Chapter 3

Abstraction and Restriction Techniques

The number of vertices of a state-transition graph of a larger QDE tends to explode as discussed in section 2.2.4 (p. 36). In this chapter I present several new methods to improve reasoning with such model ensembles. I define meaningful abstractions and subgraphs of the state-transition graph and restrict the model ensemble by including additional assumptions which cannot be expressed by a monotonic landmark ensemble. I develop algorithms to use these methods in practice.

For the first strategy the generic graph theoretical definition of abstraction techniques as supplied in section 2.2.4 is used. Graph theoretical versions of viable and invariant sets as introduced in section 2.4 (p. 45) are formulated to define subgraphs of interest. The so called no-return set appears as a new and useful concept which is associated with the notion of irreversibility. It turns out that there is a close relationship to strongly connected components, a well-known concept in graph theory. This is helpful to derive appropriate algorithms and to clarify the structure of a no-return abstraction. It can be tested in which regions of the qualitative state space the model respects certain specifications, even if the state-transition graph is too large to be visualised effectively. Then I analyse how the new abstraction technique can be combined with established ones.

For the second strategy, I posit restrictions of the space of admissible trajectories $\mathcal{E}$ and the model ensemble $\mathcal{M}$ in the sense defined in section 2.1 (p. 17). This idea is a guiding principle for the rest of the chapter. At first, $\mathcal{E}$ is restricted, which results in the elimination of edges representing unprobable marginal cases. Then, $\mathcal{M}$ is restricted by assumptions which cannot be expressed as a monotonic landmark ensemble, but still keep the model ensemble infinite, covering a broad set of functional relationships: in addition to requiring a sign matrix $\Sigma \approx [\mathcal{J}(f(x))]$, knowledge on the order of the coefficients of the Jacobian is used in the sense that for indices i, j, k, l assumptions hold like $D_i f_j(x) > D_k f_l(x)$. Finally, I further restrict $\mathcal{M}$ by prescribing quantitative intervals $u_{j,i}$ such that $D_i f_j(x) \in u_{j,i}$. Here, QDEs are combined with differential inclusions (cf. section 2.3, p. 42). The concept of an absorption basin and the viability algorithm (cf. section 2.4, p. 45) are central to determine the conditions under which one qualitative state is the successor of another one.

3.1 No-Return Abstraction

Abstraction techniques can be used to simplify a large state-transition graph. Recall that an abstracted state-transition graph G is determined from a family of disjoined subgraphs which cover G. Two important examples, chatter-box abstraction and projection, were introduced in section 2.2.4 (p. 36). The disjoined subgraphs can be displayed as clusters in G, or as a new graph H where each vertex corresponds to a subgraph, and edges are inherited from G.

In this section I introduce several new types of subgraphs which are meaningful in the context of sustainability science. Simply speaking, all of them are related to the notion of irreversibility in some sense: For example, if a region of the state or velocity space of a system is valued as problematic, the modeller wants to know whether the systems persists there once it is attained. Problems of this kind are closely related to the concepts from viability theory as introduced in section 2.4 (p. 45).

The basic ideas of this work appeared in Eisenack and Petschel-Held (2002), and are extended in this thesis. The main challenge is that the characterisation of the subgraphs exhibiting irreversible structures is not sufficient for their use as abstraction techniques – usually, they are not disjoined. Thus, further relations between these structures have to be investigated to develop an applicable method, the no-return abstraction. I show that it can be computed by combining well-known algorithms from graph theory related to reachability and connected components (e.g. Behzad et al. 1979). Finally, I explore how this new technique interferes with projection and chatter-box abstraction.

3.1.1 Characterisation of Subgraphs

Irreversibility is closely related to reachability: a system shifts from one region of the state space to another irreversibly if the former region cannot be reached from the latter. The system resides in a region forever if no state outside this region is reachable from inside it. In the following, G always denotes a state-transition graph. Reachability of a state $w \in V(G)$ from another state $v \in V(G)$ is expressed as the existence of a path $v, \ldots, w$. Hence, the basic tool in this section is the set-valued successor map $\Gamma : V(G) \rightsquigarrow V(G), v \rightsquigarrow \Gamma(v)$. By $\Gamma^*(v)$ we denote the set of successors of vertex v in the transitive closure G^* of G. The vertex $w \in \Gamma^*(v)$ if and only if there is a path $v, \ldots, w$. Recall that a state-transition graph is loop free (cf. section 2.2, p. 20), and therefore it is not generally true that $v \in \Gamma^*(v)$.

The relation between paths in G and solutions of a monotonic landmark ensemble $\mathcal{M}(\mu, C)$ should be kept in mind here. As shown in section 2.2 (p. 20), the existence of a path in G with length greater than two does not imply the existence of a solution of $\mathcal{M}(\mu, C)$ which has this path as landmark abstraction. On the other hand we know that if w is *not* reachable from v, i.e. $w \notin \Gamma^*(v)$, there is *no* corresponding solution.

We now introduce the basic types of sets $D \subseteq V(G)$ which will be investigated in this section. Let G be a state-transition graph of a monotonic landmark ensemble $\mathcal{M}(\mu, C)$.

DEFINITION 18: *A set $D \subseteq V(G)$ is*

1. ***Viable**, if for all $v_0 \in D$*

$$\exists \textit{ path } v_0, \ldots, v_i, \ldots \textit{ in } G\, \forall i \geq 0 : v_i \in D$$
$$\textit{or } \exists \textit{ path } v_0, \ldots, v_m \textit{ in } G : \Gamma(v_m) = \varnothing \textit{ and } \forall i = 0, \ldots, m : v_i \in D.$$

2. ***Invariant**, if for all $v_0 \in D$*

$$\forall \textit{ paths } v_0, \ldots, v_i, \ldots \textit{ in } G, i \geq 0 : v_i \in D.$$

3. ***No-return**, if for all $v_0 \in D$*

$$\forall \textit{ paths } v_0, \ldots, v_m, \ldots, v_i \textit{ in } G \textit{ with } v_m \in D^c, i \geq m : v_i \in D^c.$$

In a viable set a path starts from every vertex which remains in the set. Invariant sets correspond to regions in the phase space which cannot be left once they are entered, and no-return sets cannot be re-entered once they have been left. In the context of sustainability science, invariant sets correspond to robust facts under uncertainty or generality. Since there is no edge leaving an invariant set, no model of the ensemble $\mathcal{M}(\mu, C)$ has a solution leaving the associated region in the state and velocity space (i.e. every ODE with a Marchaud-map $f \in \mathcal{M}(\mu, C)$ as right-hand side has an invariance domain). In contrast, no-return sets correspond to a fragile configuration of states and velocities: Since there is no re-entering path, no solution of $\mathcal{M}(\mu, C)$ re-enters the region. A negative consequence holds for viable sets. If D is *not* viable, there are vertices in D where all successors are outside D, i.e. there is a region in the state and velocity space where any solution of $\mathcal{M}(\mu, C)$ (supposing it does not have a constant qualitative value) necessarily leaves this region – a problematic situation if such a region is valued as positive.

To find such sets in the state transition graph and to improve our understanding of these concepts, we provide further characterisation in the following propositions. They also make the connection to viability theory more clear and prepare for the development of efficient algorithms.

PROPOSITION 16: *A set $D \subseteq V(G)$ is viable iff the following criterion holds:*

$$\forall v \in D : \Gamma(v) \cap D \neq \varnothing \textit{ or } \Gamma(v) = \varnothing.$$

PROOF: First, choose $v \in D$. If $\Gamma(v) = \varnothing$, the criterion obviously holds. Otherwise, there is a path $v, w, \ldots$ in D, since D is viable. Thus, $w \in \Gamma(v) \cap D$.

Now, let D fulfil the criterion and choose $v_0 \in D$. If $\Gamma(v_0) = \varnothing$, it is obviously an element of a viable set. Otherwise, we can choose one $v_1 \in \Gamma(v_0)$ with $v_1 \in D$. This can be repeated infinitely or until some $\Gamma(v_m) = \varnothing$. Thus, D is a viable set. □

As discussed above, viable sets can only be used in a negative sense. In practice large state-transition graphs have viable sets comprising most vertices of G, making this structure not very distinctive. Viable sets were introduced here for sake of completeness and will not be considered further. This could be different if strong restriction techniques to eliminate edges are used before computing viable sets. In contrast, invariant sets, which are characterised now, will be more helpful.

PROPOSITION 17: *If $D \subseteq V(G)$ is an invariant set, this is equivalent to each of the following conditions:*

(i) $\forall v \in V(G) : \Gamma(v) \subseteq D$

(ii) $\phi(D) = D$*, where* $\phi : V(G) \rightsquigarrow V(G), v \rightsquigarrow \phi(v) := \Gamma^*(v) \cup \{v\}$.

Moreover, the set-valued map ϕ has the following properties:

1. *For all $D \subseteq V(G) : D \subseteq \phi(D)$, i.e. ϕ is* ***extensive****.*
2. *For all $C, D \subseteq V(G), C \subseteq D : \phi(C) \subseteq \phi(D)$, i.e. ϕ is* ***monotone****.*
3. *For all $D \subseteq V(G) : \phi(\phi(D)) = \phi(D)$, i.e. ϕ is* ***idempotent****.*

The properties of ϕ will be useful for various proofs in this section. As G is loop free, it holds for all $v \in V(G)$ that $v \notin \Gamma(v)$, but $v \in \phi(v)$. If $w \in \phi(v)$ then $w = v$ or there is a path from v to w in G.

PROOF: We begin with the properties of ϕ.
The map is extensive by definition.
If $C \subseteq D$, choose $w \in \Gamma^*(C)$. Then there is a path $v, \ldots, w$ with $v \in C$. Since also $v \in D$, we have $w \in \Gamma^*(D)$, and ϕ is monotone.
It holds for every set-valued map $F : X \rightsquigarrow X$ and $A, B \subseteq X$ that $F(A \cup B) = F(A) \cup F(B)$. For the successor map Γ^* it holds that $\Gamma^*(\Gamma^*(D)) \subseteq \Gamma^*(D)$, since it operates on the transitive closure of G. Thus,

$$\begin{aligned}\phi(\phi(D)) &= \phi(\Gamma^*(D) \cup D) = \Gamma^*\big(\Gamma^*(D) \cup D\big) \cup \big(\Gamma^*(D) \cup D\big)\\ &= \Gamma^*(\Gamma^*(D)) \cup \Gamma^*(D) \cup \Gamma^*(D) \cup D = \Gamma^*(D) \cup D = \phi(D),\end{aligned}$$

and ϕ is idempotent.

Equivalence to condition (i): Choose $v \in D$, D invariant. If $\Gamma(v) = \varnothing$, the condition is met. Otherwise, select an arbitrary $w \in \Gamma(v)$. Since D is invariant, it holds that $w \in D$, i.e. $\Gamma(v) \subseteq D$.
Let D fulfil the condition. If some $v_i \in D$, then all $v_{i+1} \in \Gamma(v_i) \subseteq D$. Thus, all paths starting from an $v_0 \in D$ remain in this set – it is invariant.

Equivalence to condition (ii): Let D be invariant. Since ϕ is expansive, only $\phi(D) \subseteq D$ has to be shown. If we choose $w \in \phi(D)$, there is a path $v, \ldots, w$ with $v \in D$. Due to invariance, also $w \in D$.
Let $D = \phi(D)$, take $v_0 \in D$ and an arbitrary path $v_0, \ldots, v_i, \ldots$ in G. Since $\forall i \geq 0 : v_i \in \phi(v_0) \subseteq \phi(D) = D$, the set is invariant. $\square$

The notion of an invariant set can be used to further describe no-return sets (a further relation between both types of sets will be shown below):

PROPOSITION 18: *A set $D \subseteq V(G)$ is a no-return set iff $\phi(D) \cap D^c$ is invariant.*

PROOF: First, let D be a no-return set. Choose $v_m \in \phi(D) \cap D^c$. Then there is a path $v_0, \ldots, v_m$ in G with $v_0 \in D$. Since $v_m \notin D$ and D is a no-return set, it holds for every continued path $v_0, \ldots, v_m, \ldots, v_i$ that $\forall i \geq m : v_i \in D^c$. Consequently, $v_i \in \phi(D) \cap D^c$, such that $\phi(D) \cap D^c$ is invariant.

Now, let $\phi(D) \cap D^c$ be invariant. Choose $v_0 \in D$. If there is no path leaving D, it is already a no-return set. Otherwise, there is some $v_m \in \phi(D) \cap D^c$ with $v_0, \ldots, v_m$ a path in G. Then, due to invariance, it holds for all continued paths $v_0, \ldots, v_m, \ldots, v_i, \ldots$ that $\forall i \geq m : v_i \in \phi(D) \cap D^c \subseteq D^c$, and D is a no-return set. □

3.1.2 Computing Invariant Sets and the No-Return Abstraction

Invariant sets need to be computed and displayed efficiently if they are to be exploited in applications from sustainability science. Moreover, we would like to integrate them into the generic definition of abstraction techniques as introduced in section 2.2.4 (p. 36) – requiring a disjoined family of subgraphs. In this section we will see important obstacles to this task – although the family of all invariant sets of a state-transition graph has a very regular structure. I show that no-return sets and connected components play the decisive role to overcome them.

At first we investigate the structure of the family of all invariant sets of a state-transition graph. Recall that for an arbitrary set X, a family of sets $\mathcal{L} \subseteq \mathcal{P}(X)$, ordered by inclusion $\subseteq$, is a **set lattice** if for all $A, B \in \mathcal{L}$ the supremum $A \cup B \in \mathcal{L}$ and the infimum $A \cap B \in \mathcal{L}$ (see, e.g. Davey and Priestley 1990).

