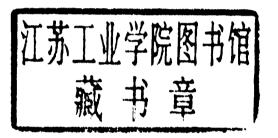
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Expert Systems for
Engineering:
Classification,
Education and Control

Editors: D. Sriram R.A. Adey





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PREFACE

Following the success of the 1st International Conference on Applications of Artificial Intelligence in Engineering Problems held in Southampton U.K. in April 1986, the second meeting was held in Cambridge, Massachusetts, U.S.A. in August 1987. This book contains a collection of the papers presented at the Conference in the area of Knowledge Based Expert Systems for classification, education and control.

The theme of the Conference and the selected papers was the application of Artificial Intelligence technology in engineering. Engineering research and development have provided powerful analytical and computational tools which have revolutionised the way in which products can be designed, tested and manufactured. However, engineering cannot be simply described by numerical models and algorithms; it involves knowledge, reasoning, heuristics and interpretation in addition to many other factors. Artificial Intelligence technology is now emerging from the research laboratory and promises to provide the same level of success as the numerical models have had with the representation of physical systems.

The papers published represent only approximately half of the total number of papers submitted for the Conference. The editors would like to express their thanks to Professor J. Gero, Dr M. Tenenbaum and Dr R. Milne and also to the International Advisory Board for their invaluable advice in the review and selection of the papers. This thorough process we believe has significantly added to the success of the Conference and the value of this book. Finally, we would like to thank all the authors for their contributions.

The Editors

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Qualitative Sketching of Parameterized Functions

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ABSTRACT

This paper describes a qualitative sketcher called QS that draws families of parameterized real univariate functions. It is useful because sketches provide better insight into global behavior than verbal or other descriptions. Existing graphics packages cannot plot parameterized functions because they require exact numerical values. Also, they cannot recognize discontinuities, singularities, and asymptotes or graph infinite domains. QS avoids these limitations by constructing and manipulating global models of functions. It can sketch functions that arise in pharmacokinetics, probability theory, circuit analysis, and other domains.

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This research was supported (in part) by National Institutes of Health Grant No. R01 LM04493 from the National Library of Medicine and National Institutes of Health Grant No. R24 RR01320 from the Division of Research Resources.

INTRODUCTION

This paper describes a qualitative sketcher called QS that draws families of parameterized real univariate functions. Qualitative sketching focuses on the high-level attributes of functions, such as extrema and discontinuities, without specifying exact values at every point. At this level of abstraction, a few sketches generally suffice to describe entire families of parameterized functions. For example, the family $f_a(x) = e^{ax}$ requires the three sketches shown in Figure 1, corresponding to a negative, zero,

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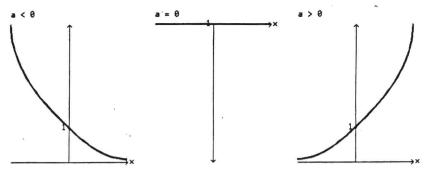


Figure 1: The qualitative sketches of e^{ax}

and positive. Qs helps its users understand the global behavior of parameterized functions by generating all possible sketches.

Qs can plot a much wider class of functions than conventional graphics packages. It handles parameterized functions with infinite domains and unbounded values, whereas conventional plotting programs require bounded numeric functions on finite domains. Also, Qs explicitly recognizes discontinuities, singularities, asymptotes, and periodicity. To sketch a parameterized function with a conventional graphics package, one must plot it for several values of each parameter and inspect the results for possible asymptotes, discontinuities, and singularities. The user must guarantee that his choices of specific parameter values generate all qualitatively distinct cases and that his choice of domain includes all interesting behaviors. He must also decide what ranges of parameter values produce the same abstract behavior. Sketching a parameterized function with Qs is equivalent to sketching all of its infinitely many instances and collapsing the results into qualitatively equivalent sets.

The next section contains a brief overview of the mathematical reasoner that the sketcher uses. In the following two sections, I describe the sketching algorithm and discuss applications in pharmacokinetics, probability theory, utility theory, and circuit analysis. The final section consists of a summary, a discussion of related work, and proposed extensions.

