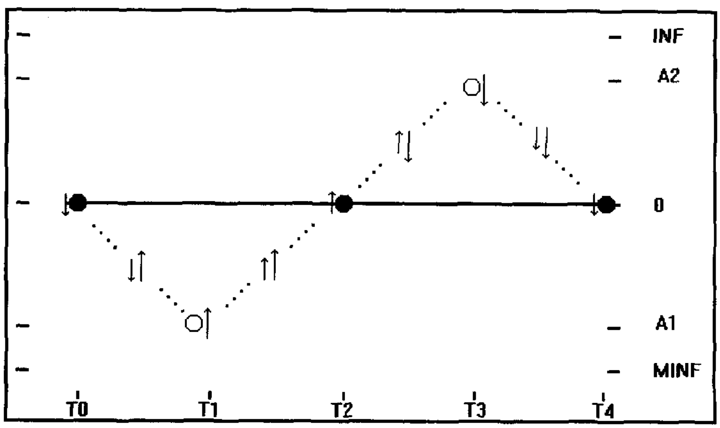
with initial states $X(t_0) = 0$, $V(t_0) = V_0$, and $A(t_0) = 0$ where the parameters X, V and A represent the displacement of the mass from the equilibrium position, velocity and acceleration of the mass respectively. The behaviors of the physical parameters obtained using QSIM2 algorithm are shown in Fig. C.1.



Behavior 1: x(t)

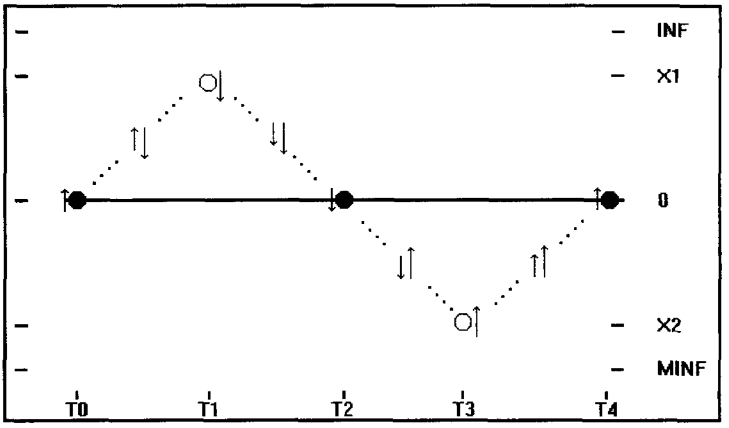


Behavior 1: V(t)

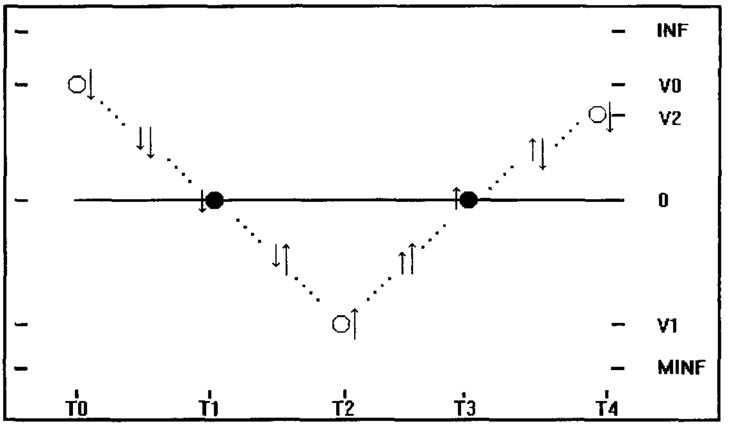


Behavior 1: A(t)