PROPOSITION 19: *The family $\mathcal{L}$ of all invariant sets of G is a finite set lattice.*

PROOF: Let $C, D \in \mathcal{L}$. Since C and D are invariant, PROP. 17 yields

$$\phi(C \cup D) = \phi(C) \cup \phi(D) = C \cup D,$$

such that also $C \cup D$ is invariant by PROP. 17.
It holds for every set-valued map $F : X \rightsquigarrow X$ and $A, B \subseteq X$ that $F(A \cap B) \subseteq F(A) \cap F(B)$. Since C and D are invariant and ϕ is extensive, we can use PROP. 17 (p. 54) again to see that

$$C \cap D \subseteq \phi(C \cap D) \subseteq \phi(C) \cap \phi(D) = C \cap D,$$

and $C \cap D$ is invariant. □

Furthermore, this lattice can be constructed from simple invariant sets of the form $\phi(v)$ which are the atoms of $\mathcal{L}$:

PROPOSITION 20: *For all $v \in V(G)$, $\phi(v)$ is an invariant set.*
For all invariant sets D of G,

$$D = \bigcup_{v \in D} \phi(v).$$

PROOF: The set $\phi(v)$ is invariant by PROP. 17 (p. 54) since ϕ is idempotent.
By definition, $v \in \phi(v)$, and thus $D \subseteq \bigcup_{v \in D} \phi(v)$.
Now choose $w \in \bigcup_{v \in D} \phi(v)$. Then there is a $v \in D : w \in \phi(v)$, i.e. $w = v$ or there is a path $v, \ldots, w$. Since D is invariant, also $w \in D$, and $\bigcup_{v \in D} \phi(v) \subseteq D$. □

This situation seems comfortable at first, as ϕ can be easily obtained from the transitive closure of G for which various efficient algorithms are well-known. However, the sets $\phi(v)$ have a nested structure:

PROPOSITION 21: *Let $v, w \in V(G)$. Then $\phi(w) \subseteq \phi(v)$ iff $v = w$ or there is a path $v, \ldots, w$ in G.*

PROOF: If $w \in \phi(w) \subseteq \phi(v)$, then $w = v$ or there is a path $v, \ldots, w$.
Suppose there is a path $v, \ldots, w$, then $w \in \phi(v)$. Since ϕ is monotone and idempotent, we conclude that $\phi(w) \subseteq \phi(\phi(v)) = \phi(v)$. □

This makes it impossible to compute an abstracted state-transition graph (cf. DEF. 8, p. 37) directly from the invariant sets, since this needs disjoined subgraphs. To display all invariant sets of a state-transition graph, we would lose the overview due to the variety of nested clusters. Moreover, invariant sets need not be connected, e.g. if there is no path between $v, w \in V(G)$ and $D = \phi(v) \cup \phi(w)$. The basic idea for the solution of this problem lies in the following proposition which draws a new connection between invariant sets and no-return sets. I will go on to show that there is a “basis” of disjoined no-return sets from which all invariant sets can be constructed in a unique way.

PROPOSITION 22: *Let $D \in \mathcal{L}$ be an invariant set, and $D_1, \ldots, D_n \in \mathcal{L}$ the family of all invariant sets D_j with $D_j \subsetneqq D$. Then,*

$$B_D := D \setminus \bigcup_{j=1,\ldots,n} D_j$$

is a no-return set.

PROOF: Choose $v_0 \in B_D$ and a path $v_0, \ldots, v_m, \ldots, v_i, \ldots$ with $v_m \notin B_D$ (if there is no such path, B_D is a no-return set obviously). Since also $v_0 \in D$, due to invariance $v_m \in D$, and therefore $v_m \in \bigcup_{j=1,\ldots,n} D_j$, i.e. there is one j such that $v_m \in D_j$. Since D_j is invariant, $\forall i \geq m : v_i \in D_j \nsubseteq B_D$. Therefore, B_D is a no-return set. □

In other words, we obtain a no-return set by taking an invariant set and eliminating all included invariant sets. When this proposition is applied to the basic invariant sets $\phi(v)$, we obtain a family of no-return sets with stronger properties as building blocks for the no-return abstraction:

PROPOSITION 23: *For $v \in V(G)$ define*

$$B_v := \phi(v) \setminus \bigcup_{\substack{D_j \in \mathcal{L} \\ D_j \subsetneqq \phi(v)}} D_j.$$

Then, $v \in B_v$ and B_v is a single vertex or is strongly connected.

PROOF: Suppose, that $v \notin B_v$. Since $v \in \phi(v)$, there would be a $D_j \in \mathcal{L}$ with $D_j \subsetneqq \phi(v)$ and $v \in D_j$. Hence, since ϕ is monotone and D_j is invariant, this would imply that

$$\phi(v) \subseteq \phi(D_j) = D_j \subsetneqq \phi(v),$$

which is a contradiction. Therefore, $v \in B_v$.

If $|B_v| \geq 2$, take $w \in B_v, w \neq v$. As w is also an element of $\phi(v)$, there is a path $v, \ldots, w$. Supposing there is no path $w, \ldots, v$, then from PROP. 21 (p. 56) we yield the contradiction that $\phi(v) \nsubseteq \phi(w) \subseteq \phi(v)$. Thus, B_v is strongly connected. ☐

Taken with PROP. 22, it follows that all B_v consisting of more than one vertex are strongly connected no-return sets. The following proposition guarantees that they can be computed by standard algorithms from graph theory to detect strongly connected components (e.g. van Leeuwen 1990, p. 571). It is also another characterisation of no-return sets.

PROPOSITION 24: *A set $D \subseteq V(G)$ of a graph G is a strongly connected no-return set if and only if it is a strongly connected component.*

PROOF: Assume that D is a strongly connected no-return set. If it were not a strongly connected component, there would be a path $v, \ldots, w$ with $v \in D, w \notin D$, and a path $w, \ldots, v$. The latter is a contradiction since D is a no-return set.

If D is a strongly connected component, we have to show that D is a no-return set. Choose $v_0 \in D$ and a path $v_0, \ldots, v_m, \ldots, v_i$ with $v_m \notin D$. Suppose D is a no-return set. Then there is some $v_i \in D$ with $i \geq m$. Consequently, there is a cycle $v_0, \ldots, v_m, \ldots, v_i, \ldots, v_0$ since D is strongly connected. Hence, $v_m \notin D$ belongs to the same connected component as v_0, which is a contradiction to maximality. Thus, D is a no-return set. ☐

Thus, if the strongly connected components are computed, a large part of the set

$$\mathcal{B} := \{B_v \mid v \in V(G)\}$$

is known. What remains are the single vertices which are not part of any component. Luckily, all these vertices are no-return sets:

PROPOSITION 25: *If $v \in V(G)$ is not an element of any strongly connected component of G, then it is a no-return set and $B_v = \{v\} \in \mathcal{B}$.*

PROOF: If $v_0 \in V(G)$ does not belong to any strongly connected component, there is no cycle $v_0, \ldots, v_i, \ldots, v_0$, and thus it holds for every path $v_0, \ldots, v_i$ with $v_i \neq v_0$ that $\forall i \geq 1 : v_i \notin \{v_0\}$, making v a no-return set.

Due to PROP. 23, $v \in B_v$. If there were another $w \in B_v$ distinct from v, it would be an element of the same strongly connected component. ☐

We conclude from these results that:

PROPOSITION 26: *The family $\mathcal{B}$ is a cover of $V(G)$, which contains only no-return sets.*

PROOF: Due to PROP. 23 (p. 56), $\bigcup_{v \in V(G)} B_v = V(G)$. It holds for all $B_v, B_w \in \mathcal{B}$ that $B_v = B_w$ or $B_v \cap B_w = \varnothing$, since strongly connected components and/or single states not being part of a strongly connected component are always disjoined.

The elements of $\mathcal{B}$ are no-return sets due to PROP. 24 and PROP. 25. □

Thus, we arrive at the first of our aims: $\mathcal{B}$ has the necessary properties to compute an abstracted state-transition graph (cf. DEF. 8, p. 37):

DEFINITION 19: *Let G be a state-transition graph and $\mathcal{B} = \{B_v \mid v \in V(G)\}$ the disjoined partition of $V(G)$ with B_v as defined in* PROP. *23 (p. 56). The resulting abstracted state-transition graph G' with $V(G') = \mathcal{B}$ is the* ***no-return abstraction*** *of G.*

The other result is that there is a one-to-one correspondence between the atoms of the lattice $\mathcal{L}$ of invariant sets, $\phi(v), v \in V$, and the "no-return basis" $\mathcal{B}$: together with PROP. 20 (p. 55), where each invariant set is constructed from appropriate $\phi(v)$, every invariant set can be constructed by a union of appropriately chosen elements of $\mathcal{B}$, and every union of appropriately chosen elements of $\mathcal{B}$ yields an invariant set.

PROPOSITION 27:

(i) *For all $v \in V(G) : \phi(v) = \phi(B_v)$.*

(ii) *For all $v \in V(G)$:*

$$\phi(v) = \bigcup_{\substack{B_w \in \mathcal{B} \\ B_w \subseteq \phi(B_v)}} B_w.$$

(iii) *If $D \subseteq V(G)$ is an invariant set, then*

$$D = \bigcup_{\substack{B_v \in \mathcal{B} \\ v \in D}} B_v.$$

PROOF: Part (i): By PROP. 23 (p. 56), $v \in B_v \subseteq \phi(v)$. Since ϕ is monotone and idempotent, $\phi(v) \subseteq \phi(B_v) \subseteq \phi(\phi(v)) = \phi(v)$.

Part (ii): Generally,

$$\bigcup_{\substack{B_w \in \mathcal{B} \\ B_w \subseteq \phi(B_v)}} B_w \subseteq \phi(B_v) \subseteq \phi(v).$$

For the inclusion in the other direction take $u \in \phi(v)$. Since $\phi(u) \subseteq \phi(v)$, it holds by PROP. 21 (p. 56) and (i) that $u \in B_u \subseteq \phi(u) \subseteq \phi(v) = \phi(B_v)$, i.e. $u \in \bigcup_{\substack{B_w \in \mathcal{B} \\ B_w \subseteq \phi(B)}} B_w$.

Part (iii): It holds that $D \subseteq \bigcup_{\substack{B_v \in \mathcal{B} \\ v \in D}} B_v$ since $v \in B_v$ (cf. PROP. 23, p. 56).
Now, take a $u \in \bigcup_{\substack{B_v \in \mathcal{B} \\ v \in D}} B_v$. Then, by (i) and PROP. 20 (p. 55),

$$u \in \bigcup_{\substack{B_v \in \mathcal{B} \\ v \in D}} \phi(B_v) = \bigcup_{v \in D} \phi(v) = D.$$

□

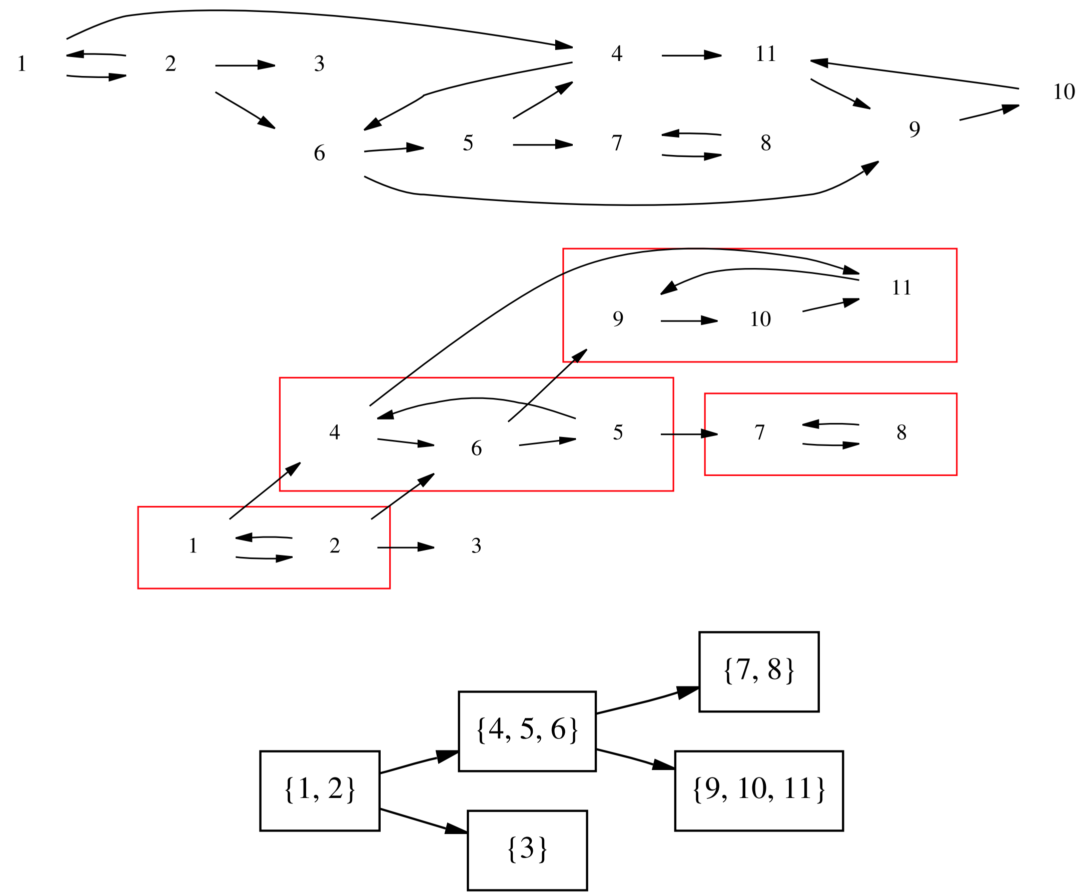

Figure 3.1: Stylised example for a no-return abstraction of a state-transition graph (top: a graph G, middle: the family $\mathcal{B}$ displayed as clusters, bottom: no-return abstraction of G).

In practice, it is sufficient to compute and display only the basic no-return sets $\mathcal{B}$ to obtain the no-return abstraction of G. It is quite simple for the end-user to find all relevant invariant sets from such a presentation: It is well-known in graph theory that directed graphs can be decomposed as an acyclic graph of strongly connected components (van Leeuwen 1990): If G' is the no-return abstraction of G, for all $B_0 \in V(G') = \mathcal{B}$ and for all paths $B_0, \ldots, B_i$ in G' it holds that $B_i \neq B_0$ for $i > 0$. Otherwise, there would be a path $v_0, \ldots, v_i, \ldots, v_0$ with $v_0 \in B_0$ and $v_i \notin B_0$, which is impossible since B_0 is a no-return set. Thus, by picking a no-return set $B \in V(G')$, one can trace “downstream” to all other vertices in G' which are attainable from B – which is straightforward in an acyclic graph – to obtain an invariant set. Of course, there are other invariant sets, but the most likely question when performing a no-return abstraction is: Where do irreversible changes of the qualitative state occur? This happens exactly for all edges entering a $B \in \mathcal{B}$, because $\phi(B)$ is an invariant set (see Fig. 3.1 for a stylised example).

