Analytic Abduction from Qualitative Simulation

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Abstract

We describe how to obtain mathematical formulae capturing the approximate behaviour of simple dynamic systems. We call such formulae approximate functional solutions of the associated ordinary differential equation. We show how approximate functional solutions can be of greater practical utility than numerical, qualitative or even exact closed form representations of behaviour.

1. Introduction

Many types of dynamic system can be modelled using ordinary differential equations. Recently, there has been much interest in the A.I. community in reasoning about a dynamic system by reasoning from this underlying differential equation model. Current approaches fall on a spectrum ranging from numerical [Yip 87, Yip 88], interval [Berleant & Kuipers 88, Davis 87b] through qualitative [Forbus 84, de Kleer & Brown 84, Kuipers 85, Kuipers 86], order of magnitude [Raiman 86, Mavrovouniotis & Stephanopoulos 87, Dague *et al.* 87, Davis 87a] to exact analytic representations [Sacks 85a, Sacks 85b, Sacks 87, Sacks 88].

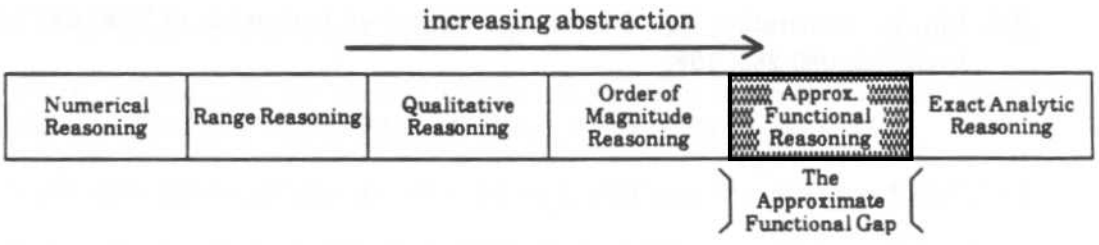


Figure 1. Spectrum of Reasoning Systems

In all these systems the principal emphasis is on correctness. We contend that this misses the whole point of why we were doing the analysis. In many engineering applications the major concern is to obtain a behavioural description which is 1) *comprehensible* and 2) of *practical use*. Such issues are the focus of this paper. We have developed a system which combines qualitative and mathematical reasoning to produce behavioural descriptions which emphasize comprehensibility, utility and adequacy rather than mere correctness. We call this level of description an approximate functional solution.

The first question to be addressed is what are the characteristics of a comprehensible, useful and adequate behavioural description?

1.1 Criteria for a Comprehensible Description

Comprehensibility is an elusive concept in part because it is dependent on one's education but also because it is necessarily subjective. A formal definition of what constitutes a "comprehensible" description is therefore a pipe dream. At the very least, however, we need to identify the class of individuals and their necessary educational background such that for them our behavioural descriptions will indeed be comprehensible. We chose college-educated engineers as our target audience.

We take it as an axiom that a college-educated engineer has a certain body of mathematical knowledge, is acquainted with physical concepts and knows how to interpret simple formulae in terms of those concepts. For example, the formulae would include forms such as exponentials and sinusoids and the physical concepts would encompass ideas such as half-life, completion time and frequency. We want to capitalize on the fact that a great deal of this information is in the form of clichés *i.e.* mathematical formulae which provoke an immediate and mandatory interpretation of the physical significance of their subterms. For example, if told that "t" represents time and given the formula "$\exp(-t/\tau)$" any engineer would immediately identify τ as a time constant. The prevalence of clichés suggests one principle: the behavioural descriptions we ultimately obtain should contain the kinds of interpretable sub-terms with which engineers are familiar. In practice this amounts to saying any behaviour is expressed as being "close" to one of a library of standard forms.

A second principle emerges from considering the tradition of approximation in engineering. Approximate descriptions are often found to be more easily comprehended than exact ones by stripping away the detailed relationships to leave only the most coarse trends. Such formulae, whilst still fully fledged mathematical descriptions are nevertheless rendered more comprehensible by their greater simplicity. So a second principle is that the formulae in our standard library should be fairly simple.

Both these principles can be summarized as "a mathematical formula is comprehensible if it is familiar and concise". We only admit a formula to our library of standard forms if it meets both these criteria.

1.2 Criteria for a Useful Description

Next we turn to the question of what constitutes a genuinely "useful" behavioural description. We claim the following criteria need to be met:

- The qualitative form should be easily accessible.
- The key functional relationships between system parameters should be explicit.
- The effects of perturbations should be easily computable.
- The timescale of processes in the model should be apparent.

Such features appear those most keenly sort by human engineers when performing "back of the envelope" calculations.

1.3 Criteria for an Adequate Description

Whilst we want to take the emphasis off fatuous accuracy it is, of course, important that any description we obtain should be adequate for predictive purposes. A general characterisation is difficult because it is intimately connected with the intended application *e.g.* in some cases accuracy to 10% is acceptable whilst for others accuracy to 1% is demanded. What we can ask, is that the user be able to assert a required tolerance and then allow the system to enforce accuracy to this value.

However, as we are deliberately avoiding exact methods of solution we can hardly base our estimate of adequacy by direct comparsion of the approximate solution with the exact one. Consequently, in practical terms the criteria for an adequate solution need to be:

- The adequacy of the behavioural description should be verifiable by an indirect procedure.
- The description lies within the tolerance bound.

1.4 Failure of Previous Methods

Neither exact nor qualitative behavioural descriptions are guaranteed to meet either the comprehensibility or utility criteria. For example, here are just some of the ways in which exact descriptions can fail.