THE MATHEMATICAL REASONER

The qualitative sketcher uses the QMR mathematical reasoner¹ to derive the properties of parameterized functions. QMR handles a large class of functions on the real numbers, including the extended elementary functions: polynomials and compositions of exponentials, logarithms, trigonometric functions, inverse trigonometric functions, absolute values, maxima, and minima. It infers their qualitative properties: signs of the first and second derivatives, discontinuities, singularities, and asymptotes,

which it records in data structures called *Q-behaviors*. For example, the Q-behavior for the function $(x-a)^{-1}$ appears in Table 1.

Table 1: The Q-behavior of
$$f(x)=(x-a)^{-1}$$

$$f(x) \quad (x-a)^{-1}$$
 sign of $f'(x)$ negative on $(-\infty,a)$ and (a,∞) sign of $f''(x)$ negative on $(-\infty,a)$; positive on (a,∞) discontinuities $f(a)$ undefined; $\lim_{x\to a^-} f(x) = -\infty$; $\lim_{x\to a^+} f(x) = \infty$ singularities $f'(a)$ undefined; $\lim_{x\to a} f'(x) = -\infty$

QMR can either analyze simple functions from first principles of calculus or match them against stored patterns. It analyzes complex functions by recursively analyzing their constituents and combining the results. Three combination algorithms suffice because each complex function must consist of a sum, product, or functional composition of its constituents. QMR may produce several alternate Q-behaviors, depending on algebraic relations between parameters. For example, composing e^x with ax produces a decreasing, constant, or increasing function, depending on a's sign, as shown in Figure 1.

QMR invokes the BOUNDER inequality prover² to resolve inequalities over sets of constraints. Given the constraint a < b, for example, BOUNDER can prove $e^a < e^b$ and refute b - a < 0, but can neither prove nor refute $a^2 < b^2$. It can also derive upper and lower bounds for symbolic expressions over constraint sets. When BOUNDER pronounces an inequality ambiguous, QMR constructs a Q-behavior for each possibility. This strategy certainly derives all possible Q-behaviors for any input, but may produce spurious ones as well. These arise when BOUNDER fails to prove valid inequalities. This is a fundamental limitation because no program can prove all inequalities between arbitrary extended elementary functions, as shown by Richardson.³ However, BOUNDER can handle all the examples in this paper as well as many more complicated inequalities.

THE SKETCHING ALGORITHM

QS sketches a function by invoking QMR to construct its Q-behaviors and sketching each of them separately. It chooses a set of interesting points for each Q-behavior, picks an appropriate scale, lays out the points on the plane, and connects them with smooth curves. The interesting points for a Q-behavior consist of its boundaries, extrema, inflection points, discontinuities, singularities, and any additional points designated by the user. QMR can infer every type of interesting point (except for user designated ones) directly from Q-behaviors.

Qualitative scales

A QS scale is a function from symbolic expressions to real numbers that preserves inequalities and bounds derivable by BOUNDER. Put symbolically, if s is a scale, a and b expressions, and C a set of constraints then

$$a \stackrel{c}{<} b \Rightarrow s(a) < s(b)$$
 (1)

$$a \stackrel{c}{\leq} b \Rightarrow s(a) \leq s(b)$$
 (2)

$$INF_C(a) \le s(a) \le SUP_C(a)$$
 (3)

where $a \stackrel{c}{<} b$ or $a \stackrel{c}{\le} b$ holds iff BOUNDER can deduce a < b or $a \le b$ from C and $INF_C(a)$ and $SUP_C(a)$ denote BOUNDER's bounds on a given C. Since a number is its own lower and upper bound, equation (3) implies that scales map numbers to themselves. Scales also preserve linear relations whenever possible, that is

$$a \stackrel{*}{=} mb + n \Rightarrow s(a) = m[s(b)] + n \tag{4}$$

where x = y means that QS can prove x equal to y, m and n denote numbers, and a and b denote symbolic expressions. Equation (4) cannot be strengthened by substituting = for = because equality between arbitrary extended elementary functions is undecidable, as shown by Richardson.³ Nonetheless, the powerful MACSYMA algebraic simplifier, which QS uses, recognizes all straightforward equalities and many more subtle ones. As a special case, each scale maps $-\infty$ to a very small number and ∞ to a very large number. These numbers satisfy equations (1) and (2), but violate equations (3) and (4).