3.1.3 Consistency of Projection, No-Return and Chatter-Box Abstraction

For the analysis of large state-transition graphs we would like to combine no-return abstraction with other methods, e.g. projection and chatter-box abstraction (cf. section 2.2.4 (p. 36), DEF. 9 and DEF. 11). Since all abstraction methods take an input graph and produce a new one which is not larger than the input graph, the idea is to apply the abstraction methods subsequently to substantially improve the clarity of the model result. The result is a sequence of graphs $G_0, \ldots, G_n$, where G_{i+1} is an abstraction of G_i, determined by the abstraction methods used.

For a chosen set of abstraction methods, does the result G_n depend on the sequence in which they are computed? In other words, if the methods are regarded as operators, do they commute? As I will show below, they do not, so the appropriate sequence has to be determined. Since the objective of this exercise is to reveal properties of the state-transition graph which would not be easy accessible otherwise, there is a pragmatic criterion for appropriateness: If we observe a certain type of structure in G_n, we want to be sure that the structure also exists in G_0. In the following, I infer the sequence in which projection, chatter-box, and no-return abstraction should be applied. Start with a simple observation.

PROPOSITION 28: *Every chatter-box is contained in a no-return set.*

PROOF: If D be a chatter-box of G, it is strongly connected in the subgraph $G^- = G \cap G^{-1}$ by definition (cf. DEF. 9, p. 38). Since $E(G^-) \subseteq E(G)$, D is part of a strongly connected component of G, and thus also part of a no-return set due to PROP. 24 (p. 57). □

The consequence of this proposition is that we do not "split" chatter-boxes when we compute a no-return abstraction as second step after chatter box abstraction. On the other hand, the chatter-boxes are not visible any more in the no-return abstraction – we may only note the sets $B \in \mathcal{B}$ which contain a chatter-box. However, it makes no sense to apply the abstraction procedures the other way round, since there are no chatter-boxes in the no-return abstraction due to its acyclic structure. Now consider the case where projection is combined with no-return abstraction.

PROPOSITION 29: *For G and an index set I, denote $G' := \pi_I(G)$. If D' is a no-return set in G', then $D := \pi_I^{-1}(D')$ is a no-return set in G.*

PROOF: Suppose that D is *not* a no-return set. Then there is a path $v_0, \ldots, v_m, \ldots, v_n$ in G with $v_0, v_n \in D$ and $v_m \notin D$. By taking $\pi_I(v_0), \ldots, \pi_I(v_m), \ldots, \pi_I(v_n)$ and eliminating all elements of this sequence which are identical to their predecessor, we obtain a path $v'_0, \ldots, v'_k, \ldots, v'_l$ in G' with $v'_0 = \pi_I(v_0) \in \pi_I(D)$, $v'_l = \pi_I(v_n) \in \pi_I(D)$, and $v'_k = \pi_I(v_m)$. Therefore, since D is the inverse image of D', it holds that $v'_k \notin \pi_I(D)$. Thus, $\pi_I(D)$ is not a no-return set. Since surjectivity of π_I guarantees that $\pi_I(D) = \pi_I(\pi_I^{-1}(D')) = D'$, this is a contradiction to D' being a no-return set. □

This means that if there is a no-return set in a projection, it corresponds to a no-return set in the original state-transition graph. Conversely, the property of being a no-return set is not

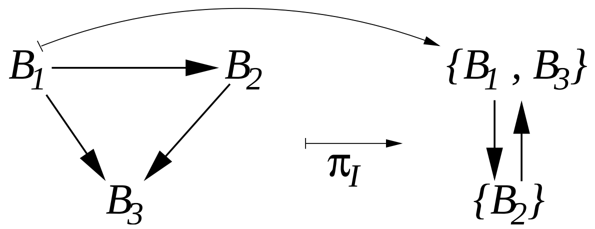

Figure 3.2: Example for a projection not preserving no-return sets. The graph to the left is the no-return abstraction G' of some state-transition graph with $V(G') = \mathcal{B} = \{B_1, B_2, B_3\}$. We consider a projection π_I and assume that $\forall v, w \in B_1 \cup B_3 : \pi_I(v) = \pi_I(w)$, and that $\forall v, w \in B_2 : \pi_I(v) = \pi_I(w)$, i.e. B_1 and B_3 are projection equivalent. The resulting projection $H = \pi_I(G')$ is displayed to the right. Although the vertex B_1 is a no-return set in G', it's image $\pi_I(B_1) = \{B_1, B_3\}$ is obviously not a no-return set in H.

generally preserved under projection, as the example in Fig. 3.2 shows. Thus, a no-return abstraction should be performed after a projection. To be complete, we consider the third possible combination of abstractions: projection and chatter-box abstraction.

PROPOSITION 30: *Let G be a state-transition graph and $H := \pi_I(G)$ its projection. If D is a chatter-box in G, then $D' := \pi_I(D) \subseteq V(H)$ is a single vertex or induces a chatter-box in H.*

PROOF: The subgraph induced by D is strongly connected in $G^- = G \cap G^{-1}$ by definition. It follows that $D' = \pi_I(D)$ is a single vertex in H or it is strongly connected in $\pi_I(G^-)$ (cf. p. 39). We show that $\pi_I(G^-) = \pi_I(G)^- = H^-$, making D' a chatter-box in H.
Since $V(G^-) = V(G)$, we have that $V(\pi_I(G)^-) = V(\pi_I(G)) = V(\pi_I(G^-))$. For the edges,

$$\begin{aligned}
E(\pi_I(G)^-) &= E(\pi_I(G)) \cap E(\pi_I(G^{-1})) = \\
&= \{(\pi_I(v), \pi_I(w)) \mid (v, w) \in E(G)\} \cap \\
&\qquad \{(\pi_I(v), \pi_I(w)) \mid (w, v) \in E(G)\} = \\
&= \{(\pi_I(v), \pi_I(w)) \mid (v, w) \in E(G) \wedge (w, v) \in E(G)\} = \\
&= E(\pi_I(G^-))
\end{aligned}$$

holds. $\square$

Simply speaking, chatter-boxes remain chatter-boxes under projection. Again, the converse is not generally true: If D' is a chatter-box in $\pi_I(G)$, it cannot be concluded that $\pi_I^{-1}(D')$ is a chatter-box in G (see example in Fig. 3.3). Hence, one has to be careful when applying chatter-box abstraction after projection. To sum up, for a large state-transition graph the different abstraction methods should be applied in the following sequence:

1. Chatter-box abstraction

2. Projection

3. No-return abstraction

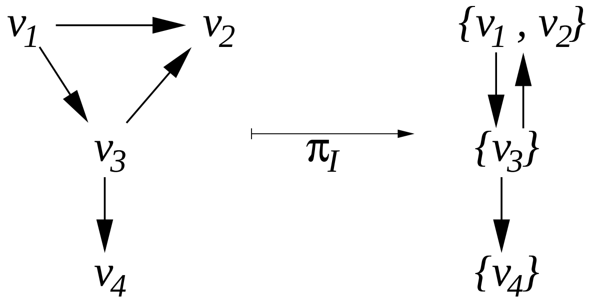

Figure 3.3: Example for a projection producing "artifical" chatter-boxes. The diagram to the left represents a state-transition graph G with $V(G) = \{v_1, v_2, v_3, v_4\}$. We consider a projection π_I and assume that $\pi_I(v_1) = \pi_I(v_2)$, but $\pi_I(v_1) \neq \pi_I(v_3) \neq \pi_I(v_4) \neq \pi_I(v_1)$, i.e. only v_1 and v_2 are projection equivalent. The resulting projection $H = \pi_I(G)$ is displayed to the right. The set $\{\{v_1, v_2\}, \{v_3\}\} \subseteq V(H)$ induces a chatter-box in H, while its inverse image $\{v_1, v_2, v_3\} \subseteq V(G)$ does not so in G.

3.2 Marginal Edges

In this section I present two techniques to simplify the state-transition graph of a QDE by eliminating edges which are of little relevance in most applications. They also preserve connectedness properties of the graph, thus being a special type of transitive reduction. Main ideas appeared in Eisenack and Petschel-Held (2002) and are formulated here more rigorously. There is related work of Bouwer and Bredeweg (2002), who compute another type of transitive reduction of the state-transition graph. Along some edges two or more qualitative directions or qualitative magnitudes change at the same time. This implies the existence of a solution which passes through the intersection of two main isoclines or the intersection of a main isocline with a landmark. It can be shown that for many systems the set of trajectories with such features is of measure zero (Bernard and Gouze 2002). The completeness of the QSIM algorithm guarantees that also the abstractions of such solutions are represented in the state-transition graph. By restricting the space of admissible trajectories $\mathcal{E}$ to functions which do not attain values on such intersections of measure zero, we obtain a graph with fewer edges. The implied loss of information is acceptable, since no features of relevance are left out.

3.2.1 Characterising Marginal Edges

In the following let S be a qualitative state space with n quantity spaces, and G the state-transition graph of a monotonic landmark ensemble $\mathcal{M}(\mu, C)$. For each edge $(v, w) \in E(G)$, there is at least one component i such that $\mathrm{qdir}_i(v \wedge w) = 0$ or that $\mathrm{qmag}_i(v \wedge w) = \lambda$ with a landmark $\lambda \in Q_i$. If $\mathrm{qdir}_i(v) \neq \mathrm{qdir}_i(w)$, we say in the first case that the edge **transgresses the ith main isocline**, while in the second we say that it **transgresses the landmark** λ if $\mathrm{qmag}_i(v) \neq \mathrm{qmag}_i(w)$. This corresponds to the existence of a solution $x(\cdot)$ of a system of the monotonic landmark ensemble such that for one $t \in \mathbb{R}_+ : f_i(x(t)) = 0$ (if it transgresses a main isocline), or that $x_i(t) = \lambda$, where $\lambda \in \mathbb{R}$ is defined by the landmark vector Λ associated with the system (cf. PROP. 2, p. 25, DEF. 4, p. 29 and Eq. 2.12).

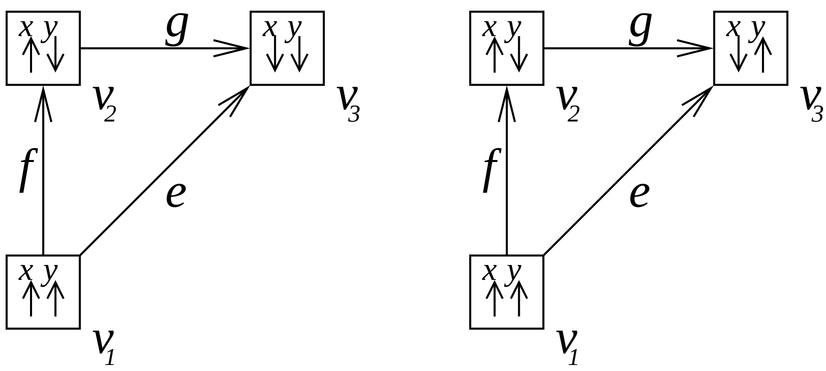

Figure 3.4: Different types of composed edges. Arrows in the boxes show qualitative directions of two variables.

Some edges $e = (v_1, v_3)$ in the state transition graph are composed in the sense that there are two other edges $f = (v_1, v_2)$ and $g = (v_2, v_3)$, in simple words, e is a "shortcut". If all landmarks or main isoclines which are transgressed along f and g are also transgressed along e, it is tempting to elemi nate e: Along this edge the transgressions occur simultaneously although they do not necessarily have to by the model assumptions (otherwise only the edge e would exist, but not the edges f and g). Eliminating all edges (v_1, v_m) for which a path $v_1, \ldots, v_m$ exists is conceptualised as transitive reduction in graph theory. However, it is well-known that – in contrast to transitive closure – this operation cannot be defined in a unique way (cf. van Leeuwen 1990). There is another subtlety: what happens along alternative paths from v_1 to v_3? Two cases have to be distinguished (see Fig. 3.4):

1. Along f some components change their qualitative direction or transgress a landmark, while along g other qualitative values change. Along the edge e the qualitative values change at the same time.

2. Along g some qualitative directions change back to the value they had in v_1 or transgress the same landmark in the other direction, while other components change to a new qualitative value. Along e only landmarks or main isoclines not transgressed along g are affected.

The first case is a marginal edge, since along e the landmarks or main isoclines are transgressed simultaneously "by accident". This interpretation is not valid for the second case, since some landmarks or main isoclines are crossed twice. Here, the edge e exhibits – compared to f and g – a notable new property which should not be ignored. Only composed edges e of the first type can be omitted, where transgressions coincide which do not necessarily have to. Usually, they have no special relevance: Nothing basically new happens, the result of both paths is the same (namely the system being in state v_3), and e is not likely to be observed in empirical studies.

Now, these considerations are formalised. Note that, since the quantity spaces $Q_i, i = 1, \ldots, n$ are ordered (cf. section 2.2.2, p. 27), expressions like "λ is between $\mathrm{qmag}_i(v)$ and $\mathrm{qmag}_i(w)$" and $\max(\mathrm{qmag}_i(v))$ are well-defined. If $\mathrm{qdir}_i(v) \neq \mathrm{qdir}_i(w)$, then $\mathrm{qdir}_i(v \wedge w) = 0$, and if $\mathrm{qmag}_i(v) \neq \mathrm{qmag}_i(w)$, then $\mathrm{qmag}_i(v \wedge w) = \lambda$ is a landmark (by Eq. 2.12).

Before defining a marginal edge, the following "qualitative intermediate value theorem" is formulated.

PROPOSITION 31: *Let* $v_1, \dots, v_m$ *be a path in* G *and* $i \in \{1, \dots, n\}$. *Then, for every landmark* λ *between* $\mathrm{qmag}_i(v_1)$ *and* $\mathrm{qmag}_i(v_m)$ *there is a* $j \in \{1, \dots, m-1\}$ *such that the edge* (v_j, v_{j+1}) *transgresses* λ.

PROOF: Since paths of length 1 in G correspond to abstractions of reasonable trajectories, an edge (v, w) can only transgress landmarks $\lambda \in \mathrm{qmag}_i(v) \cap \mathrm{qmag}_i(w)$ with $\lambda \in Q_i$ by continuity (cf. Eq. 2.12). Thus, along the path $v_1, \dots, v_m$ there must be an edge (v_j, v_{j+1}) with $\mathrm{qmag}_i(v_j \wedge v_{j+1}) = \lambda$. □

DEFINITION 20: *Let* $v_1, \dots, v_m$ *with* $m \geq 3$ *be a path in* G. *Then, an edge* $(v_1, v_m) \in E(G)$ *is called* ***marginal edge*** *if for all* $i = 1, \dots, n$ *there are not two edges* $(v_j, v_{j+1}), j = 1, \dots, m-1$ *which transgress the same landmark or the* i*th main isocline more than once.*

The concept is further clarified by the following equivalent characterisation, which is helpful for the elimination techniques. For its formulation we define for $(v, w) \in E(G)$ the **change set** $\mathrm{Ch}(v, w) := \{i \mid \mathrm{qmag}_i(v) \neq \mathrm{qmag}_i(w)\} \cup \{j = n + i \mid \mathrm{qdir}_i(v) \neq \mathrm{qdir}_i(w)\}$.