- *Impossible*. Many differential equations have solutions which can only be written as an infinite series. Extracting the qualitative properties, the coarse functional relationships and the effects of perturbations from such a representation is extremely difficult.
- *Impenetrable*. Moreover, even when the equations can be solved in closed form, the ultimate formula can be so unweildy and involve such esoteric functions that it is difficult to interpret its meaning.
- *Spurious impression of accuracy* Even after prodigious computation any so-called exact solution is only as good as the quality of the original model. In many cases, the apparent precision is fictitious as the real physical system may differ from the idealisations implicit in its mathematical model. In such circumstances it would be inappropriate to expend a great deal of effort in solving the equations exactly as there is no guarantee that it would lead to significant predictive power or physical insight.

Similarly the qualitative level of description does not provide the kind of information an engineer would typically want. Here are some of its problems:

- *Loss of quantitative timescale*. In a qualitative behavioural description, there is no notion of timescale, merely a total ordering on the distinguished time points. Thus it is impossible to tell whether a process completes in seconds, days or months.

- *Lack of functional relationships* The final output does not embody any information as to the functional relationships underlying the observed behaviour. At best it might be possible to infer a monotonic connection but this is rarely precise enough to be of use in engineering applications.

- *Low level state sequence description of behaviour*. Most qualitative reasoners specify behaviour as sequences of state transitions; a very low level representation. Whilst the ease with which such descriptions are comprehended is a much vaunted claim, there is little evidence to support this. In engineering applications one usually wants something more concrete than state sequence information.

The latter two criticisms apply equally to numerical integration methods.

These criticisms suggest that comprehensibility and utility have been sub-ordinated to positions of lesser importance than accuracy. What we are striving for is the kind of description an engineer might obtain after performing a back-of-the-envelope calculation; enough mathematical detail to capture the key functional dependencies and timescale yet not so cluttered with esoterica that the overall structure is swamped in detail.

2. Pathways to Approximation

There are two basic ways, starting from an ordinary differential equation, to build an approximate functional solution. One way is to solve the equation exactly and approximate the resulting expression and the other is to abstract the equation, reason in the abstraction space and map what is learnt back to the mathematical level.

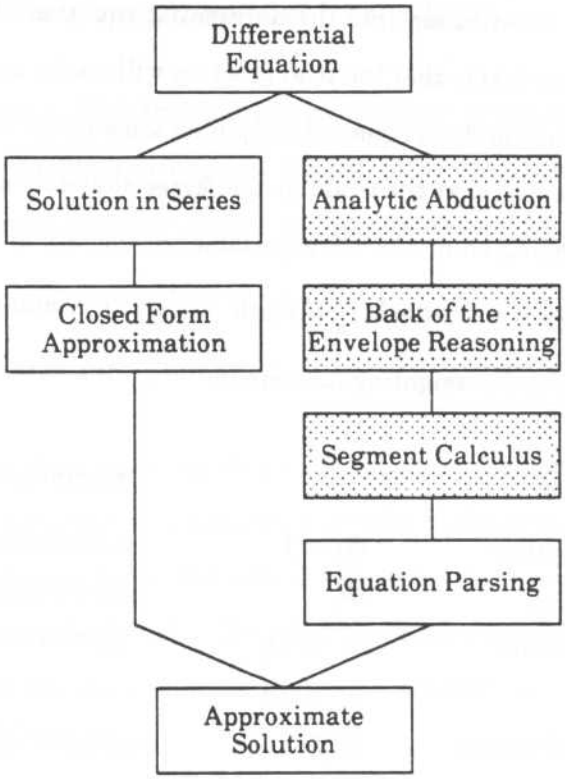


Figure 2. Pathways to Approximation

In my thesis [Williams 89] I develop both approaches. In this paper I shall focus on the second. The principal technique is called analytic abduction because it abduces an analytic function from a qualitative behaviour but we shall also mention two ancillary techniques, back-of-the-envelope reasoning and segment calculus.

3. Traditional Weighted Residual Procedure

Such a philosophy of approximation is new to A.I. but not to the physical sciences. Engineers have long faced up to the difficulties of solving awkward differential equations which in fact constitute the majority arising in real world problems. One technique, known as the method of weighted residuals works as follows: A "trial function" (*i.e.* a guess at the solution) is constructed from a finite sum of orthogonal polynomials containing adjustable parameters. If, by chance, we had guessed the right

solution then on substitution into the differential equation all terms would cancel out identically. However, it is more likely that the trial function will not be an exact solution. In this case, when the substitution is made and the equation simplified some terms will remain. These so called "residuals" must be minimized to make the trial function agree as closely as possible with the exact solution. This is achieved by finding values for the adjustable parameters in the trial function such that a weighted integral involving the residual, $\int_a^b \omega_i R_e \, dt \; / \; \int_a^b \omega_i \, dt$ is minimised. Different methods obtain from different choices for the weighting function ω_i:

Method	ω_i	**Explanation**
Collocation	$\delta(t-t_i)$	a Dirac delta function
Galerkin	Φ_i	an orthogonal polynomial
Subdomain	1 $t \in D_i$	a square hump
	0 $t \notin D_i$	
Least Squares	$\partial R_e / \partial t_i$	the partial derivative of the residual

If, after optimization the approximation is still inadequate then higher members from the family of orthogonal functions are added to the trial function and the cycle repeated.

4. Failure to Satisfy the Comprehensibility and Utility Criteria

For our purposes this approach is not immediately useful as the description it yields violates most of the criteria we set down at the outset: the qualitative form of the sum is difficult to gauge; the coarse functional information is absent, it does not conform to a cliché because the sum could contain arbitrarily many terms. The easiest way to fix this is to find a good single-term trial function in the belief that the qualitative properties of such an object may more easily be comprehended than those of a sum of orthogonal polynomials.

5. Knowledge Based Weighted Residual Procedure

This introduces a new difficulty. With the algorithmic approach we can choose a set of basis functions arbitrarily so long as they form an orthogonal family. However, if we want to make single-term approximations we had better pay due regard to the qualitative properties of the *exact* solution (whatever it may be).