Equations (1-4) guarantee that scaling preserves known relations between interesting points. Other relations between scaled values reflect arbitrary decisions. For example, consider the Q-behavior of (x-a)(x-b) with zeros at a and b. When no constraints exist, QS must arbitrarily draw a greater than b or b greater than a, even though either relation could hold. Sketches cannot express partial orders.

Sketching

After choosing a scale for the interesting points $\{x_1, \ldots, x_n\}$ of a behavior and a scale for their images $\{f(x_1), \ldots, f(x_n)\}$, QS prints each x_i at its scaled location on the x axis and each $f(x_i)$ at its scaled location on the y axis. However, it does not print large expressions because they would obscure the sketch. It chooses a new label (x_i) for the independent variable x and y_i for the dependent variable), attaches it to the expression, and prints it. Next, QS fills in the sketch. All discontinuities, singularities, extrema, and inflection points are interesting points, so the function must be continuous, differentiable, monotone, and of fixed convexity on the

intervals between them. This enables QS to capture the portion of a function between adjacent interesting points with a smooth curve. Since we are only interested in qualitative behavior, the exact path of the curve is unimportant, as long as it has the correct end points and convexity. QS uses a modified cubic spline, but any curve with four degrees of freedom would serve.

For the sake of brevity and clarity, the following discussion refers to points even though the program manipulates their scaled values. Let p and q be two finite adjacent interesting points. If f is continuous at p and q, QS draws a smooth curve between the pairs (p, f(p)) and (q, f(q)) with initial derivative f'(p) and final derivative f'(q). If f is discontinuous and bounded at p or q, QS uses the left or right limit respectively in place of the (possibly undefined) value. Similarly, it substitutes the left and right derivatives for f'(p) and f'(q) at sharp points and cusps. An unbounded discontinuity at p is asymptotic to the line x = p. Qs extends the sketch to the top of the y axis when the limit is ∞ and to the bottom when it is $-\infty$. It marks the asymptote with a dashed line. Infinite interesting points are treated analogously to unbounded finite ones. Qs extends the sketch to the left end of the x axis for $-\infty$ and the right end for ∞ . If the limit is a finite number $\lim_{x \to \infty} f(x) = \lim_{x \to \infty} f(x)$ with a dashed line.

Figure 2 illustrates these ideas with two sketches. All constants are declared positive in these examples and throughout the rest of the paper. The left-hand figure contains the sketch of $x^3 - 3ax$; its interesting points are: boundaries at $\pm \infty$, extrema at $\pm \sqrt{a}$, and an inflection point at 0. The right-hand figure contains the sketch of $\frac{x-a}{x-3a}$ with interesting points: $-\infty$, a, 3a and ∞ . The sketch includes (a,0) because zero crossings have been designated interesting. There is a vertical asymptote at x = 3a and a horizontal one at y = 1.

All the functions discussed so far have a finite number of interesting points. They are continuous and monotone for all sufficiently large and small values. QMR can also represent periodic functions with infinitely many extrema and discontinuities, although it cannot represent functions with infinitely many extrema in a finite region, such as $\sin 1/x$. The algorithm described thus far would fail on periodic functions, since it could not lay out an infinite number of points. Instead QS uses this basic algorithm to sketch one period of the function, marks it with a broken line, and prints its length. Figure 3 contains the sketches of $\sin(ax)$ which has a period of $2\pi/a$ and $\tan(ax)$ which has a period of π/a . The tangent has asymptotes at $\pm \pi/2a$ indicated, as usual, by dashed lines.