PROPOSITION 32: *An edge* $(v_1, v_m) \in E(G)$ *is marginal if and only if there is a path* $v_1, \dots, v_m$ *in* G, $m \geq 3$, *such that the change sets* $\mathrm{Ch}(v_j, v_{j+1}), j = 1, \dots, m-1$, *are pairwise disjoined.*

PROOF: If the change sets are pairwise disjoined, every $i = 1, \dots, 2n$ occurs no more than once in a change set. Since only changing components can transgress a landmark or main isoclines, (v_1, v_m) is a marginal edge.

Now assume that no landmark or main isocline is transgressed twice. Take an arbitrary $i = 1, \dots, 2n$.
For $i > n$, there is not more than one j such that $\mathrm{qdir}_{i-n}(v_j \wedge v_{j+1}) = 0$ and $\mathrm{qdir}_{i-n}(v_j) \neq \mathrm{qdir}_{i-n}(v_{j+1})$, and consequently not more than one j with $i \in \mathrm{Ch}(v_j, v_{j+1})$ – the intersections of the change sets with $\{n+1, \dots, 2n\}$ are pairwise disjoined.
For $i \leq n$ define $\lambda_0 := \mathrm{qmag}_i(v_1 \wedge v_m)$. Choose the smallest j such that $i \in \mathrm{Ch}(v_j, v_{j+1})$ and set $\lambda_j := \mathrm{qmag}_i(v_j \wedge v_{j+1})$. If $\lambda_j < \lambda_0$, then

$$\mathrm{qmag}_i(v_{j+1}) \leq \lambda_j \leq \mathrm{qmag}_i(v_j) = \mathrm{qmag}_i(v_1) \leq \lambda_0 \leq \mathrm{qmag}_i(v_m).$$

Due to PROP. 31, λ_j will be transgressed a second time on $v_{j+1}, \dots, v_m$, which is a contradiction. If $\lambda_0 < \lambda_j$, the analogue contradiction applies. Thus $\lambda_0 = \lambda_j$. The same argument applies for the next smallest $k > j$ with $i \in \mathrm{Ch}(v_k, v_{k+1})$. Therefore, it holds for all $l = 1, \dots, m-1$ with $i \in \mathrm{Ch}(v_l, v_{l+1})$ that $\mathrm{qmag}_i(v_l \wedge v_{l+1}) = \lambda_0$. Since λ_0 cannot be transgressed twice, also the intersection of the change sets with $\{1, \dots, n\}$ are pairwise disjoined. □

Later we will need the following property of the change sets to show the applicability of the restriction techniques:

PROPOSITION 33: *If* $(v_1, v_m) \in E(G)$ *and there is a path* $v_1, \ldots, v_m, m \geq 3$ *in* G *with pairwise disjoined change sets* $\mathrm{Ch}(v_j, v_{j+1}), j = 1, \ldots, m-1$*, then*

$$\bigcup_{j=1,\ldots,m-1} \mathrm{Ch}(v_j, v_{j+1}) = \mathrm{Ch}(v_1, v_m).$$

PROOF: Let $i \in \mathrm{Ch}(v_1, v_m)$. Since $\mathrm{qval}_i(v_1) \neq \mathrm{qval}_i(v_m)$ there must be at least one $j \in \{1, \ldots, m-1\}$ with $i \in \mathrm{Ch}(v_j, v_{j+1})$.

Now suppose that $i \notin \mathrm{Ch}(v_1, v_m)$, i.e. $\mathrm{qval}_i(v_1) = \mathrm{qval}_i(v_m)$. It is not possible that there is one and only one j such that $i \in \mathrm{Ch}(v_j, v_{j+1})$, since otherwise $\mathrm{qval}_i(v_1) = \mathrm{qval}_i(v_j) \neq \mathrm{qval}_i(v_{j+1}) = \mathrm{qval}_i(v_m)$. Because the change sets are disjoined, there also cannot be more than one such j, and therefore $i \notin \bigcup_{j=1,\ldots,m-1} \mathrm{Ch}(v_j, v_{j+1})$. □

3.2.2 Eliminating Marginal Edges

I present two algorithms to eliminate marginal edges. One uses a preprocessing approach, the other a postprocessing approach. Both can be combined. The preprocessing strategy requires the modeller to reason about marginal edges which are likely to occur. This can be based on earlier qualitative simulations, on algebraic reasoning or on knowledge about the application domain. Removing marginal edges means preventing simultaneous changes of qualitative values which can also occur subsequently. If two such changes are identified, associated edges can be filtered out by introducing a new constraint into the qualitative landmark system, called **correspondence-not**,

```
((cornot x y) <(lx ly)>)
```

with a sequence of m pairs `(lx ly)`, where `lx` represents a landmark of the variable `x` (associated with index i) and `ly` a landmark of variable `y` (associated with index j), denoting sequences of landmarks $\lambda_{i,1}, \ldots, \lambda_{i,m}$ and $\lambda_{j,1}, \ldots, \lambda_{j,m}$. An edge $(v, w) \in E(G)$ satisfies this constraint if

$$\begin{aligned} & i \notin \mathrm{Ch}(v, w) \\ \text{or } & j \notin \mathrm{Ch}(v, w) \\ \text{or } & \forall l = 1, \ldots, m : \mathrm{qmag}_i(v \wedge w) \neq \lambda_{i,l} \text{ or } \mathrm{qmag}_j(v \wedge w) \neq \lambda_{j,l}, \end{aligned}$$

i.e. if no pair of changing components transgresses the given landmarks at the same time. All marginal edges can be excluded if the qualitative directions of the state variables are included as additional qualitative magnitudes of auxiliary variables with indices $i = n+1, \ldots, 2n$, i.e. by augmenting the qualitative state space with the qualitative velocity space (as default in the QSIM algorithm, cf. section 2.2.3, p. 32).

PROPOSITION 34: *If the qualitative state space is augmented with the velocity space and* (v_1, v_m) *is a marginal edge, there is a correspondence-not constraint which contradicts the edge* (v_1, v_m)*, but all edges along the path* $v_1, \ldots, v_m$ *satisfy it.*

PROOF: At first recall that for the augmented qualitative state space $\forall v \in V(G), i = n+1, \ldots, 2n : [\mathrm{qmag}_i(v)] = \mathrm{qdir}_{i-n}(v)$, and consequently $\mathrm{Ch}(v,w) \cap \{1,\ldots,2n\}$ in the augmented state space equals $\mathrm{Ch}(v,w)$ in the original state space.
Let (v_1, v_m) be a marginal edge. Choose $k, l \in \{1,\ldots,m-1\}, k \neq l$ and $i \in \mathrm{Ch}(v_k, v_{k+1}) \cap \{1,\ldots,2n\}$, $j \in \mathrm{Ch}(v_l, v_{l+1}) \cap \{1,\ldots,2n\}$, $i \neq j$, such that $\lambda_{i,1} = \mathrm{qmag}_i(v_k \wedge v_{k+1})$ is between $\mathrm{qmag}_i(v_1)$ and $\mathrm{qmag}_i(v_m)$, and also $\lambda_{j,1} = \mathrm{qmag}_j(v_l \wedge v_{l+1})$ is between $\mathrm{qmag}_j(v_1)$ and $\mathrm{qmag}_j(v_m)$. This is possible since for a marginal edge, by PROP. 32, the change sets are pairwise disjoined. The correspondence-not constraint given by the components i, j and the pair of landmarks $\lambda_{i,1}, \lambda_{j,1}$ has the required properties: Since $i \neq j$, all edges along $v_1, \ldots, v_m$ satisfy the constraint. However, (v_1, v_m) does not, because due to PROP. 33, $i, j \in \mathrm{Ch}(v_1, v_m)$, $\mathrm{qmag}_i(v_1 \wedge v_m) = \lambda_{i,1}$, and $\mathrm{qmag}_j(v_1 \wedge v_m) = \lambda_{j,1}$, because $\lambda_{i,1}$ is between $\mathrm{qmag}_i(v_1)$ and $\mathrm{qmag}_i(v_m)$, while $\lambda_{j,1}$ is between $\mathrm{qmag}_j(v_1)$ and $\mathrm{qmag}_j(v_m)$, and PROP. 31 (p. 64) holds. □

This strategy can substantially reduce computing costs, since fewer edges have to be generated during simulation.

The second method avoids the problem of the first – namely having to know potential marginal edges in advance – and is completely automatic. On the other hand, it requires the state-transition graph of the QDE to be determined first. Taking this as input, all marginal edges are determined and eliminated from the state transition graph by exploiting PROP. 32 (p. 64). In the basic version, the change set $\mathrm{Ch}(v,w)$ is assigned to every edge (v,w) of the state-transition graph. The method subsequently starts a depth first search (DFS) from every vertex $v_1 \in V(G)$, such that maximal paths $v_1, \ldots, v_m$ with disjoined change sets are traversed. Efficient algorithms are well-established for depth first search with a given criterion (cf. van Leeuwen 1990). If there is an edge (v_1, v_j), $j \in \{3,\ldots,m\}$, then it is marked as a marginal edge. After all the paths starting from all vertices in G are traversed, the marked edges are eliminated. Of course, there are various possibilities to increase the computational efficiency of the method, e.g. by not re-considering vertices which have already been visited. A problem would occur with this procedure if eliminating a marginal edge interrupts the path defining another marginal edge. Then, vertices which were connected in G would become unconnected. However, this can be excluded:

PROPOSITION 35: *Let G' be the graph obtained from the state-transition graph G by eliminating all edges which are marginal edges. There is a path $v_1, \ldots, v_m$ in G iff there is also a path $v_1, \ldots, v_m$ in G'.*

PROOF: Obviously, paths in G' are also paths in G, since $V(G) = V(G')$ and $E(G') \subseteq E(G)$.

Now, let $v_1, \ldots, v_m$ be a path in G. We have to clarify that there is still a path from v_1 to v_m in G' if some edges of G are marginal (and do not occur in G'). Suppose that $(w_1, w_k) \in E(G)$ is such a marginal edge with $w_1 = v_j$ and $w_k = v_{j+1}$, $j \in \{1,\ldots,m-1\}$. Then, there is a path $w_1, \ldots, w_k$ not containing the edge (w_1, w_k). If this path does not contain another marginal edge, there is a path $v_1, \ldots, w_1, \ldots, w_k, \ldots v_m$ which also exists in G', but there is no edge (v_j, v_{j+1}).

If there are multiple marginal edges in $v_1, \dots, v_m$, or if one edge of $w_1, \dots, w_k$ is marginal again, this argument can be repeated iteratively. The procedure stops when no further marginal edge is contained – with the consequence that there is still a path from v_1 to v_m in G'.
It would not stop if one of the paths from the source to the target of a marginal edge contains another marginal edge which was considered before during the iteration, yielding a cyclic procedure. To show that this can be excluded, consider a path $v_1, \dots, w_1, \dots, w_k, \dots v_m$ in G and let $(v_1, v_m), (w_1, w_k)$ be marginal edges. Then, by PROP. 32 (p. 64) and PROP. 33, the change sets $\mathrm{Ch}(v_1, v_2), \dots, \mathrm{Ch}(w_1, w_2), \dots, \mathrm{Ch}(w_{k-1}, w_k), \dots, \mathrm{Ch}(v_{m-1}, v_m)$ are pairwise disjoined. If the path $w_1, \dots, w_k$ contains the marginal edge (v_1, v_m) again, we must conclude for the same reasons that the change sets

$$\begin{aligned}&\mathrm{Ch}(v_1, v_2), \dots, \mathrm{Ch}(w_1, w_2), \dots,\\ &\mathrm{Ch}(v_1, v_2), \dots, \mathrm{Ch}(v_{m-1}, v_m), \dots,\\ &\mathrm{Ch}(w_{k-1}, w_k), \dots, \mathrm{Ch}(v_{m-1}, v_m)\end{aligned}$$

are also pairwise disjoined – a contradiction. □

To sum up, marginal edges can be defined so as to simplify a state-transition graph by restricting the space of admissible functions in a way that is not an obstacle from the application perspective. Two techniques with different advantages have been presented for this task.

3.3 Ordinal Assumptions

To define a monotonic landmark ensemble $\mathcal{M}(\mu, C)$, the signs of the components of the Jacobian $\mathcal{J}(f), f \in \mathcal{M}(\mu, C)$ are considered. Usually, this leads to a large state-transition graph G due to the generality of $\mathcal{M}(\mu, C)$. The no-return abstraction developed in section 3.1 (p. 52) helps to identify and display structural features in this case, and the elimination of marginal edges (section 3.2, p. 62) brings about more structure in G by restricting the space of admissible trajectories. However, practice shows that restriction techniques like the elimination of marginal edges together with eliminating non-analytical states (cf. section 2.2.4, p. 36) are not always sufficient to bring about enough interpretable subgraphs as no-return and invariant sets. In many cases, the graph consists of one connected component. If more edges can be eliminated, the value of abstraction techniques increases substantially. This is only possible if model ensembles are further restricted by including more assumptions than can be expressed by mere sign and landmark properties. We can use quantitative information (which will be investigated in section 3.4, p. 77), but when uncertainty or generality is high, this might not be available: we need to integrate additional, but not quantitative, information which is likely to be available when reasoning, for example, with causal loop diagrams.