5.1 A Model Intended for Manual Application

Acton & Squire [Acton & Squire 85] present a model, intended for manual application, of an approximation procedure whose first step is to conjecture the qualitative form of the solution which is then used to constrain the search for a plausible, single-term trial function. This model is based on years of practical experience in "solving" awkward differential equations and teaching the acquired heuristics to undergraduate engineering students. Their emphasis, like ours, is on comprehensibility and utility rather than fatuous accuracy.

5.2 Automation & Extension of the Model

However, for our purposes, Acton & Squire's model is deficient in three respects:

1) The initial step consists of guessing the qualitative form of the behaviour. This difficult point is finessed by appealing to the reader's "physical intuition". A machine however, needs to be able to compute the properties explicitly. Moreover, unless we give the machine extensive knowledge about the physical world we will need to derive this qualitative information *from* the differential equation.

2) There is no advice given as to what to do in the event of the first trial function proving to be inadequate. In contrast, our extended model has three repair strategies (discussed below).

3) Finally, the control of mathematical manipulation is simply a non-issue for Acton & Squire because they can rely on the pre-existing abilities students bring to the

problem. For the computer, faced with a multitude of legal manipulations, choosing which one to pursue is a difficult problem.

The solution we advocate combines qualitative simulation (a reconstructed **QSIM** algorithm [Kuipers 85, Kuipers 86a]) with algebraic manipulation (an extended **PRESS** algorithm [Bundy & Welham 81, Bundy 83, Bundy & Silver 81, Bundy & Sterling 81, Sterling *et al.* 82]) in the context of a goal directed problem solver. As the resulting technique conjectures an analytic function from a qualitative behaviour we term it **analytic abduction**.

QSIM is used to envision the qualitative properties of an exact solution and **PRESS** to control the subsequent mathematical manipulations. It is conceivable that the qualitative description of the behaviour could be obtained by other means *e.g.* by considering an ensemble of numerical integrations. However, the advantages of using **QSIM** are twofold: first, its behavioural predictions are provably complete *i.e.* guaranteed to include all qualitatively distinct modes of system behaviour and second, it works solely with the differential equation.

PRESS [Bundy & Welham 81, Bundy 83, Bundy & Silver 81, Bundy & Sterling 81, Sterling *et al.* 82] is a program which solves algebraic equations of the standard demanded by 'A' level (college entrance) mathematics courses. **PRESS** exploits the distinction between reasoning *about* an equation and reasoning *with* it. The former type of reasoning is called meta-level inference and the latter object-level inference. The key insight is that inference at the meta-level can be used to guide that at the object level.

The meta-level description of an equation is in terms of features such as the position or number of occurrences of a variable. This information is used to verify the preconditions for the invocation of various strategies for solving the equation. These include *isolation* (which solves equations containing a single occurrence of a variable by applying the inverse function to both sides), *collection* (which reduces the number of occurrences of an unknown in an equation thereby often enabling *isolation*) and *attraction* (which, as a preparatory step for *collection*, brings the occurrences of an unknown closer together).

PRESS has no notion about the relative magnitudes of the terms it manipulates. Consequently, we extended the orignal with a heuristic algebraic simplifier called **BOTHER** (for **B**ack-**O**f-**TH**e-**E**nvelope-**R**easoner).

We present the overall algorithm and then describe the operation of its parts in the context of a running example. Note that although this problem is taken from the Acton & Squire text, their proposed solution turns out to be an inadequate approximation. In contrast our system solves the problem without user intervention by invoking various repair strategies. This example therefore demonstrates not only the automation of the analytic abduction procedure but also the greater power of the underlying algorithm.

5.3 Analytic Abduction Algorithm

Given an ordinary differential equation and an intial state description, the goal of analytic abduction is to predict an approximate functional solution. The method consists of abstracting the equation to qualitative constraints, finding a qualitative form for the solution, constraining the search for a plausible trial function using knowledge of the qualitative form, optimising the trial function with respect to the differential equation and finally verifying its adequacy. If inadequate, the trial function is modified and the cycle repeated. This is summarized in figure 3b.

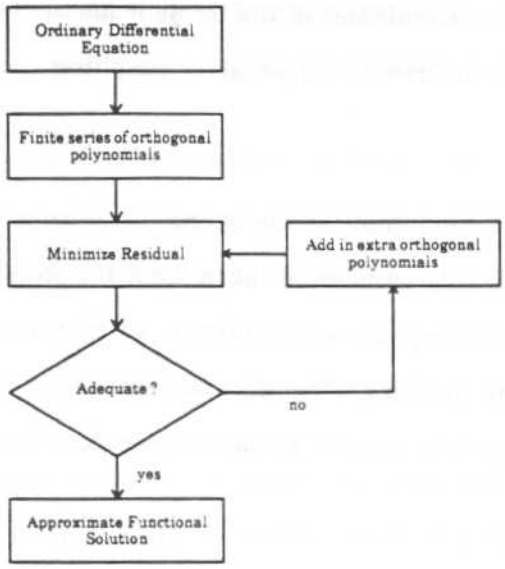


Figure 3(a).
Traditional Weighted Residual Algorithm

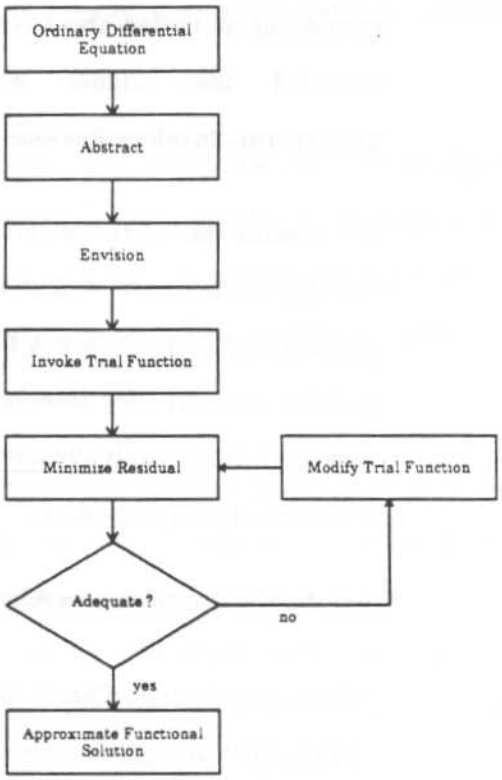


Figure 3(b).
Analytic Abduction Algorithm

6. Running Example

Consider a chemical reaction in which a molecule of substance A combines with two of B to make the product C. Mathematically the rate equation is