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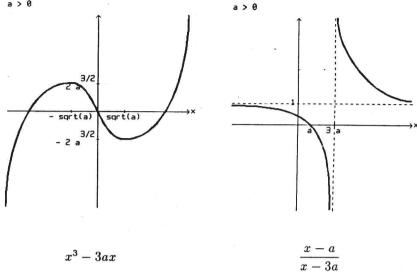


Figure 2: Sample QS sketches

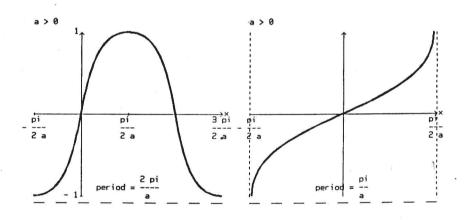


Figure 3: Two periodic functions

tan(ax)

sin(ax)

APPLICATIONS

Qualitative sketching applies to systems describable by univariate real functions. These arise in many domains, including pharmacokinetics, probability theory, utility theory, and circuit analysis.

Pharmacokinetics

Pharmacokinetics is the study of how drug concentrations vary over time in the body. Wagner⁵ (ch. 1-6) analyzes several pharmacokinetic models and plots the results. In a typical example, reproduced in Figure 4a, he plots the function

 $f_E(f_u) = \frac{f_u p_u}{1 + f_u p_u} \tag{5}$

for several specific values of the parameter p_u . Qs summarizes all the instances of (5) in a single sketch, shown in Figure 4b. Unlike the numeric plots, this sketch establishes that every instance of equation (5) has the same form: each increases monotonically, passes through the origin, approaches 1 asymptotically as f_u increases toward ∞ , and is concave. In this case, the Qs sketch is too abstract to serve Wagner's purpose, finding combinations of f_u and p_u that produce specific f_E values. He could either use Qs to sketch f_E for specific numeric values of p_u , or invoke the QMR utility that calculates inverses.

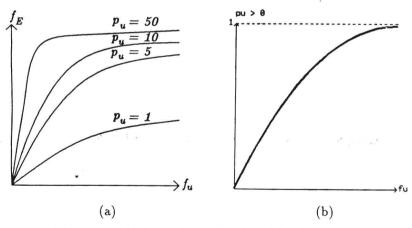


Figure 4: (a) Wagner's graph of f_E (b) The QS sketch

Probability theory

Qualitative sketches can help probability theorists and statisticians derive the properties of continuous probability distributions. For example, Freund⁶ (sec. 5.3) discusses the four important probability distributions

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that appear in Table 2 and constructs their qualitative sketches by hand. Qs can sketch all four of them. The uniform distribution has a trivial sketch consisting of a line segment, while the exponential distribution is a scaled version of the left-hand sketch in Figure 1. Figure 5 reproduces Freund's sketch of the gamma distribution for several values of a and b and Figure 6 shows the Qs version. This example demonstrates that qualitative sketches can be more informative and general than multiple numerical plots. Figure 7 contains the Qs sketch of the normal distribution.

Table 2: Four important probability distributions

uniform
$$\frac{1}{b-a}$$
 on the interval $[a,b]$ and 0 elsewhere exponential $\frac{1}{\theta}e^{-x/\theta}$ for $x>0$ and 0 elsewhere gamma $\frac{1}{b^a\Gamma(a)}x^{a-1}e^{-x/b}$ for $x>0$ and 0 elsewhere normal $\frac{1}{s\sqrt{2\pi}}e^{-\frac{1}{2}\left(\frac{x-m}{s}\right)^2}$

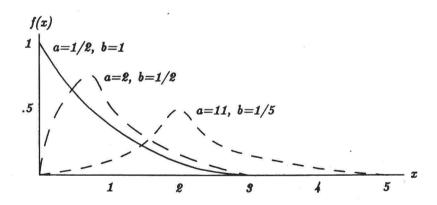


Figure 5: Freund's sketch of the gamma distribution

Utility theory

Wellman⁷ (chap. 3) uses QMR to analyze single-attribute utility functions u(x) and their risk functions:

$$r(x) = -\frac{u''(x)}{u'(x)} \tag{6}$$

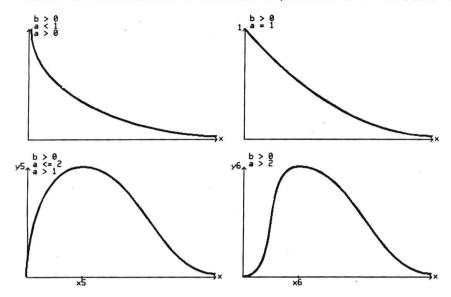


Figure 6: The QS sketch of the gamma distribution

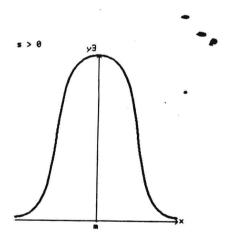


Figure 7: The QS sketch of the normal distribution

The utility functions are extended elementary functions, as are their risk functions. Figure 8 contains the sketch of a typical utility function: $u(x) = x^{1-c}$. Other common utility functions that QS can handle include linear functions, exponentials, and logarithms. Wellman tested QMR on all the examples and exercises appearing in the unidimensional utility theory chapter of Keeney and Raiffa's text⁸ (chap. 4). It analyzed 17 out of the 18 cases correctly, enabling QS to sketch them.

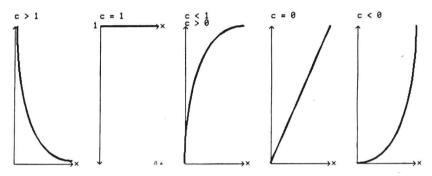


Figure 8: The QS sketch of $u(x) = x^{1-c}$

Circuit analysis

Graphic reasoning plays a significant role in circuit analysis. For example, electrical engineers infer the characteristics of a linear system by sketching the magnitude and phase of its transfer function $H(j\omega)$ against the frequency ω . The most common format, called a Bode plot, plots the quantities $20\log_{10}|H(j\omega)|$ and $\mathcal{L}H(j\omega)$ in a logarithmic scale. Qs can sketch the Bode plot of any transfer function that it can factor, including all numeric functions and many containing symbolic parameters. For example, Figure 9 contains the magnitude plot of

$$H(j\omega) = \frac{j\omega - a}{(j\omega - 2a)(j\omega - 3a)} \tag{7}$$

with a real and positive. The Bode plot of a symbolic transfer function expresses the characteristics common to all its instances. Engineers can observe them directly with QS instead of plotting several instances and generalizing the results.

CONCLUSIONS

This paper has described a qualitative sketcher for parameterized univariate functions on the real numbers. Its sketches capture the significant properties of functions better than verbal descriptions such as "f increases

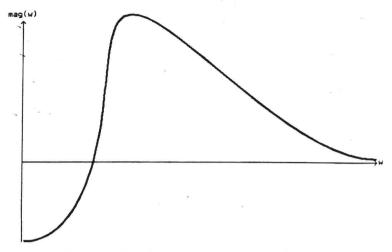


Figure 9: The Bode plot of equation (7).

between 0 and 1" or mathematical descriptions such as $\lim_{x\to\infty} f(x) = 2$. Qs can sketch any function that the QMR mathematical reasoner can analyze. As the previous section illustrates, this class includes interesting models from diverse fields.

Qualitative sketching seems to be a new idea. The only related system that I found appears in Kuipers. His system plots the qualitative values of a function at discrete qualitative time points and connects the results with straight lines. It marks increasing values with an ascending arrow, decreasing values with a descending arrow and steady values with a horizontal line. Although adequate for Kuipers's purposes, this algorithm ignores many important properties of functions, including convexity, discontinuities, singularities, asymptotes, and periodicity.

Many interesting models, including most nonlinear ones, cannot be solved in closed form. Qs cannot sketch these models because QMR is unable to construct their Q-behaviors. I am developing a new technique called piecewise linear abstraction (PLA) for analyzing systems describable by finite sets of ordinary differential equations. PLA constructs and analyzes piecewise linear approximations of complicated models instead of solving them directly. It uses a phase space representation to derive the behavior of a piecewise linear system over its entire domain from its local behavior on linear subregions. The resulting phase diagram provides extensive insight into the qualitative behavior of the system. For example, Figure 10 contains the phase diagram for the system of equations

$$\begin{bmatrix} z_1' \\ z_2' \end{bmatrix} = \begin{bmatrix} -\mu & 0 \\ 0 & \lambda \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \text{ with } \lambda, \mu > 0$$
 (8)

appearing in Brauer and Nohel¹⁰ (p. 172). It is clear from the figure

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