3.3.1 The Effect of Ordinal Assumptions

Ordinal assumptions represent one such type of information. By these we mean statements that the value of some functions on the state space are always above or below the values of other functions. In this section I concentrate on ordinal assumptions for partial derivatives of models f of a monotonic ensemble $\mathcal{M}(\Sigma)$ of the form

$$\forall x \in X : D_k f_i(x) > D_l f_j(x),$$

with prescribed $i, j, k, l \in \{1, \dots, n\}$, $\Sigma = (\sigma_{i,j})_{i,j=1,\dots,n}$, $\sigma_{i,j} \in \mathcal{A}_*$ a matrix of (extended) signs and X the state space. In practice, ordinal assumptions are often supplied together with causal loop diagrams, when not only the positive or negative influences are stated, but also comparative propositions are made about their strengths. Such statements can be like "the influence of x_1 on x_3 is more important than the influence of x_2 on x_3, but it is not known how strong the influence of x_4 on x_3 is in comparison to the other two". This can be interpreted as a partial order of the partial derivatives of the models to be considered. In some cases we can deduce from such knowledge that a main isocline can be transgressed by trajectories only once. Before giving a general proposition to eliminate edges, the idea is illustrated with a simple qualitative model.

EXAMPLE 9: Define

$$\Sigma = \begin{pmatrix} + & + \\ - & - \end{pmatrix}.$$

The resulting state-transition graph is depicted in Fig. 3.5. It has one trivial no-return set, the graph itself, exhibiting a cycle through all four states. We perform a phase plane analysis. From Σ we derive – using the implicit function theorem – the monotonicity properties of both main isoclines $\dot{x}_1 = f_1(x) = 0, \dot{x}_2 = f_2(x) = 0$ (supposed they exist), which are denoted by

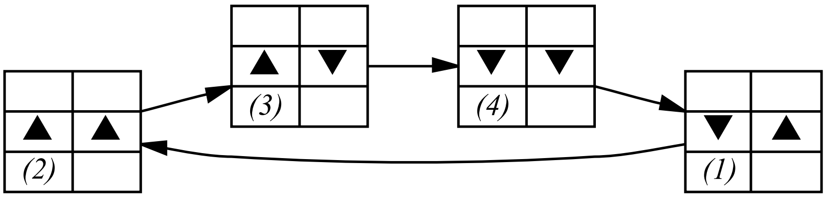

Figure 3.5: State-transition graph of the QDE of the monotonic system $M(\Sigma)$ (computer-generated output, one non-analytic state is eliminated).

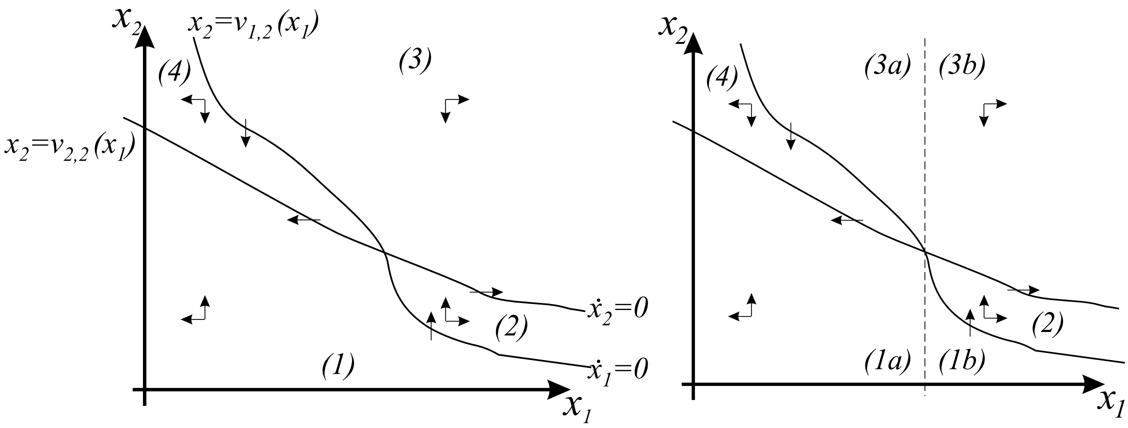

Figure 3.6: Phase plane analysis of an exemplary system $f \in \mathcal{M}(\Sigma)$. To the left: areas with constant direction of change, indicated by arrows and numbers corresponding to Fig. 3.5. To the right: area (1) and (3) are split to $(1a)$, $(1b)$ and $(3a)$, $(3b)$, respectively.

the functions $v_{2,2}, v_{1,2}$ (the indices will become clear in the next subsection). The functions $v_{2,2} : \mathbb{R} \to \mathbb{R}$ and $v_{1,2} : \mathbb{R} \to \mathbb{R}$ solve $f_1(x_1, v_{1,2}(x_1)) = 0$ and $f_2(x_1, v_{2,2}(x_1)) = 0$, yielding

$$\begin{aligned}
[D_1 v_{1,2}] &= \big[-\frac{D_1 f_1}{D_2 f_1}\big] = [-], \\
[D_1 v_{2,2}] &= \big[-\frac{D_1 f_2}{D_2 f_2}\big] = [-],
\end{aligned}$$

i.e. both functions are decreasing. In Fig. 3.6, left, see the phase plane structure of an ODE with $f \in \mathcal{M}(\Sigma)$ where both isoclines exist and intersect exactly once. It can be verified that the state-transition graph is correct: From area (4), corresponding to the qualitative state (4), only area (1) can be reached. If the system is somewhere in area (1) only area (2) can be reached, etc. The result is a cycle in the state-transition graph. However (considering Fig. 3.6, right), it is possible to split areas (1) and (3), such that (2) and $(1b)$ cannot be reached from $(1a)$, while (4) and $(3a)$ cannot be reached from $(3b)$. It is tempting to draw a modified graph (Fig. 3.7), which exhibits a stronger invariance structure than the original state-transition graph. □

Why is it not possible to derive this structure directly from Σ? This stems from the fact that there are other systems $f \in \mathcal{M}(\Sigma)$ with a different phase plane structure. Suppose there is

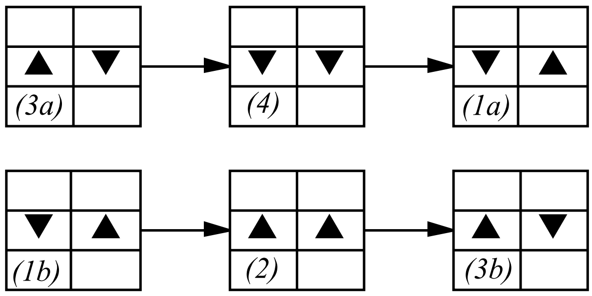

Figure 3.7: Modified state-transition graph derived from the example in Fig. 3.6.

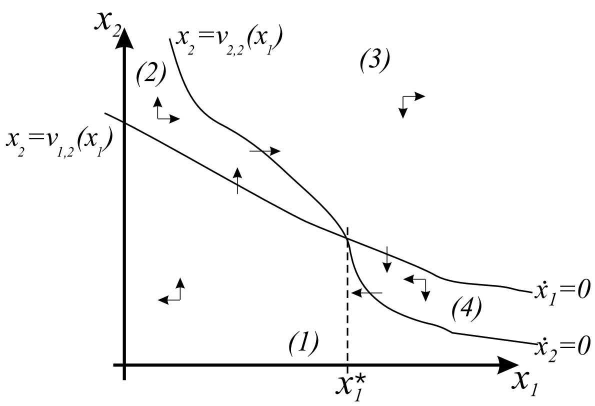

Figure 3.8: Phase plane analysis of a system with property Eq. (3.1).

an equilibrium for $x_1 = x_1^*$, i.e. $v_{1,2}(x_1^*) = v_{2,2}(x_1^*)$, and the system has the property that

$$\begin{aligned} &\forall x_1 < x_1^* : v_{1,2}(x_1^*) < v_{2,2}(x_1^*), \\ &\forall x_1 > x_1^* : v_{1,2}(x_1^*) > v_{2,2}(x_1^*). \end{aligned} \tag{3.1}$$

Then, the phase plane analysis may look like Fig. 3.8, showing that a cycle is possible under these conditions. This is also the case when there are multiple intersections of main isoclines. Since the state-transition graph covers all these cases, it is a strongly connected component. To exclude the cycle case, the model has to be supplied with additional information. If, for example, we impose the ordinal assumptions

$$\begin{aligned} \forall x \in X: \ & D_1 f_1(x) > D_2 f_1(x) (> 0), \\ & D_2 f_2(x) < D_1 f_2(x) (< 0), \end{aligned}$$

it follows that

$$\frac{D_1 f_1}{D_2 f_1} > \frac{D_1 f_2}{D_2 f_2},$$

and thus

$$\begin{aligned} 0 &< -\frac{D_1 f_2}{D_2 f_2} + \frac{D_1 f_1}{D_2 f_1} \\ &= D_1 \big(v_{2,2}(x_1) - v_{1,2}(x_1) \big), \end{aligned}$$

meaning that the distance between the main isoclines strictly increases with x_1, excluding multiple intersections and a situation as characterised by Eq. (3.1).

3.3.2 The ORDAS Algorithm

I now generalise this idea to state spaces with an arbitrary dimension. The result is a criterion to eleminate paths using ordinal assumptions and the knowledge that a certain main isocline was transgressed along a path before. We assume that $\Sigma \in \mathcal{A}^{n\times n}$. At first a simple proposition is shown, showing whether – for a given sign vector $[\dot{x}(t)]$ and Σ – a state $x(t)$ is above or below the ith isocline with respect to the direction of the kth unit vector. To avoid complications only models $f \in \mathcal{M}(\Sigma)$ are considered where for a given component i the implicit equation $f_i = 0$ **is soluble for** some $k \in \{1, \ldots, n\}$, meaning that there is a unique solution $v_{i,k} : X \to \mathbb{R}$, independent from x_k, such that

$$\forall x \in X : f_i\big(x_1, \ldots, x_{k-1}, v_{i,k}(x_1, \ldots, x_n), x_{k+1}, \ldots, x_n\big) = 0.$$

Uniqueness of the solution $v_{i,k}$ is guaranteed by the implicit function theorem since f is monotonic as specified by Σ, such that the *existence* on X is the assumption here.

PROPOSITION 36: *For a given Σ, let $f \in \mathcal{M}(\Sigma)$ be a function where f_i is soluble for k. Let $v_{i,k}$ be the solution, choose an arbitrary $x \in X$, and define $\sigma_i := [f_i(x)]$. If $\sigma_{i,k} \neq 0$ then*

$$\begin{aligned} \sigma_i\, \sigma_{i,k}\, x_k &> \sigma_i\, \sigma_{i,k}\, v_{i,k}(x) && \text{if } \sigma_i \neq 0, \\ \text{or } x_k &= v_{i,k}(x) && \text{if } \sigma_i = 0. \end{aligned}$$

PROOF: The case $\sigma_i = 0$ is obvious.
If $\sigma_i > 0$ then

$$\begin{aligned} &f_i(x_1, \ldots, x_{k-1}, x_k, x_{k+1}, \ldots, x_n) > 0 = \\ &= f_i\big(x_1, \ldots, x_{k-1}, v_{i,k}(x_1, \ldots, x_n), x_{k+1}, \ldots, x_n\big), \end{aligned}$$

and thus $\sigma_{i,k} x_k > \sigma_{i,k} v_{i,k}(x)$.
By analogy for $\sigma_i < 0$, it holds that $\sigma_{i,k} x_k < \sigma_{i,k} v_{i,k}(x)$. This and the former case together yield $\sigma_i \sigma_{i,k} x_k > \sigma_i \sigma_{i,k} v_{i,k}(x)$. □

Next, we introduce assumptions about terms of the form

$$d^{i,j}_{k,l} := D_l f_j \cdot D_k f_i - D_k f_j \cdot D_l f_i, \tag{3.2}$$

defined for a differentiable function $f : X \to \mathbb{R}^n$, and $i, j, k, l \in \{1, \ldots, n\}$. It is assumed that the sign $\big[d^{i,j}_{k,l}\big]$ is constant on X. In some cases, this already follows from Σ, but in other cases it is a consequence of ordinal assumptions, as EX. 9 (p. 68) shows, where

$$\Sigma = \begin{pmatrix} + & + \\ - & - \end{pmatrix},$$

and $\big[d^{1,2}_{1,2}\big] = \big[D_1 f_1 \cdot D_2 f_2 - D_1 f_2 \cdot D_2 f_1\big]$ can be positive, negative or vanishing. If the modeller knows, e.g. that $D_2 f_1 > D_1 f_1$ and $D_2 f_2 > D_1 f_2$, then $\big[d^{1,2}_{1,2}\big] = [+]$. This kind of information is decisive for the elimination of edges:

PROPOSITION 37: *Let $\mathcal{M}(\Sigma)$ be a monotonic ensemble, G the resulting state-transition graph, v_0, v_1, v_2 a path of length 2 in G, and let the following criterion hold:*

(i) There exists an $i \in \{1, \ldots, n\}$ such that

$$-\mathrm{qdir}_i(v_0) = \mathrm{qdir}_i(v_1) = \mathrm{qdir}_i(v_2) \neq 0, \tag{3.3}$$

(ii) there is a $j \in \{1, \ldots, n\}$ such that

$$\mathrm{qdir}_j(v_0) = \mathrm{qdir}_j(v_1) = -\mathrm{qdir}_j(v_2) \neq 0, \tag{3.4}$$

(iii) for such i, j there exists a $k \in \{1, \ldots, n\}$ such that

$$\mathrm{qdir}_i(v_1)\, \sigma_{i,k} = \mathrm{qdir}_j(v_1)\, \sigma_{j,k} \neq 0, \tag{3.5}$$

(iv) for all $l \in \{1, \ldots, n\}, l \neq k$, $\left[d^{i,j}_{k,l}\right]$ is uniquely determined, fulfilling

$$\mathrm{qdir}_l(v_1)\, \mathrm{qdir}_i(v_1)\, \sigma_{j,k} \left[d^{i,j}_{k,l}\right] \geq 0. \tag{3.6}$$

Then there is no solution to an initial value problem $\dot{x} = f(x), [\dot{x}(0)] = v_0, f \in \mathcal{M}(\Sigma)$ with f_i soluble for k, which has the path v_0, v_1, v_2 as abstraction.