$$dn_c/dt = K*(n_a - n_c)*(n_b - 2n_c)^2 \qquad (1)$$

This can be solved using elliptic integrals to yield [Acton & Squire 85]:

$$t = (1/K)[\ (1/(2n_a - n_b))((1/(n_b - 2n_c) - 1/n_b) + (2/(2n_a - n_b)^2)(\log_e[(1 - (2n_c/n_b))/(1 - n_c/n_a)]\ ] \qquad (2)$$

However the question is, is this useful for most practical purposes? For example, how does the amount of product qualitatively vary with time? What determines the rate? What is the effect of increasing the initial concentration of substance A or B? What is a natural timescale for the reaction? Such information is presumably embodied in the solution somehwere but it is not immediately accessible. Let's look at analytic abduction applied to this system.

6.1 Abstraction

The first step is to map the functions in an ordinary differential equation into their **QSIM** counterparts. This is done by bottom up parsing of the expression tree representation of the differential equation. Equation (1) is mapped to the constraint set:

$$\texttt{deriv}(n_c,\texttt{f1}) \wedge \texttt{mult}(2,n_c,\texttt{f2}) \wedge \texttt{add}(\texttt{f2},\texttt{f3},n_b) \wedge \texttt{mult}(\texttt{f3},\texttt{f3},\texttt{f4}) \wedge \texttt{add}(\texttt{f5},n_c,n_a) \wedge \texttt{mult}(\texttt{f5},\texttt{f4},\texttt{f6}) \wedge \texttt{mult}(K,\texttt{f6},\texttt{f1}) \quad (3)$$

6.2 Simulation

Qualitative simulation of this system of equations reveals that initially the rate of formation of C is high but gradually falls off as the number of free molecules of reactants declines.

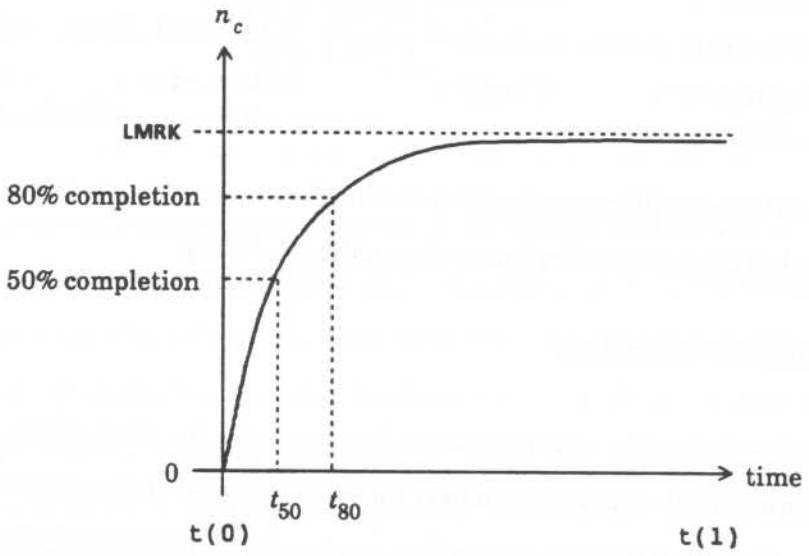


Figure 4. Qualitative Behaviour of the Chemical Reaction A + 2B → C

The qualitative behavioural description is thus

time	n_c	dn_c/dt
t(0)	<0,inc>	<[0,+inf],dec>
t(0,1)	<[0,+inf],inc>	<[0,+inf],dec>
t(1)	<LMRK,std>	<0,std>

Notice that LMRK is a newly discovered landmark value.

6.3 Behavioural Revision

Each behaviour is a sequence of tuples of qualitative states *i.e.* $\langle qval, qdir \rangle$ pairs for each system parameter. As simulation proceeds, new landmark values may be discovered and inserted between existing ones. Therefore, the landmark sets at the beginning and end of simulation may differ. We therefore revise the output into a globally consistent qualitative behaviour by propagating the knowledge of the new landmark values back through the state sequence. This turns out to be essential for efficient trial function invocation.

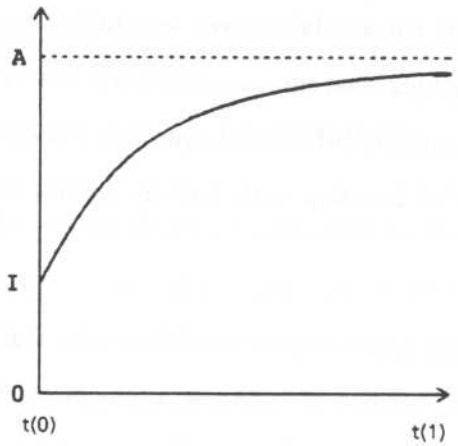
	Original		Revised	
	n_c	dn_c/dt	n_c	dn_c/dt
t(0):	[<0,inc>,	<[0,+inf],dec>]	[<0,inc>,	<[0,+inf],dec>]
t(0,1):	[<[0,+inf],inc>,	<[0,+inf],dec>]	[<[0,LMRK],inc>,	<[0,+inf],dec>]
t(1):	[<LMRK,std>,	<0,std>]	[<LMRK,std>,	<0,std>]

Knowledge of the newly discovered landmark value "LMRK" is propagated back to the earlier state over t(0,1) thereby tightening the bounds on the qualitative value.