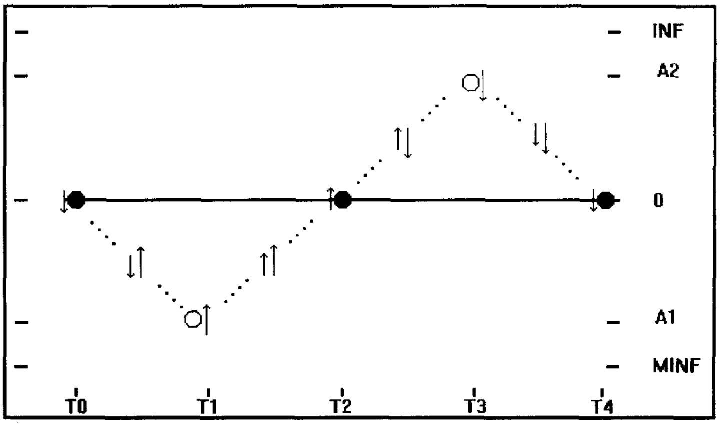
Fig. C.1. QSIM2 outputs of a spring mass system simulation gives a three-way branching at T_4 as V reaches V_0 before, after, or at the same time as X and A reach zero. Although only one behaviour is valid as in [9].



Behavior 2: X(t)

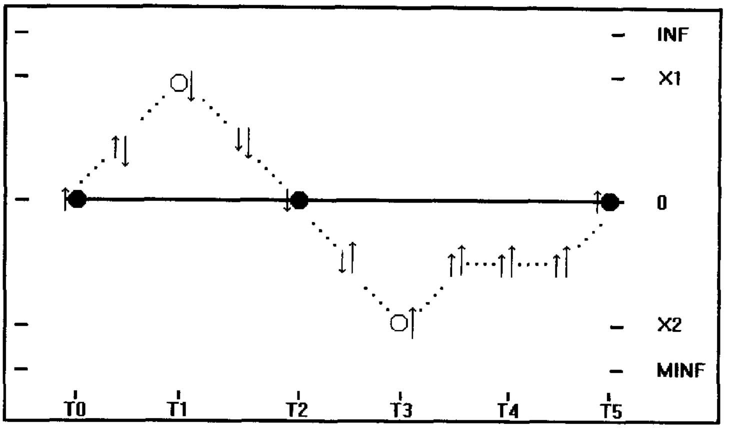


Behavior 2: V(t)

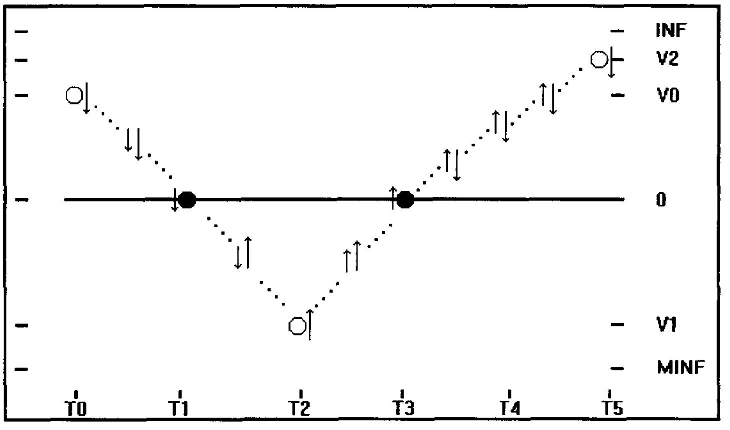


Behavior 2: A(t)

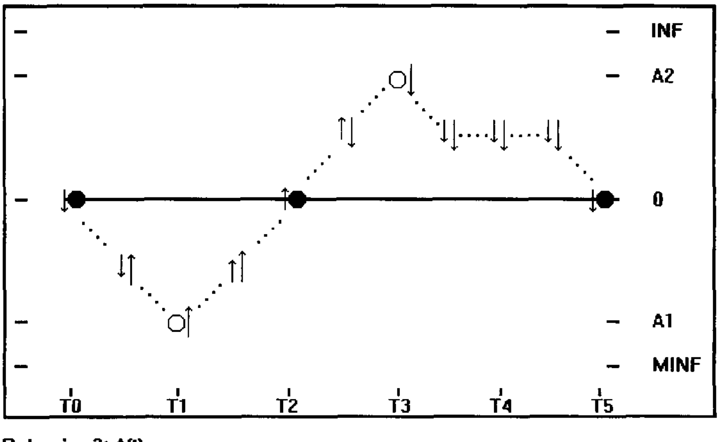
Fig. C.1 — continued.



Behavior 3: X(t)



Behavior 3: V(t)



Behavior 3: A(t)

Fig. C.1 — continued.

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