PROOF: Assume that there were a solution $x(\cdot)$ of the above type which has the path v_0, v_1, v_2 as abstraction. We demonstrate that this yields a contradiction.
For convenience, define $\sigma_i = \mathrm{qdir}_i(v_1)$ and $\sigma_j = \mathrm{qdir}_j(v_1)$. We know from Eq. (3.3) and Eq. (3.4) (using Eq. 2.2) that there are $t_1, t_2 \in \mathbb{R}_+$ with $t_1 < t_2$ such that $\dot{x}_i(t_1) = 0 = \dot{x}_j(t_2)$ and $\dot{x}_i(t_2) \neq 0 \neq \dot{x}_j(t_1)$. Eq. (3.5) has the consequence that $\sigma_{i,k}$ and $\sigma_{j,k}$ do not vanish, and thus PROP. 36 can be applied to $x(t_1)$ and $x(t_2)$. Infer that

$$x_k(t_1) = v_{i,k}(x(t_1)), \tag{3.7}$$
$$\sigma_i\, \sigma_{i,k}\, x_k(t_2) > \sigma_i\, \sigma_{i,k}\, v_{i,k}(x(t_2)), \tag{3.8}$$
$$x_k(t_2) = v_{j,k}(x(t_2)), \tag{3.9}$$
$$\sigma_j\, \sigma_{j,k}\, x_k(t_1) > \sigma_j\, \sigma_{j,k}\, v_{j,k}(x(t_1)). \tag{3.10}$$

Now consider the function $\Delta(t) := v_{i,k}(x(t)) - v_{j,k}(x(t))$. It follows from Eq. (3.7) and Eq. (3.10) that

$$\sigma_j\, \sigma_{j,k}\, \Delta(t_1) = \sigma_j\, \sigma_{j,k}\, x_k(t_1) - \sigma_j\, \sigma_{j,k}\, v_{j,k}(x(t_1)) > 0,$$

and Eq. (3.5) implies that also $\sigma_i\, \sigma_{i,k}\, \Delta(t_1) > 0$. Compare $\Delta(t_2)$ with $\Delta(t_1)$: by differentiating and applying the implicit function theorem we obtain

$$D_t\Delta = \sum_{\substack{l=1,\ldots,n\\ l\neq k}} D_l v_{i,k} \cdot \dot{x}_l - \sum_{\substack{l=1,\ldots,n\\ l\neq k}} D_l v_{j,k} \cdot \dot{x}_l = \sum_{\substack{l=1,\ldots,n\\ l\neq k}} \dot{x}_l \Big(\frac{D_l f_j\, D_k f_i - D_k f_j\, D_l f_i}{D_k f_i\, D_k f_j} \Big).$$

The criterion guarantees that $\sigma_{i,k}\,\sigma_i\,D_t\Delta \geq 0$, since $\sigma_{i,k}, \sigma_{j,k}$ do not vanish and by Eq. (3.6) for all $l \neq k$

$$
\begin{aligned}
0 &\leq \sigma_l\,\sigma_i\,\sigma_{j,k}\left[d_{k,l}^{i,j}\right] = \\
&= \sigma_l\,(\sigma_{i,k}\,\sigma_{i,k})\,\sigma_i\,\sigma_{j,k}\left[d_{k,l}^{i,j}\right] = \\
&= \sigma_l\,\sigma_{i,k}\,\sigma_i\,\frac{\left[D_l f_j\,D_k f_i - D_k f_j\,D_l f_i\right]}{\sigma_{i,k}\,\sigma_{j,k}},
\end{aligned}
$$

where the last step exploits the multiplicative cancellation law of sign algebra (Eq. 2.1). Consequently, $\sigma_i\,\sigma_{i,k}\,\Delta(t_2) \geq \sigma_i\,\sigma_{i,k}\,\Delta(t_1) > 0$, and Eq. (3.9) implies

$$
\sigma_i\,\sigma_{i,k}\,v_{i,k}(x(t_2)) > \sigma_i\,\sigma_{i,k}\,v_{j,k}(x(t_2)) = \sigma_i\,\sigma_{i,k}\,x_k(t_2),
$$

which is a contradiction to Eq. (3.8).
We must conclude that there is no trajectory $x(\cdot)$ which has the path v_0, v_1, v_2 as abstraction.
$\square$

This proposition makes it possible to eliminate paths of length 2 if appropriate assumptions about $\left[d_{k,l}^{i,j}\right]$ are supplied by the modeller. Some of them are derived directly from Σ, while others represent a new structural property of the QDE not already entailed by the sign matrix. It should be noted that these assumptions cannot be chosen independently from each other since, by symmetry,

$$
d_{k,l}^{i,j} = -d_{k,l}^{j,i} = -d_{l,k}^{i,j} = d_{l,k}^{j,i}. \tag{3.11}
$$

In contrast to the elimination of marginal edges (section 3.2), the criterion cannot be applied to singular edges. In addition to the ordinal assumptions, some information about the "past" of a qualitative state v_1 is used to exclude a potential "future" v_2. It may be the case that the path v_0, v_1, v_2 is excluded, while a path v_0', v_1, v_2 is still possible.

Thus, an elimination algorithm is not straightforward. In the following, I present the **ORD**inal **AS**sumptions algorithm. It exhausts PROP. 37 by "splitting" states as already indicated in EX. 9 (p. 68). This leads to a new graph containing multiple states with identical qualitative values. Each of them represents one case were PROP. 37 can be applied, having only the predecessors fulfilling Eq. (3.3) and Eq. (3.4), and the successors which cannot be eliminated under this condition.

DEFINITION 21: *The* ***ORDAS algorithm*** *inductively computes a sequence of graphs $H_0, \ldots, H_i$ by the following procedure, which takes as input a state transition graph G and a set of assumptions on the signs of expressions of the form Eq. (3.2).*

Define H_0 by

$$
\begin{aligned}
V(H_0) &:= \{v \times \{0\} \mid v \in V(G)\} \subseteq V(G) \times \mathbb{N}, \\
E(H_0) &:= \{(v \times \{0\}, w \times \{0\}) \mid (v, w) \in E(G)\}.
\end{aligned}
$$

For convenience, we write v_j for $v \times \{j\}$, and identify $\mathrm{qdir}(v_j)$ with $\mathrm{qdir}(v)$. Enumerate the vertices of H_0 as $v_0^1, \ldots, v_0^i, \ldots$ in an arbitrary order.

For the inductive definition of the sequence of graphs we consider the vertex v_0^i at step i and define the set of ***contradicting paths of a vertex*** *v in H_i as*

$$\mathrm{Cp}(v, H_i) := \{(u, v, w) \in V(H_i)^3 \mid (u, v) \in E(H_i), (v, w) \in E(H_i) \text{ and PROP. 37 (p. 72) can be used to eliminate the path } u, v, w\}.$$

This also defines the set of ***contradiction initiating predecessors***

$$\mathrm{Ci}(v, H_i) := \{u \in V(H_i) \mid (u, v, w) \in \mathrm{Cp}(v, H_i)\},$$

with its elements denoted by $u_1, \ldots, u_k$, $k := |\mathrm{Ci}(v, H_i)|$.

Then, H_{i+1} is given by

$$V(H_{i+1}) = V(H_i) \cup \{v_1^i, \ldots, v_k^i\},$$
$$E(H_{i+1}) = E_1 \cup E_2 \cup E_3 \cup E_4 \cup E_5,$$

where $v_1^i, \ldots, v_k^i$ are introduced as new vertices which appear in the following edges:

$$E_1 = \{(u, w) \mid (u, w) \in E(H_i) \text{ and } u \neq v_0^i \neq w\},$$
$$E_2 = \{(v_0^i, w) \mid (v_0^i, w) \in E(H_i)\},$$
$$E_3 = \{(u, v_0^i) \mid (u, v_0^i) \in E(H_i) \text{ and } u \notin \mathrm{Ci}(v_0^i, H_i)\},$$
$$E_4 = \{(u_j, v_j^i) \mid 1 \leq j \leq k \text{ and } u_j \in \mathrm{Ci}(v_0^i, H_i)\},$$
$$E_5 = \{(v_j^i, w) \mid (v_0^i, w) \in E(H_i), 1 \leq j \leq k \text{ and } (u_j, v_0^i, w) \notin \mathrm{Cp}(v_0^i, H_i)\}.$$

The set E_1 represents all edges which are not affected by considering v_0^i at induction step i and is consequently included in H_i as well as in H_{i+1}. Via E_2, all successors of v_0^i in H_i remain successors in H_{i+1}, since this vertex is made to represent all cases where PROP. 37 cannot be applied, and E_3 contains are all corresponding predecessors in H_i. In contrast, the new vertices $v_1^i, \ldots, v_k^i$ are introduced to represent a paths where the conditions of the proposition are met. The edges E_4 subsume the contradiction initiating predecessors corresponding to each of the new vertices, and E_5 subsumes all remaining successors of a v_j^i which cannot by excluded by PROP. 37. The next proposition shows that the result of the ORDAS algorithm is a graph H which contains no path of length 2 contradicting the ordinal assumptions, and maintains other important structural properties of G.

PROPOSITION 38: *The ORDAS algorithm computes a finite sequence of graphs $H_0, \ldots, H_i, \ldots, H$ such that H has the following properties:*

(i) For all vertices $v \in V(H)$ the set of contradicting paths $\mathrm{Cp}(v, H) = \varnothing$.

(ii) For all not-contradicting paths u, v, w in H_0, i.e. $(u, v, w) \notin \mathrm{Cp}(v, H_0)$, u, v, w is a path in H.

(iii) For all edges $(v', w') \in E(H)$ there exists an edge $(v, w) \in E(H_0)$ with $\mathrm{qdir}(v) = \mathrm{qdir}(v')$ and $\mathrm{qdir}(w) = \mathrm{qdir}(w')$.

The first property guarantees that all paths to which PROP. 37 applies are eliminated in H. The second property ensures that not too many paths are eliminated. The third safeguards that no essentially new edges are introduced (which would be artifacts of the procedure).

PROOF: Obviously, the algorithm terminates after a finite number of steps since the number of vertices in H_0 is finite.

To prove property (i), we show that at each induction step i it holds for all $v \in \{v_0^i, v_1^i, \ldots, v_k^i\}$ that

$$\begin{aligned} \mathrm{Cp}(v, H_{i+1}) &= \varnothing, \\ \text{and } \forall l > i : \mathrm{Cp}(v, H_l) = \varnothing &\Rightarrow \mathrm{Cp}(v, H_{l+1}) = \varnothing. \end{aligned}$$

For a given $v \in \{v_0^i, v_1^i, \ldots, v_k^i\}$ consider an arbitrary path u, v, w in H_{i+1}.
If $v = v_0^i$, then by DEF. 21 $(u, v) \in E_3$ and $(v, w) \in E_2$. Hence, in H_i there is also an edge (v, w) and an edge (u, v) with $u \notin \mathrm{Ci}(v_0^i, H_i)$. This entails $(u, v_0^i, w) \notin \mathrm{Cp}(v_0^i, H_i)$, such that the path u, v, w cannot by excluded from H_i using PROP. 37. Likewise, it is not a contradicting path in H_{i+1}.
If $v = v_j^i$, then $(v, w) \in E_5$, implying $(u_j, v_0^i, w) \notin \mathrm{Cp}(v_0^i, H_i)$, i.e. there is a path u_j, v_0^i, w in H_i which cannot be excluded by PROP. 37. Since $\mathrm{qdir}(u_j) = \mathrm{qdir}(u)$ and $\mathrm{qdir}(v_0^i) = \mathrm{qdir}(v)$, the path u, v, w can also not be excluded from H_{i+1}.
Assume for the induction step that for a given vertex $v \in V(H_l)$ there is no contradicting path u, v, w in H_l. By DEF. 21, also $v \in V(H_{l+1})$. Since $l > i$, all paths of length 2 in H_{l+1} having v as second vertex are of the form $\hat{u}, v, \hat{w}$ with $\mathrm{qdir}(\hat{u}) = \mathrm{qdir}(u)$ and $\mathrm{qdir}(\hat{w}) = \mathrm{qdir}(w)$. Thus, none of the paths can be excluded in H_{l+1}.

For property (ii), let u, v, w be a path in H_i with $(u, v, w) \notin \mathrm{Cp}(v, H_i)$, and consequently $u \notin \mathrm{Ci}(v, H_i)$. Depending on whether u, v or w equals v_0^i we can determine if (u, v) and (v, w) are elements of E_1, E_2, E_3, E_4 or E_5, making u, v, w a path in H_{i+1}.
First consider that $v = v_0^i$. Then $(v, w) \in E_2$, and as $u \notin \mathrm{Ci}(v_0^i, H_i)$, also the edge $(u, v) \in E_3$.
Now let $v \neq v_0^i$. If $u \neq v_0^i$ then the edge $(u, v) \in E_1$, if $w \neq v_0^i$ then $(v, w) \in E_1$, and if $u = v_0^i$ then $(u, v) \in E_2$. For $w = v_0^i$ and $v \notin \mathrm{Ci}(v_0^i, H_i)$, it holds that $(v, w) \in E_3$. Otherwise, $v \in \mathrm{Ci}(v_0^i, H_i)$, and since $v \neq v_0^i$ there is one $j \geq 1$ such that $(v, v_j^i) \in E_4$. Note that $\mathrm{qdir}(v_j^i) = \mathrm{qdir}(w)$.
Thus, in any case there is a corresponding path in H_{i+1} which cannot be eliminated using PROP. 37 since it has the same qualitative directions as (u, v, w). By induction, the correspondence also holds from H_0 to H.

To show property (iii), consider an edge $e = (v, w) \in E(H_{i+1})$. Distinguish whether e is an element of E_1, E_2, E_3, E_4 or E_5. If $e \in E_1$, it is also an edge in $E(H_i)$. If $e \in E_2$, then $v = v_0^i$, and the edge (v_0^i, w) exists in H_i (and $\mathrm{qdir}(v_0^i) = \mathrm{qdir}(v)$). For $e \in E_3$, we have that $w = v_0^i$, making (v, v_0^i) an edge in H_i, and for $e \in E_5$ it is $v = v_j^i$, making (v_0^i, w) an edge in H_i. In the case that $e \in E_4$, it is $v = u_j$ and $w = v_j^i$ with $v \in \mathrm{Ci}(v_0^i, H_i)$, such that $(u_j, v_0^i) \in E(H_i)$ and $\mathrm{qdir}(v_j^i) = \mathrm{qdir}(v_0^i)$. Since there are no other types of edges in H_{i+1}, all of them correspond to an edge in H_i with identical qualitative directions. By induction, there is also a correspondence from H to H_0. $\square$

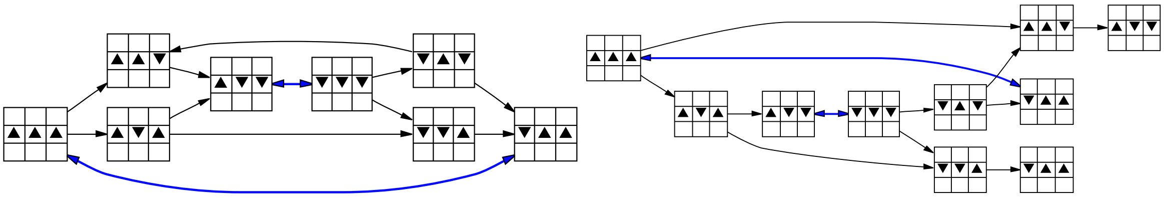

Figure 3.9: The state-transition graph of EX. 10 (left) and the result of the ORDAS algorithm (right).