6.4 Trial Function Invocation

The next task is to invoke a trial function hypothesis on the basis of the qualitative behavioural prediction. To do this it is necessary to have an explicit representation of the qualitative properties of each library entry. Each function is therefore represented in a manner similar to that shown below for the rising exponential function.

name: rising-exponential



rising exponential

function: `F = A - (A-I)*exp( - b*t)`

descriptor:
```
{t(0):   [<I,inc>,      <[0,+inf],dec>],
 t(0,1): [<[I,A],inc>, <[0,+inf],dec>],
 t(1):   [<A,std>,      <0,std>]}
```

consequences:
```
{A>I,
asymptotic-approach(F,A),
horizontal-shift(0),
vertical-shift(I),
vertical-scale(A),
is-infinite(t(1))}
```

parameters: `[b]`

Matching occurs by attempting to unify the revised qualitative behavioural description of the exact solution with the descriptor template of each library entry. If an entry is found which does unify with the qualitative behaviour then they must share the same sequence of critical points, convexities and bounding intervals. Such a function therefore makes a plausible trial function hypothesis. For example, the rising exponential unifies with the behaviour of the chemical system provided `I = 0` and `A = LMRK`. Notice that it was necessary to revise the qualitative behaviour produced by `QSIM` so that the intervals were specified in a way consistent with the syntax for library descriptor templates.

6.5 Optimization

As the exact solution is not available (even as a table of numerical data) the trial function cannot be optimised directly (*e.g.* by a least squares procedure). Instead, the optimisation must be done indirectly *via* its "fit" with the original differential equation. This is accomplished by finding values of the free parameters in the trial function such that it agrees as closely as possible with the differential equation.

We have implemented two methods for doing this: Collocation (for non-oscillatory systems) and Harmonic Balance (for oscillatory systems). Other methods are possible [Crandall 56] but all involve the calculation of integrals and consequently have a higher computational overhead. For the purpose of this paper we will ignore harmonic balance.

Collocation works by making the trial function satisfy the differential equation at as many points as there are adjustable parameters in the trial function. If we assume that the real solution does not stray too far from the trial function in between these points (a common engineering inference *c.f.* drawing a smooth curve through data) then the trial function will be a reasonable approximation of the true solution.

Although we do not know the formula of the exact solution we do know its range expressed in terms of the landmark values from the qualitative simulation. We can therefore find a value of the exact solution expressed as a fraction of the range. By equating the trial function to a fraction of the range we implicitly determine a time, expressed in terms of the adjustable parameters and landmarks, at which the trial function and exact solution agree. By substituting this value into the residual equation we can then find an expression for the adjustable parameter such that the residual equation is satisfied at this particular time. For example, in the present case, the trial function is

```
F = A - (A-I)*exp( - b*t)
```
(4)

(instantiated and simplified to n_c = LMRK(1 – exp(– bt) with LMRK = $\frac{1}{2}n_b$) and the function ranges between the initial point I (=0) and the asymptotic value A (=LMRK). Hence, we could collocate at 50% through the change by setting

$$F_{50} = A - (A-I)*\exp(- b_{50}*t_{50}) = (A+I)/2 \quad (5)$$

or at 80% through the change by choosing

$$F_{80} = A - (A-I)*\exp(- b_{80}*t_{80}) = 4(A+I)/5 \quad (6)$$

Or anywhere else we please. The precise choice of collocation points is, in principle, arbitrary in the sense that, for a good trial function approximation, parameter values computed at different collocation fractions will be the same. However, better results might be expected if "representative points" are chosen *i.e.* points neither too close together nor too near to the boundaries and preferably in the vicinity of maximum change in the function. Therefore, bounding the range of the trial function between **min** and **max** we invent two heuristics to guide the choice of collocation fractions:

Heursitics for Choosing Collocation Fractions

coverage heuristic:	the collocation fractions should be roughly evenly distributed over (**min, max**) or
curvature heuristic:	weighted towards the region of maximum curvature

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Turning to the particular example, the collocation equations are used to derive a numerical substitution for the time dependent sub-term *viz*:

$$\exp(- b_{50}*t_{50}) = 1/2 = c_{50}$$

and

$$\exp(- b_{80}*t_{80}) = 1/5 = c_{80}$$

Although it is possible to isolate t_i by inverting the exponential, this will be unnecessary as derivatives of the exponential function (linear in t) do not generate t in isolation. Hence when this trial function is substituted into the original differential equation, which did not contain time dependent

coefficients to begin with, t will never appear outside the exponential. Other trial functions, however, such as an exponential quadratic in t, *i.e.* $\exp(-bt^2)$, *will* have to be inverted to find t explicitly as their derivatives do generate new terms in t. Conceptually it is best to imagine that t is always isolated.

To save subsequent work the system replaces the sub-term substitutions with the indexed "c" symbol. The motivation is that when the adequacy of the approximation is being assessed the same general formula for a parameter can be used and the different numerical substitutions (the c_i) simply swapped in. This makes the verification stage much more efficient.

Having obtained the numerical substitutions the system then computes the residual equation. In this case, the original differential equation was

$$dn_c/dt = K*(n_a - n_c)*(n_b - 2n_c)^2$$

and the residual equation therefore becomes

$$^1/_2\, n_b\, b_i\, c_i = K*(n_a - {}^1/_2\, n_b(1 - c_i))\, n_b{}^2\, c_i{}^2$$

The adjustable parameter b_i may now be isolated by **PRESS** to yield

$$b_{50\%} = K*n_a*n_b*(1 - {}^1/_4(n_b/n_a))$$

$$b_{80\%} = ({}^2/_5)*K*n_a*n_b*(1 - {}^2/_5(n_b/n_a))$$

In other cases we need the extended version of **PRESS** which is able to bound expressions containing symbolic constants of unknown absolute value. But for clarity we will ignore this in the present paper.

