CORRECTION March 3rd 2014

MPRI C2-19 Examination, Part II, F. Fages
Model calibration with respect to Temporal Logic constraints: patterns and solvers

We consider the fundamental problem of calibrating an ODE model with respect to a temporal logic specification of the behavior of the system, observed in experiments. More precisely, we consider the following grammar of Linear Time Logic formulae with linear constraints over the Reals, LTL($\mathbb{R}_{\text{lin}}$):

$$\phi ::= \quad c \ \mid \phi \Rightarrow \psi \mid \phi \wedge \phi \mid \phi \vee \phi \mid \mathbf{X}\phi \mid \mathbf{F}\phi \mid \mathbf{G}\phi \mid \phi\mathbf{U}\phi \ \mid \phi\mathbf{R}\phi \mid \exists x \ \phi$$

where c denotes a linear constraint over molecular concentrations, their first derivative, and a set of variables $\boldsymbol{x}$, including the Time variable.
Timing constraints can be expressed with the time variable and free variables to relate the time of differents events. For instance, the formula

$$\mathbf{G}(Time \leq t_1 \Rightarrow [A] < 1 \wedge Time \geq t_2 \Rightarrow [A] > 10) \wedge (t_2 - t_1 < 60)$$

expresses that the concentration of molecule A is always less than 1 up to some time t_1, always greater than 10 after time t_2, and the switching time between t_1 and t_2 is less than 60 units of time.
We have seen in the course that the validity domains of the free variables of an LTL($\mathbb{R}_{\text{lin}}$) formula on a finite trace $(s_0, ..., s_n)$, can be computed by finite unions and intersections of the validity domains of the linear constraints, as follows:

$\mathcal{D}_{(s_0,...,s_n),\phi} = \mathcal{D}_{s_0,\phi}$,
$\mathcal{D}_{s_i,c(\boldsymbol{x})} = \{\boldsymbol{v} \in \mathbb{R}^k \mid \ s_i \models c[\boldsymbol{v}/\boldsymbol{x}]\}$ for a constraint $c(\boldsymbol{x})$,
$\mathcal{D}_{s_i,\phi\wedge\psi} = \mathcal{D}_{s_i,\phi} \cap \mathcal{D}_{s_i,\psi}$,
$\mathcal{D}_{s_i,\phi\vee\psi} = \mathcal{D}_{s_i,\phi} \cup \mathcal{D}_{s_i,\psi}$,
$\mathcal{D}_{s_i,\mathbf{X}\phi} = \mathcal{D}_{s_{i+1},\phi}$,
$\mathcal{D}_{s_i,\mathbf{F}\phi} = \bigcup_{j=i}^{n} \mathcal{D}_{s_j,\phi}$,
$\mathcal{D}_{s_i,\mathbf{G}\phi} = \bigcap_{j=i}^{n} \mathcal{D}_{s_j,\phi}$,
$\mathcal{D}_{s_i,\phi\mathbf{U}\psi} = \bigcup_{j=i}^{n} (\mathcal{D}_{s_j,\psi} \cap \bigcap_{k=i}^{j-1} \mathcal{D}_{s_k,\phi})$,
$\mathcal{D}_{s_i,\exists x\phi} = \Pi^x \mathcal{D}_{s_i,\phi}$,

where the projection operator Π^x returns the domain with all possible values for x.
This serves to compute a continuous violation degreee for a LTL($\mathbb{R}_{\text{lin}}$) formula with objective values v^* for the variables as the euclidian distance between the validity domain and the objective values:

$$vd^{v^*}_{s_i,\phi} = dist(\mathcal{D}_{s_i,\phi}, v^*)$$

Furthermore, a "robustness" degree can be estimated as the interior distance to the borders of the validity domain, i.e. as the distance to the complement of the validity domain:

$$ro^{v^*}_{s_i,\phi} = dist(\overline{\mathcal{D}_{s_i,\phi}}, v^*).$$

We are interested in finding more efficient algorithms for computing these values for some common patterns of LTL($\mathbb{R}_{\text{lin}}$) formulae. For instance, for the constraint

$$A \geq v$$

where v is a free variable, we have

$$\mathcal{D}_{s_i, A \geq v} =]-\infty, val_{s_i}(A)]$$

$$vd^{v^*}_{s_i, A \geq v} = max(0, v^* - val_{s_i}(A))$$

$$ro^{v^*}_{s_i, A \geq v} = max(0, val_{s_i}(A) - v^*)$$

where $val_{s_i}(A)$ is the value of A in state s_i,
For the reachability formula