I present an example for the ORDAS algorithm.

EXAMPLE 10: Let a monotonic ensemble be given by

$$\Sigma = \begin{pmatrix} + & + & - \\ - & - & 0 \\ - & 0 & + \end{pmatrix}.$$

The resulting state-transition graph is displayed in Fig. 3.9 (left). If we impose the assumptions

$$-d_{1,2}^{1,2} = -d_{2,1}^{2,1} = d_{1,2}^{2,1} = d_{2,1}^{1,2} = [+],$$
$$-d_{1,3}^{3,1} = -d_{3,1}^{1,3} = d_{1,3}^{1,3} = d_{3,1}^{3,1} = [+],$$

the ORDAS algorithm yields the result as also given in Fig. 3.9 (right). As the result H of the ORDAS algorithm is a graph where vertices represent qualitative states, abstractions techniques can also be applied to H. Performing a no-return abstraction yields a new result: The is a non-trivial no-return set D, i.e. there is no path in H which re-enters $D \subseteq V(H)$ after it is left: all solutions $x(\cdot)$ given by a model $f \in \mathcal{M}(\Sigma)$ which respects the ordinal assumptions and which is soluble for the appropriate components cannot re-enter D. If there is one $t_1 > 0$ such that $[f(x(t_1))] \in D$, and a $t_2 > t_1$ such that $[f(x(t_2))] \notin D$, then $\forall t > t_2 : [f(x(t))] \notin D$. Since there are paths in G which do not occur in H, no-return sets are more likely to occur in H (see Fig. 3.10 for the example). □

Thus, there is a synergy between the new abstraction and reduction techniques presented in this chapter, making qualitative models more valuable for questions of sustainable system design. I illustrate this added value in more detail in Chapter 4. But first the sequence of restricted model ensembles is completed in the next section.

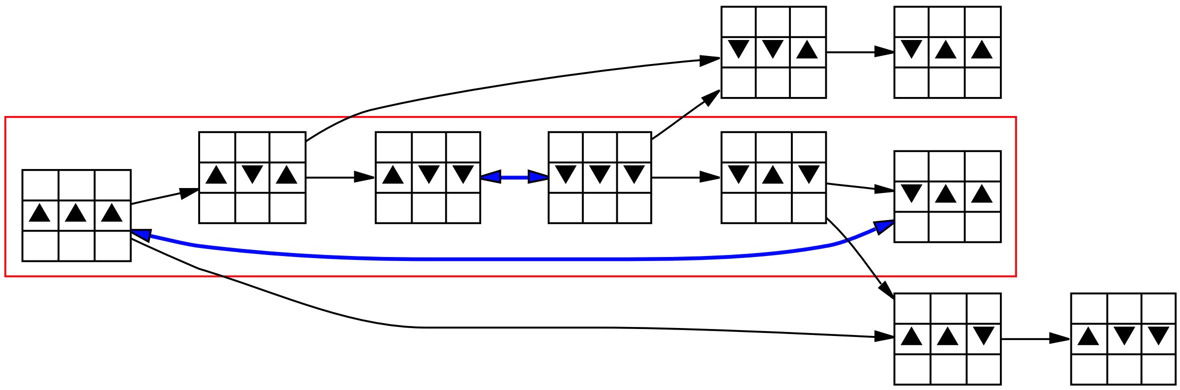

Figure 3.10: No-return abstraction of the result of the ORDAS algorithm for Ex. 10. The no-return set consisting of more than one vertex is displayed as a cluster.

3.4 Quantitative Bounds

In this section I introduce linear-interval differential inclusions, which restrict a monotonic ensemble $\mathcal{M}(\Sigma)$ to models for which interval constraints hold for the components of the Jacobian. If there are multiple successors of a single vertex in the state-transition graph, the question which of them will be attained can be formulated as a viability problem. After defining linear-interval maps and investigating their absorption basins, I show how this can be used to analyse the state-transition graph of a QDE.

3.4.1 Absorption Basins of Linear-Interval Differential Inclusions

Linear-interval differential inclusions are given by set-valued maps. Throughout this section we regard singletons as intervals and consider a state space $X \subseteq \mathbb{R}^n$.

DEFINITION 22: *Let U be a matrix of compact intervals $(u_{i,j})_{i,j=1,\dots,n}$, where each interval either vanishes or does not contain 0. A set-valued map $F : X \rightsquigarrow \mathbb{R}^n, F(x) := Ux$, where the latter denotes interval-valued multiplication, is called a* ***linear-interval map****.*

Interval-valued multiplication is defined in the usual way by $Ux := \{Mx \mid M \in U\}$, where a matrix $M = (m_{i,j})_{i,j=1,\dots,n} \in U$ if and only if $\forall i, j = 1, \dots, n : m_{i,j} \in u_{i,j}$. DEF. 22 guarantees that every coefficient of U has a prescribed sign (which will be related to Σ below). Note that a linear-interval map F defines a model ensemble (cf. section 2.3, p. 42) which includes nonlinear models $f : X \to \mathbb{R}^n$ such that $\forall x \in X : f(x) \in F(x)$. Before analysing absorption basins, the regularity properties of linear-interval maps are investigated. Based on a matrix norm $\|\cdot\|$ on $\mathbb{R}^{n\times n}$, we define the norm $\|F\| := \max_{M\in U} \|M\|$.

PROPOSITION 39: *A linear-interval map F has compact interval-valued images. It is Marchaud, Lipschitz (both with constant $\|F\|$) and homogeneous, i.e. $\forall \lambda \in \mathbb{R} : F(\lambda x) = \lambda F(x)$.*

PROOF: (i) F has interval-valued images: Each component $F_i, i = 1, \dots, n$ has the form $\sum_{j=1,\dots,n} u_{i,j} x_i$, where $u_{i,j}$ are compact intervals. The properties of interval arithmetic imply that this yields an interval. As it results from a continuous operation on a compact set, it is also compact.

(ii) F is Marchaud: $Dom(F) = \mathbb{R}^n$ is obviously closed. It has convex values, because they are interval-valued. It has linear growth, because $\|F(x)\| = \|Ux\| \leq \|U\|\|x\| = \|F\|\|x\| \leq \|F\|(\|x\| + 1)$. Its graph is closed, because F has compact values and the upper and lower bounds of the values depend continuously on x (cf. p. 43).
(iii) F is Lipschitz: Let $x, x' \in \mathbb{R}^n$. Since U is compact we can choose a matrix $M \in U$ such that $\|M(x' - x)\| = \|F\|\|x' - x\|$, and define

$$e := -\frac{M(x' - x)}{\|M(x' - x)\|} \in B(0, 1).$$

Therefore,

$$M(x' - x) + \|F\|\|x' - x\|e = M(x' - x) - \frac{\|F\|\|(x' - x)\|}{\|M(x' - x)\|}M(x' - x) = 0,$$

and $0 \in B\big(U(x' - x), \|F\|\|x' - x\|\big)$. Hence, $Ux \subseteq B\big(Ux', \|F\|\|x' - x\|\big)$, i.e. $F(x) \subseteq B\big(F(x'), \|F\|\|x' - x\|\big)$ (cf. p. 42).
(iv) F is homogeneous: Choose arbitrary $x \in \mathbb{R}^n, \lambda \in \mathbb{R}$. Due to the properties of interval arithmetic it holds for all $i = 1, \dots, n$ that

$$\begin{aligned} F_i(\lambda x) &= \sum_{j=1,\dots,n} u_{i,j}(\lambda x_i) = \sum_{j=1,\dots,n} \lambda u_{i,j} x_i \\ &= \lambda \sum_{j=1,\dots,n} u_{i,j} x_i = \lambda F_i(x). \end{aligned}$$

□

As discussed below, we need to compute absorption basins of linear-interval differential inclusions $\dot{x} \in F(x)$. In principle, this can be done with the viability kernel algorithm (cf. section 2.4, p. 45). But since it is designed for a bounded constrained set and target, and we will have to deal with (unbounded) cones, some remarks are necessary. We start with an observation resulting from the homogeneity of linear-interval maps.

PROPOSITION 40: *Let F be a linear-interval map, $x(\cdot) \in \mathcal{S}_F(x_0)$ a solution for $x_0 \in \mathbb{R}^n$, and $\lambda \in \mathbb{R}$. Then $y(\cdot) := \lambda x(\cdot) \in \mathcal{S}_F(x_0)$.*

PROOF: For almost every $t \in \mathbb{R}_+$ it holds that $\dot{y}(t) = \lambda \dot{x}(t) \in \lambda F(x(t))$. Due to PROP. 39, the last term equals $F(\lambda x(t)) = F(y(t))$, making $y(\cdot)$ a solution. □

As a consequence, the absorption basin of a cone is also a cone:

PROPOSITION 41: *Let $C, K \subseteq \mathbb{R}^n, C \subseteq K$ be cones, and $F : \mathbb{R}^n \rightsquigarrow \mathbb{R}^n$ a linear-interval map. Then $D = \mathrm{Abs}_F(K, C)$ is a cone.*

PROOF: Choose $x_0 \in D$ and $\lambda > 0$. We show that $y_0 := \lambda x_0 \in D$.
By definition of the absorption basin, for all solutions $x(\cdot) \in \mathcal{S}_F(x_0)$ there exists a $T > 0$ such that $x(T) \in C$ and $\forall t \in [0, T] : x(t) \in K$ (see DEF. 13, p. 46). Define $y(\cdot) := \lambda x(\cdot)$, which is an element of $\mathcal{S}_F(y_0)$ by PROP. 40. Since C, K are cones, this proposition also implies that $y(T) = \lambda x(T) \in \lambda C = C$ and $\forall t \in [0, T] : y(T) = \lambda x(t) \in \lambda K = K$. Therefore, $y_0 \in D$. □

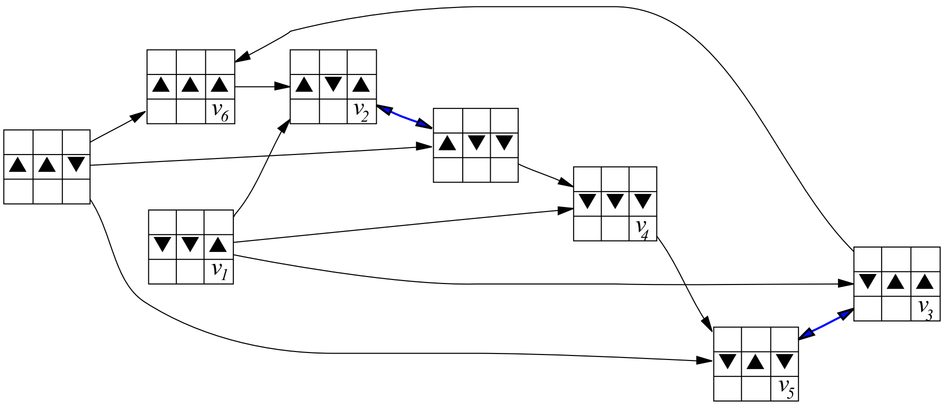

Figure 3.11: State-transition graph of the QDE defined in EX. 11 after removing marginal edges, non-analytical and equilibrium states. The vertices $v_1, \ldots, v_6$ are discussed in the text.

For cones C, K we can compute the bounded set $D_\lambda := \text{Abs}(K \cap \lambda Q, C \cap \lambda Q)$, where $\lambda > 0$ and Q is an appropriately chosen bounded set.

PROPOSITION 42: *Let* $C, K \subseteq \mathbb{R}^n, C \subseteq K$ *be cones,* $Q \subseteq \mathbb{R}^n$ *and* $\lambda > 0$. *Then* $D_\lambda = \lambda D_1$.

PROOF: For $x_0 \in D_\lambda$, we show that $y_0 := \frac{1}{\lambda} x_0 \in D_1$: Choose $x(\cdot) \in \mathcal{S}_F(x_0)$ and set $y(\cdot) := \frac{1}{\lambda} x(\cdot)$, which is an element of $\mathcal{S}_F(\frac{1}{\lambda} x_0)$ due to PROP. 40. If $\exists T > 0 : x(T) \in C \cap \lambda Q = \lambda C \cap \lambda Q = \lambda(C \cap Q)$, then $y(T) \in C \cap Q$. If $\forall t \in [0, T] : x(t) \in K \cap \lambda Q = \lambda(K \cap Q)$, then $y(t) \in K \cap Q$. Thus $y_0 \in D_1$, i.e. $D_\lambda \subseteq \lambda D_1$.
By symmetry, $\lambda D_1 \subseteq D_\lambda$ also holds. □

Finally, the absorption basin $\text{Abs}_F(K, C)$ can be recovered from D_λ by the following property:

PROPOSITION 43: *If* $0 \in \text{Int}(Q)$ *then* $\text{Abs}_F(K, C) = \bigcup_{\lambda > 0} D_\lambda$.

PROOF: If $x_0 \in \bigcup_{\lambda > 0} D_\lambda$ there exists one $\lambda > 0$ such that $x_0 \in D_\lambda$. Thus, for all $x(\cdot) \in \mathcal{S}_F(x_0) \exists T > 0 : x(T) \in C \cap \lambda Q \subset C$ and $\forall t \in [0, T] : x(t) \in K \cap \lambda Q \subset K$. Therefore, $x_0 \in \text{Abs}(K, C)$.