Although the numerical substitutions for sub-terms are easily computed it is more efficient to record them as collocation schemata which are invoked whenever the corresponding function is conjectured. This means that as soon as a trial function is hypothesised, the variables in it are automatically instantiated to the appropriate landmark symbols and its derivatives and substitutions for various collocation fractions are retrieved. Although this may seem rather rigid remember that the choice of

collocation fractions is, theoretically speaking, arbitrary so there is little to be gained performing unnecessary symbolic manipulation at run time.

6.6 Verification

Once the trial function has been optimized it is necessary to determine whether it is an adequate approximation. Had the exact solution been chosen the optimum parameter values would be independent of the choice of collocation fraction. Hence one measure of the accuracy of the approximation is the degree to which the optimum values are sensitive to collocation fraction. This is simple to determine by selecting alternative random collocation fractions and computing the ratio of optimum parameter values obtained at different collocation fractions. If this ratio exceeds a factor of 2 either way, the trial function is deemed to be inadequate.

In the current example, the value of b computed at 50% and 80% completion are

$$b_{50\%} = K*n_a*n_b*(1 - {}^1/_4(n_b/n_a))$$

$$b_{80\%} = ({}^2/_5)*K*n_a*n_b*(1 - {}^2/_5(n_b/n_a)).$$

Hence their ratio is

$$b_{50\%}/b_{80\%} = ({}^5/_2)*(1 + ({}^3/_{20})(n_b/n_a))$$

As $b_{50\%}/b_{80\%} > 2.5$, the hypothesis that $n_c = \text{LMRK}*(1 - \exp(-bt))$ must be rejected. The complete chain of reasoning is described in [Williams 89].

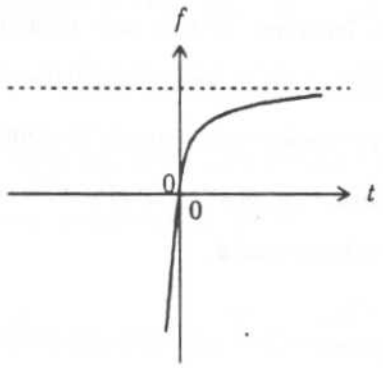
6.7 Modification

In the event of a trial function proving to be an inadequate approximation, it can be modified in one of three ways:

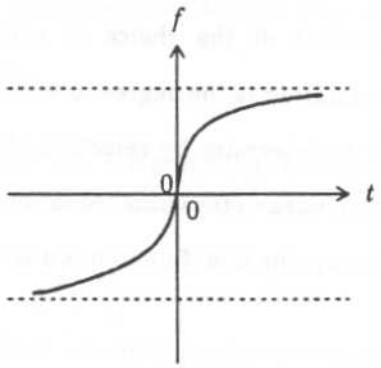
- replaced by a *congruent* trial function
- replaced by an *almost everywhere congruent* trial function

- replaced by an *exaggerated* trial function

The first repair strategy trivial. The second and third work by sacrificing agreement at the initial state in favour of a better fit overall. Almost congruent trial functions differ only in the sign of the curvature at the initial time point. For example, the tanh(bt) is almost everywhere congruent to 1–exp(–bt)) for $t \geq 0$.



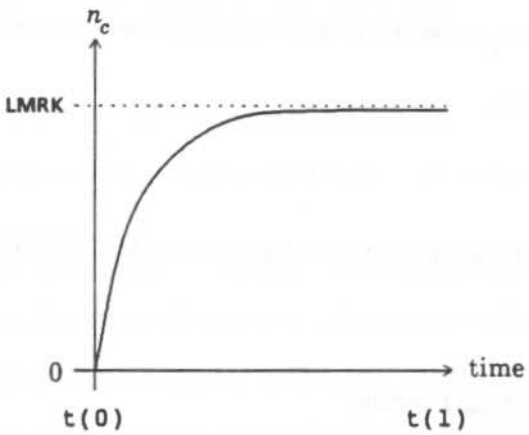
$f = (1\text{-}\exp(\text{-}bt))$



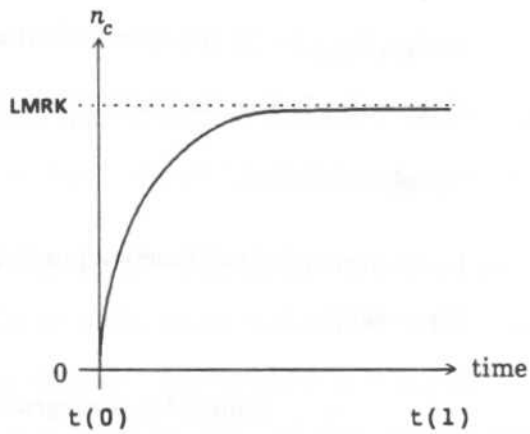
$f = \tanh(bt)$

The rationale being that a negligible positive or negative curvature can be approximated by zero.

Exaggerated trial functions differ only in the magnitude of the gradient at the initial time point. For example, the function $f =$ LMRK$(1 - \exp(-at^b))$ $(b<1)$ differs from $f =$ LMRK$(1 - \exp(-bt))$ in having a positive infinite initial gradient instead of a positive finite one..



$n_c =$ LMRK $(1 - \exp(-bt))$



$n_c =$ LMRK $(1 - \exp(-at^b))$

The rational in this case is that a large finite gradient is effectively infinite.

Despite the error incurred in satisfying the initial condition, almost everywhere congruent or exaggerated trial functions are sensible alternatives to pursue because the fit overall may be better. Information pertaining to timescale and gross functional relationships over most of the behaviour will in that case still provide valid information.