$$\mathbf{F}(A \geq v)$$

we have

$$\mathcal{D}_{s_i, \mathbf{F}(A \geq v)} =]-\infty, max_{s_i}(A)]$$

$$vd^{v^*}_{s_i, \mathbf{F}(A \geq v)} = max(0, v^* - max_{s_i}(A))$$

$$ro^{v^*}_{s_i, \mathbf{F}(A \geq v)} = max(0, max_{s_i}(A) - v^*)$$

where $max_{s_i}(A)$ is the maximum value of A over the trace $(s_i, ..., s_n)$, which can be computed in one pass over the trace, in time $O(n - i)$.

Give similar expressions for the constraint $A \leq v$

$$\mathcal{D}_{s_i, A \leq v} = \quad [val_{s_i}(A),\ +\infty[$$

$$vd^{v^*}_{s_i, A \leq v} = \quad max(0,\ val_{s_i}(A) - v^*)$$

$$ro^{v^*}_{s_i, A \leq v} = \quad max(0,\ v^* - val_{s_i}(A))$$

Give similar expressions and justify them for the formula $\mathbf{F}(A \leq v)$

$$\mathcal{D}_{s_i, \mathbf{F}(A \leq v)} = \quad \bigcup_{j=i}^{n} \mathcal{D}_{s_j, A \leq v} \ = \ \bigcup_{j=i}^{n} [val_{s_j}(A),\ +\infty[\ = \ [min_{s_i}(A),\ +\infty[$$

$$vd^{v^*}_{s_i, \mathbf{F}(A \leq v)} = \quad dist([max_{s_i}(A),\ +\infty[,\ v^*) \ = \ max(0,\ min_{s_i}(A) - v^*)$$

$$ro^{v^*}_{s_i, \mathbf{F}(A \leq v)} = \quad dist(]-\infty,\ max_{s_i}(A)[,\ v^*) \ = \ max(0,\ v^* - min_{s_i}(A))$$

Give similar expressions for the formula $\mathbf{G}(A \leq v)$

$$\mathcal{D}_{s_i,\mathbf{G}(A\leq v)} = \bigcap_{j=i}^{n} \mathcal{D}_{s_j,\ A\leq v} = \bigcap_{j=i}^{n} [val_{s_j}(A),\ +\infty[= [max_{s_i}(A),\ +\infty[$$

$$vd^{v^*}_{s_i,\mathbf{G}(A\leq v)} = dist([max_{s_i}(A),\ +\infty[,\ v^*) = max(0,\ max_{s_i}(A) - v^*)$$

$$ro^{v^*}_{s_i,\mathbf{G}(A\leq v)} = dist(]-\infty,\ max_{s_i}(A)[,\ v^*) = max(0,\ v^* - max_{s_i}(A))$$

Give similar expressions for the amplitude constraint $\exists v(\mathbf{F}(A \leq v) \wedge \mathbf{F}(A \geq v + a))$

The vector of variables by the tuple (v, a) in this order.

$$\mathcal{D}_{s_i,\mathbf{F}(A\leq v)\wedge\mathbf{F}(A\geq v+a)} = \{(v,a) \in \mathbf{R}^2 \mid min_{s_i} \leq v \wedge max_{s_i} \geq v + a\}$$

$$\begin{aligned}\mathcal{D}_{s_i,\exists v\mathbf{F}(A\leq v)\wedge\mathbf{F}(A\geq v+a)} &= \Pi^v(\{(v,a) \in \mathbf{R}^2 \mid min_{s_i} \leq v \wedge max_{s_i} \geq v + a\}) \\ &= (\mathbf{R},\ ]-\infty,\ max_{s_i}(A) - min_{s_i}(A)])\end{aligned}$$

$$vd^{a^*}_{s_i,\exists v\mathbf{F}(A\leq v)\wedge\mathbf{F}(A\geq v+a)} = max(0,\ a^* - max_{s_i}(A) + min_{s_i}(A))$$

$$ro^{a^*}_{s_i,\exists v\mathbf{F}(A\leq v)\wedge\mathbf{F}(A\geq v+a)} = max(0,\ max_{s_i}(A) - min_{s_i}(A) - a^*)$$