Now choose $x_0 \in \text{Abs}_F(K, C)$ and a solution $x(\cdot) \in \mathcal{S}_F(x_0)$. By DEF. 13 (p. 46), there is one $T > 0$ such that $x(T) \in C$ and $\forall t \in [0, T] : x(t) \in K$. Since $x(\cdot)$ is continuous, $x(T)$ finite and $0 \in \text{Int}(Q)$, there is one $\lambda > 0$ such that $x(T) \in C \cap \lambda Q$ and $\forall t \in [0, T] : x(t) \in K \cap \lambda Q$. Therefore, $x_0 \in \bigcup_{\lambda > 0} D_\lambda$. □

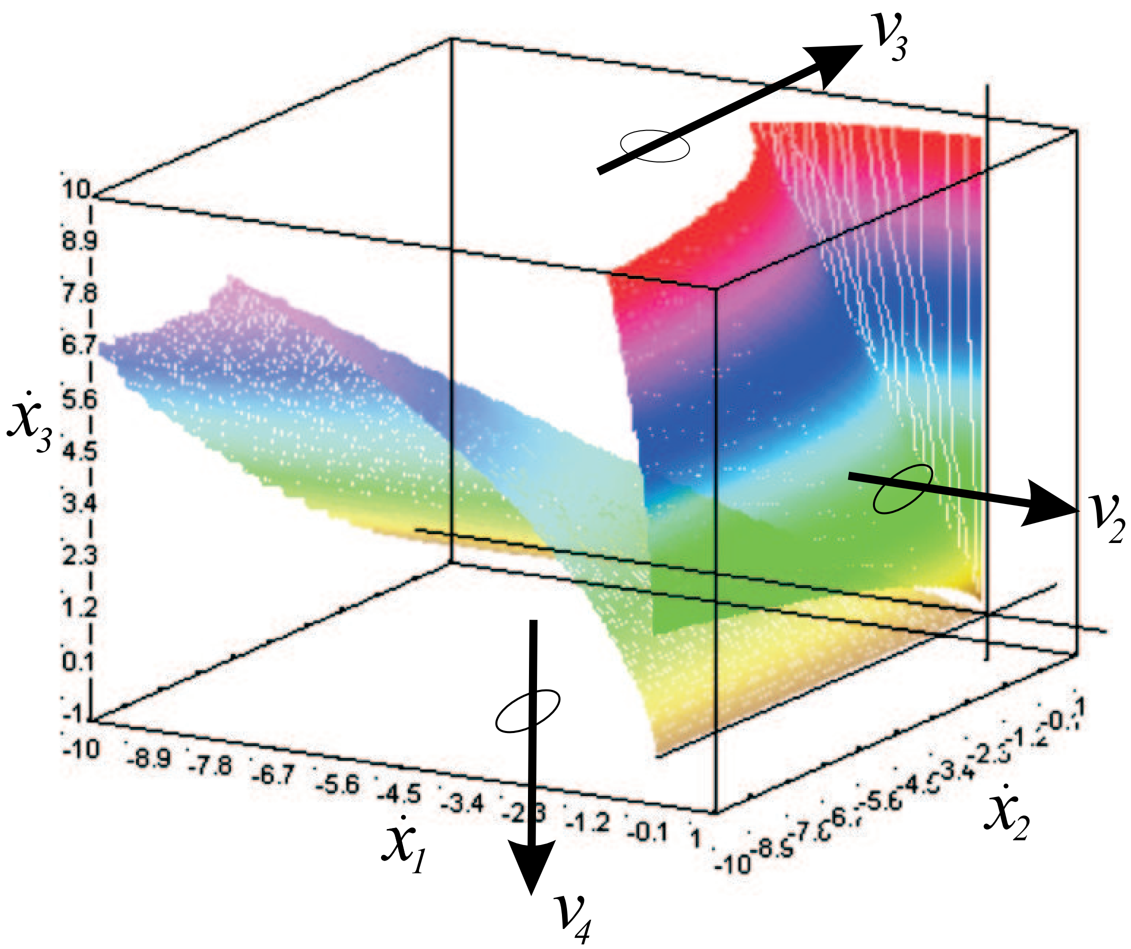

Figure 3.12: Boundaries of the absorption basins of v_1 with target v_2, v_3, v_4 restricted to a cube Q. Large arrows indicate the directions towards successors. Qualitative transitions to v_2 necessarily occur from $Abs_F\big(\bar{K}(v_1)) \cap Q, \bar{K}(v_1) \cap \bar{K}(v_2) \cap Q\big)$, the region between the surface to the right and the plane given by $\dot{x}_1 = 0$. A shift to v_4 happens from $Abs_F\big(\bar{K}(v_1) \cap Q), \bar{K}(v_1) \cap \bar{K}(v_4) \cap Q\big)$ between the lower surface and the plane given by $\dot{x}_3 = 0$. $Abs_F\big(\bar{K}(v_1) \cap Q, \bar{K}(v_1) \cap \bar{K}(v_3) \cap Q\big)$, which would lead to state v_3, is empty.

3.4.2 Analysing a State-Transition Graph with Linear-Interval Differential Inclusions

I now show how the absorption basins of linear-interval differential inclusions can be used infer system knowledge from a QDE when quantitative bounds are available. Starting with a sign matrix Σ, we set-up a monotonic ensemble and solve it with the QSIM algorithm. Then, quantitative bounds are considered by setting up a linear-interval differential inclusion where the signs of the intervals correspond to the signs of Σ. I give a precise definition of the differential inclusion and discuss its relation to the associated QDE. Recall that a monotonic ensemble $\mathcal{M}(\Sigma)$ defines a set of systems $\dot{x} = f(x)$ such that for all $x \in X : \big[\mathcal{J}(f(x))\big] \approx \Sigma$. Changing the perspective from the state space to the velocity space, we saw in section 2.3

(p. 42) that it is not possible to investigate a QDE by considering a differential inclusion

$$\ddot{x} \in \hat{F}(\dot{x}) := \{A\dot{x} \mid [A] \approx \Sigma\},$$

since the set-valued map $\hat{F}$ is unbounded. However, if intervals $u_{i,j}$ are known such that $\forall x \in X : D_j f_i(x) \in u_{i,j}$, the linear-interval differential inclusion

$$\ddot{x} \in F(\dot{x}) = U\dot{x},$$

can be set-up. It is very regular by PROP. 39 (p. 77), and "simulates" the monotonic ensemble $\mathcal{M}(\Sigma)$ in the following sense. Define the restricted model ensemble

$$\mathcal{M}'(\Sigma, U) := \{f \in M(\Sigma) \mid \forall x \in X : \mathcal{J}(f)(x) \in U\} \subseteq \mathcal{M}(\Sigma).$$

with the solution operator $\mathcal{S}_{\mathcal{M}'(\Sigma,U)}(\cdot)$. Then $\forall x_0 \in X, x(\cdot) \in \mathcal{S}_{\mathcal{M}'(\Sigma,U)}(x_0) : \dot{x}(\cdot) \in \mathcal{S}_F(\dot{x}(0))$. On the other hand, the differential inclusion also covers solutions of non-autonomous ODEs $\dot{x} = f(x,t)$ with $\mathcal{J}(f)(x,t) \in U$ for all $t \in \mathbb{R}_+$. Linear-interval differential inclusions are more general than QDEs in the sense that they also include non-autonomous models, and are more specific in the sense that they only include bounded models.

When the state-transition graph G of the QDE is computed and a linear-interval differential inclusion F is defined, I propose the following procedure. The modeller takes a close look at the state-transition graph of the QDE and identifies subgraphs of importance, i.e. vertices with multiple successors (some of which may be problematic or preferable by value judgement). We want to identify conditions for a given successor to be reached. If there is an edge (v, w) in G, we know from section 2.2.1 (p. 21) that there is an initial valued $x_0 \in X$ and a solution $x(\cdot) \in \mathcal{S}_{\mathcal{M}(\Sigma)}(x_0)$ such that $[\dot{x}(0)] = v$ and it $\exists T > 0 : [\dot{x}(T)] = v \wedge w$ and $\forall t \in [0, T) : \operatorname{sgn}(\dot{x}(t)) = v$.

To describe these reachability conditions we define – in the velocity space – the cones $K(v) := \{\dot{x} \in \mathbb{R}^n \mid [\dot{x}] = v\}$ for $v \in \mathcal{A}^n$. For the linear-interval differential inclusion $\ddot{x} \in F(\dot{x}) = U\dot{x}$, the absorption basin $\mathrm{Abs}_F(\bar{K}(v), \bar{K}(v) \cap \bar{K}(w))$ of the closure of such cones contains all initial velocities $\dot{x}_0$ such that for all solutions $\dot{x}(\cdot) \in \mathcal{S}_F(\dot{x}_0)$ with $[\dot{x}_0] = v$ there exists a $T > 0$ with $\dot{x}(T) \in \bar{K}(v \wedge w)$ and $\forall t \in [0, T] : \dot{x}(t) \in \bar{K}(v)$. The results from the previous subsection can be used to compute this absorption basin with the viability kernel algorithm as outlined in section 2.4 (p. 45). If $\mathrm{Abs}_F(\bar{K}(v), \bar{K}(v) \cap \bar{K}(w))$ is empty, the edge (v, w) can be eliminated. Otherwise, the algorithm provides insights about the velocities for which a qualitative state is reached from another one. This can be valuable in the context of sustainability science, as such conditions yield early warning indicators of the form "once the rates of change are in such and such a relation, the following trend will necessarily reverse at a later time".

EXAMPLE 11: We present an application of the method, where the monotonic ensemble is described by the sign matrix

$$\Sigma := \begin{pmatrix} 0 & 0 & + \\ - & 0 & 0 \\ + & + & 0 \end{pmatrix}.$$

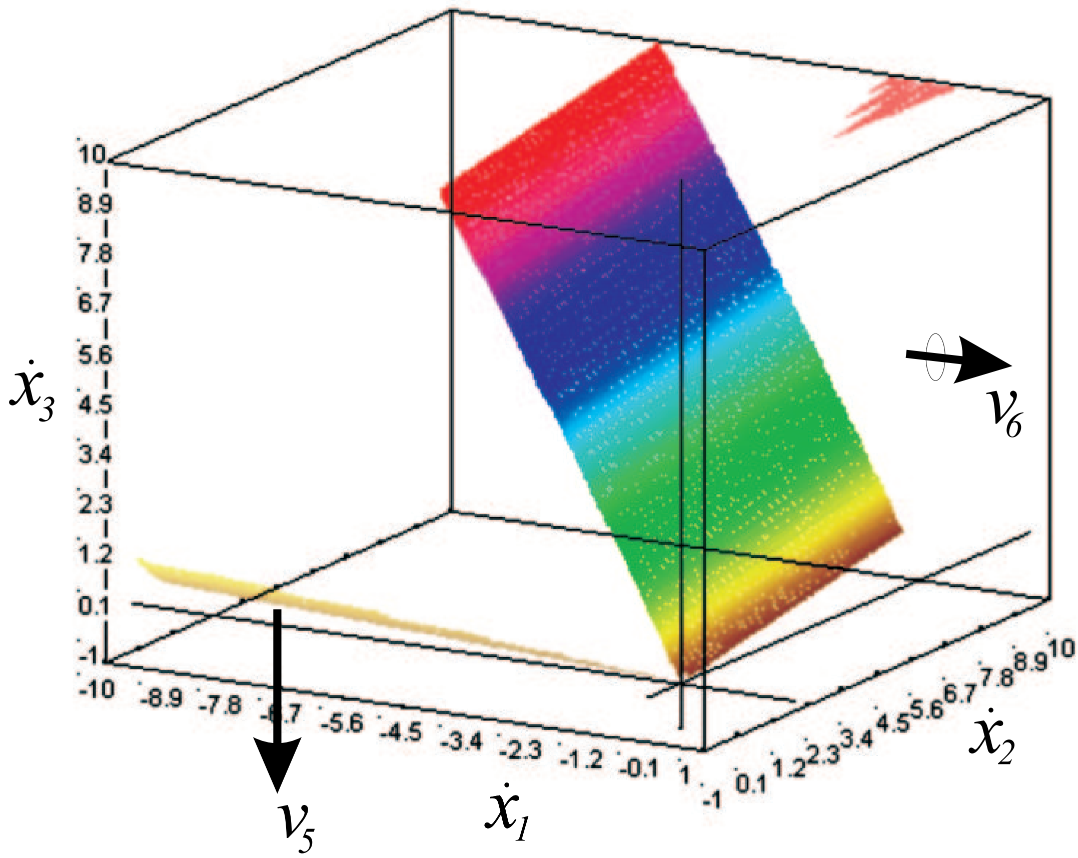

Figure 3.13: Boundaries of the absorption basins of v_3, with target v_5, v_6, restricted to a cube Q. $Abs_F\big(\bar{K}(v_3) \cap Q, \bar{K}(v_3) \cap \bar{K}(v_5) \cap Q\big)$ is a very small cone, whereas the boundary of $Abs_F\big(\bar{K}(v_3) \cap Q, \bar{K}(v_3) \cap \bar{K}(v_6) \cap Q\big)$ appears to be a plane separating a large part of the quadrant. The small part of the boundary to the upper right is an artifact resulting from restricting the absorption basin to Q, which can be eliminated due to PROP. 43 (p. 79).

The resulting graph after eliminating marginal edges (cf. section 3.2, p. 62) and non-analytical state (cf. section 2.2.4, p. 36) is shown in in Fig. 3.11. Supposing that quantitative information is available we set up an interval matrix

$$U := \begin{pmatrix} 0 & 0 & [0.7, 0.9] \\ [-0.7, -0.4] & 0 & 0 \\ [0.5, 3.0] & [0.5, 3.0] & 0 \end{pmatrix},$$

where the coefficients have signs corresponding to Σ. This defines the linear-interval differential inclusion $\ddot{x} \in U\dot{x}$. We now analyse two exemplary qualitative states $v_1 = ([-]\,[-]\,[+])^t$, $v_3 = ([-]\,[+]\,[+])^t$ in G where multiple successors occur (numbers in Fig. 3.11 correspond to indices). The computed absorption basins of state v_1 with targets v_2, v_3, v_4 are shown in Fig. 3.12. One absorption basin is empty. The boundaries of the other basins are smooth except along one ray from the origin. There are no combinations of velocities which safeguard that v_3 is reached, but there is a considerable likelihood that v_2 is a guaranteed successor. However, a large part of this quadrant necessarily leads to v_4. In state v_3, we have the successors v_5 and v_6. Since there is no edge (v_3, v_1) the corresponding absorption basin $Abs_F\big(\bar{K}(v_3)), \bar{K}(v_3) \cap \bar{K}(v_1)\big)$ (and even the respective capture basin) has to be empty. The size of the regions necessarily leading from v_3 to one of the outcomes is considerably different (Fig. 3.13). As both absorption basins of state v_3 intersect $K(v_1 \wedge v_3)$, in some cases the successor of v_3 can already be predicted at a time t, when $[\dot{x}(t)] = v_1$. If v_5 is reached, (which may be less likely as the absorption basin is significantly smaller than the other), the state-transition graph implies that the only possible subsequent qualitative transition is (v_5, v_3). $\square$