For simplicity in our running example I will ignore the procedure by which congruence and almost everywhere congruence fail in their attempts. So, suppose we are now at the point of trying to find an exaggerated trial function *i.e.* a function whose qualitative form at t(0) is shown below

	time	function	derivative
original	t=t0	<0,inc>	<[0,+inf],dec>
exaggerated	t=t0	<0,inc>	<+inf,dec>

Such a qualitative behavioural description unifies with the function descriptor of a rising exponential with polynomial exponent. Hence, the new conjecture becomes

$$n_c = \text{LMRK}(1 - \exp(-at^b))$$

Notice that this contains two adjustable parameters and so we need to choose three collocation points (two to set up simultaneous residual equations and one extra for verification purposes). However, conceptually the procedure is exactly as before. The new residual equations become (for collocation fractions c_i: $i = 33\%, 50\%, 80\%$):

$$a^{(1/b)}(\log_e(1/c_i)^{1-1/b} = 2Kn_a n_b c_i (1-(n_b/2n_a)(1-c_i)$$

BOTHER solves these simultaneously to yield

$$b = 0.51$$

$$a = 0.78*(2Kn_a n_b)^{0.51}[1 - 0.28(n_b/2n_a)]$$

Computing the ratio of parameter values computed at any two collocation fractions now yields a result close to one. Hence, the trial function n_c = LMRK(1–exp(–at^b)) is an adequate approximation to the behaviour of the chemical system.

7. The Payoff

What has been gained from doing this? To answer this consider the criteria laid down at the outset. We said we wanted:

- qualitative form
- key functional relationships
- an estimate of the timescale

The approximate functional solution meets all three criteria: the qualitative form is explicitly available from the analytic abduction procedure; n_c rises from zero approximately exponentially to attain the final value $\frac{1}{2}n_b$; if n_a is increased the reaction will reach completion quicker; the timescale is inversely proportional to $\sqrt{(n_a n_b)}$ modulated by a slowly varying term in n_b/n_a. These commonsense engineering inferences were buried under the complexity of the exact solution (equation (2)). Hence for all practical purposes the approximate functional solution is more useful.

8. Limitations

Notwithstanding its successes, analytic abduction can fail in a number of ways. There are three categories of limitations.

8.1 Limitations Inherited from QSIM

First we inherit the limitations of the QSIM algorithm. For example, we cannot deal with systems containing time dependent coefficients *e.g.* forced oscillators. Second, spurious behaviours will often be generated [Kuipers 86, Struss 88a]. Third the number of qualitatively distinct behaviours can become large. Attempts have been made to eliminate the spurious behaviours [Lee & Kuipers 88, Berleant & Kuipers 88, Struss 88b] and to contain the size of the envisionment [Kuipers 87, Kuipers & Chiu 87] but more still needs to be done.

8.2 Limitations Instrinsic to Analytic Abduction

A second limitation is that the library of "known" functions is finite whilst the number of qualitatively distinct functions is infinite. Hence, there must be many functions (in fact an infinite number!) which are unrecognisable. The situation is not too bleak if we refer to the basic motivation: comprehensibility. It isn't that important that we can't think of a simple function characterisingv a behaviour with 64 turning points or whatever! Neither would a real engineer.

What is important is to decide what to do with behaviours containing more critical points than any function known to the standard library. We make two technical suggestions: smoothing and segment calculus.

If we know of order of magnitude assertions between landmark values it may be possible to "smooth" a qualitative behaviour by reducing the number of critical points it contains. For example, the final curve in figure 5 is a smoothed version of either of the curves to its left.

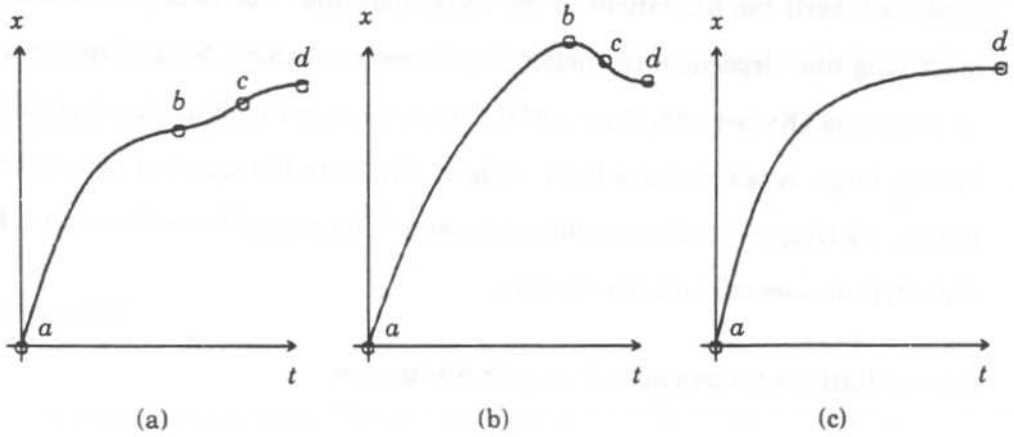


Figure 5. The Effects of Smoothing a Behaviour

A second idea, which is fully implemented, is that of segment calculus. In this technique, a complex behaviour, containing *n* critical points, is explained as the interaction of two simpler behaviours (*i.e.* each containing less than *n* critical points) under addition, multiplication, composition or exponentiation. For example, figure 6 shows how a "hump" may be explained as the interaction of something like a half-parabola multiplied by something like a decaying exponential.

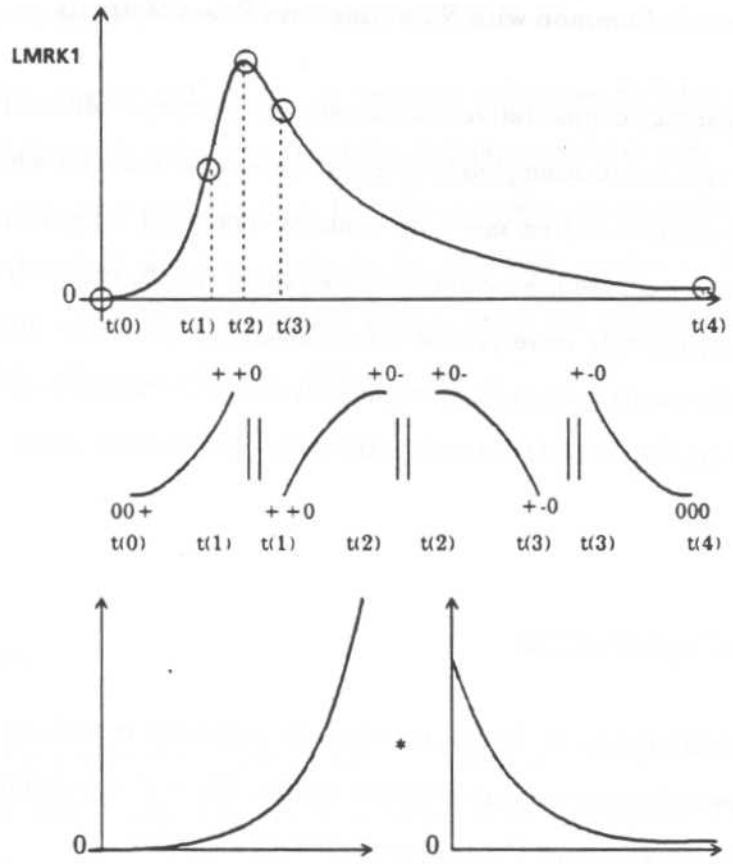


Figure 6. Explaining Behaviours as Interactions

In order to explain a whole behaviour, it is partitioned into its component monotone segments, each is explained separately and then the partial results are stitched together. Each separate explanation consists of a left segment, s_i^k, an operator, **R**, and a right segment, s_j^k. The intended interpretation is that the observed segment can arise from the interaction of segments s_i^k and s_j^k under **R**. Once all possible explanations of every component of the input behaviour have been found, an explanation spanning the whole input behaviour can be built by concatenating members of consecutive left explanations and consecutive right explanations in all legal ways. Eventually this process finds all possible spanning interpretations.

Oscillators introduce an additional complication because the phase of some compound oscillator (*e.g.* $\exp(-t)*\cos(t)$) may not match that of the simpler one (in this case $\cos(t)$). However, segment calculus can accomodate these too.

8.3 Limitations in Common with Numerical and Exact Methods

The major advantage of qualitative simulation over the more traditional mathematical approaches is that it can reason about incompletely specified systems *i.e.* those for which some coefficient is known only to be monotonic and no more. By contrast numerical integration, symbolic integration and analytic abduction all require complete mathematical specifications. However, the payoff is that one can say correspondingly more precise things about the behaviour. In the real world an engineer, confronted with partial information might well use his intuition to guess an approriate functional form for some coefficient and then explore the consequences of the choice.

9. Areas of Application

Analytic abduction has so far been tested on equations describing chemical kinetics, unforced oscillation, particle scattering and damped motion. We envisage applications in design support and intelligent tutoring systems. Consider the following scenarios.

9.1 Intelligent Tutoring Systems

We envisage a physics tutoring system. Suppose one of the aims of the system is to encourage correct "physical intuitions". This is an elusive quality. In current Intelligent Tutoring Systems [Wenger 87] it is, at best, assumed to be induced by exposure to an apposite problem set. More often, it is ignored in favour of inculcating problem solving schemata.

We want to address a student's intuitions head-on and foresee approximate functional reasoning as a valuable tool for this application. In this scenario, the tutoring system would derive a rough approximate functional solution to some problem and the student would be asked to suggest justifications for both its qualitative features and its functional relationships. This would encourage thought about the relative importance of competing processes as well as general physical principles. Moreover, if the system were then to proceed to solve the problem exactly, the student could then compare his or her intuitive predictions with the exact behaviour.

9.2 Design Support Systems

Second, in a design support application, we envisage a designer defining a model of a device and submitting it to approximate functional reasoning to determine its principal features. This may prove to be better than numerical techniques as there is an explicit proposal for the principal functional dependencies. Moreover, it may prove to be better than exact symbolic solution as the differential equations corresponding to the device models may be extremely difficult, if not impossible, to solve exactly or perhaps would not possess a closed form solution.

10. Conclusions

It is our belief that engineering support tools should focus on what a college-educated engineer actually needs in order to build an approximate mathematical description of behaviour. This is a level of description engineers typically communicate with and is meaningful to them by emphasising comprehensibility and utility over fatuous accuracy.

Analytic abduction presents one way of building such approximate solutions which exploits knowledge of the qualitative form of the exact solution to constrain the search for a plausible trial function which may then be optimized with respect to the differential equation.

Analytic abduction is founded on an extension and formalization of Acton & Squire's model of approximate engineering inference. Their model was intended for manual application assuming a certain level of mathematical facility. Consequently it ignored the mechanisms by which the qualitative behaviour of a system was envisioned and the control of subsequent mathematical inference (especially the incorporation of order of magnitude reasoning). Moreover, it failed to explain what to do in the event of the first trial function proving to be inadequate.

Analytic abduction addresses all these problems. As this permits automation of a procedure taught to undergraduate engineers we believe it holds the promise of becoming a genuinely useful tool.

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Combined Qualitative and Numerical Simulation with *Q3**

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Abstract

Combining numerical and qualitative simulation into one technique allows simulation to be performed even when there is insufficient information for a numerical simulation. Predictions are also guaranteed correct. Also, numerical simulations predict just one behavior; combined simulations can predict more than one when this is warranted. Thus, combined simulation is an improvement over numerical simulation.

Combined simulation is also an improvement over qualitative simulation. Qualitative simulation provides weak predictions, because it relies on weak model descriptions. Combined simulation allows adding numbers to model descriptions, resulting in stronger and potentially more practical predictions.

Q3 is a system for doing combined simulation. It uses intervals to express partial information about values, because intervals can express values anywhere from fully specified numbers, to partially specified numbers, to very vague qualitative values. Q3 also explicitly represents qualitatively significant values, like qualitative simulation, and other values, like numerical simulation. Thus, Q3 represents, and reasons, in ways that neither numerical simulation nor qualitative simulation do alone.

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