

# Using the Picard Contraction Mapping To Solve Inverse Problems For ODEs

postdoc work with E. Vrscay

(paper in *Inverse Problems*, 1999)

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# Question

Given a function  $x(t)$ , possibly an interpolation of data points, with  $t \in [0, 1]$ , find an ODE

$$\dot{x} = f(x, t), \quad x(0) = x_0,$$

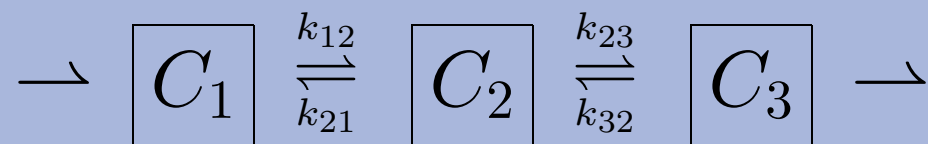
that admits  $x(t)$  as a solution as closely as desired, where  $f$  is restricted to a class of functional forms (affine, quadratic in  $x$ , etc.).

# Motivation

1. **Ecology**: determination of parameters in ecological models (and relative importance of each parameter).

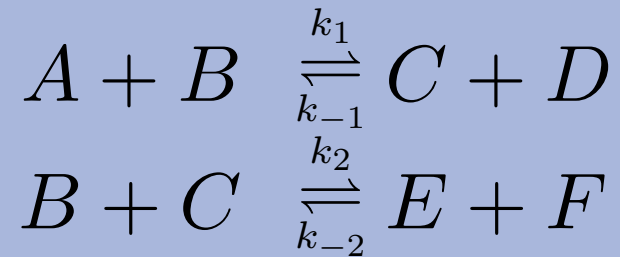
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2. **Compartmental Models:** schematically,



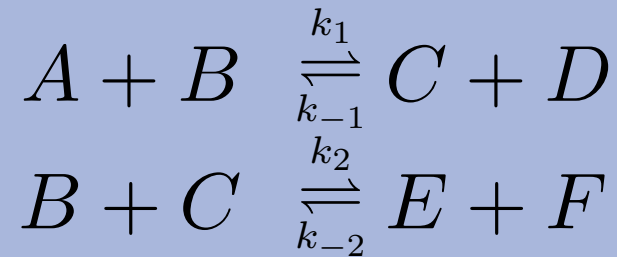
e.g. drug ingestion, metabolism.

3. **Chemical Kinetics:** determination of rate constants in chemical reaction systems. For example,



induces ODEs for the concentrations involving  $k_i$ s.

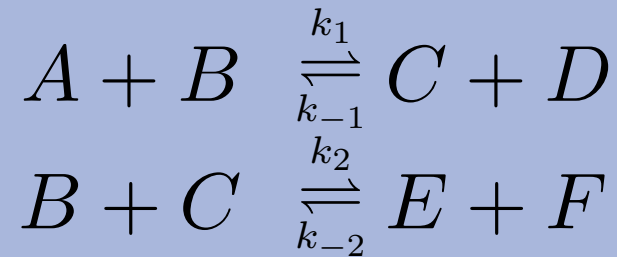
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4. **Tracer Kinetics:** concentrations of radioactive elements in a system.
5. **Structural Dynamics:** vibration of structures - determination of “Hooke’s constants.”

# References

A very useful reference on inverse problems is *Inverse Problems in the Mathematical Sciences* by C.W. Groetsch (F. Vieweg und Sohn, 1993). The book contains a particular study of damped vibrations that uses a collage-type method.

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The approach outlined in this presentation has been used systematically in the literature in a number of applications (although with little or no rigorous justification!).

1. R. Bellman, H. Hagiwara, and R. Kalaba, “Inverse Problems in Ecology,” *J. Theoret. Biol.*, **11**, pp 164–176, 1965. (Lotka-Volterra system)
2. W. Squire, “A Simple Integral Method for System Identification,” *Math Biosci.*, **10**, pp 145–147, 1971. (Lotka-Volterra system,  $\mathcal{L}^2$  collage method)
3. D.M. Himmelblau, C.R. Jones, and K.B. Bischoff, “Determination of Rate Constants for Complex Kinetic Models,” *Ind. Eng. Chem. Fundam.*, **6**, pp 539–542, 1967.

4. J. Milstein, “The Inverse Problem: Estimation of Kinetic Parameters,” in *Modeling of Chemical Reaction Systems*, K. Ebert et. al. eds., Springer, 1981.
5. H.G. Bock, “Numerical Treatment of Inverse Problems in Chemical Reaction Kinetics,” in *Modeling. . .*, *ibid.*

# Formulation

Consider the IVP

$$\dot{x}(t) = f(x, t), \quad x(0) = x_0, \quad (1)$$

with  $x \in \mathbb{R}$ ,  $f : \mathbb{R} \times \mathbb{R} \mapsto \mathbb{R}$ . A solution to (1) satisfies the integral equation

$$x(t) = x_0 + \int_0^t f(x(s), s) ds.$$

The **Picard operator**  $T$  associated with (1) is defined as

$$(Tu)(t) = x_0 + \int_0^t f(u(s), s) ds.$$

In the appropriate setting,  $T$  is a contraction mapping. This property will allow us to apply the collage theorem.

# Existence-Uniqueness Refresher

Define  $I = [-a, a]$ ,  $a > 0$ , and  $C(I) = \{\text{Banach space of continuous functions on } I \text{ with sup norm}\}$ . Then  $T : C(I) \mapsto C(I)$ ; a solution  $x(t)$  to (1) is a fixed point of  $T$ .

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Furthermore, define  $D = \{|x| \leq b, |t| \leq a\}$ ,  $\bar{C}(I) = \{u \in C(I) \mid \|u\|_\infty \leq b\}$  (a Banach space), and let  $\mathcal{F}(D)$  be the set of all functions  $f(x, t)$  on  $D$  satisfying

1.  $\max_{(x,t) \in D} |f(x, t)| < \frac{b}{a}$  and
2.  $|f(x_1, t) - f(x_2, t)| \leq K|x_1 - x_2|$ ,  $\forall (x_i, t) \in D$ , such that  $c = Ka < 1$ .

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Assuming  $f \in \mathcal{F}(\mathcal{D})$ ,

$$\|Tu - Tv\|_\infty \leq c\|u - v\|_\infty, \quad \forall u, v \in \bar{C}(I).$$

This contractivity implies that the solution to (1) is unique.

# Contractivity for the ODEs Inverse Problem

Define

$$I = [-a, a], \quad a > 0,$$

$C(I)$  = Banach space of continuous functions on  $I$   
with sup norm,

$$S = [-\delta, \delta], \quad 0 < \delta \ll 1,$$

$$D = \{|x| \leq b + \delta, |t| \leq a\},$$

$\mathcal{F}(D)$  as before,

$\Pi(I)$  = set of all Picard operators  $T : C(I) \mapsto C(I)$   
with  $x_0 \in S$  and  $f \in \mathcal{F}(\mathcal{D})$ .

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**Prop:** Let  $T \in \Pi(I)$ . Then

$$\|Tu - Tv\|_2 \leq \frac{c}{\sqrt{2}} \|u - v\|_2, \quad \forall u, v \in \bar{C}(I) \cap \mathcal{L}^2(I),$$

where  $c = Ka < 1$ .

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where  $c = Ka < 1$ .

Now use the collage theorem: instead of finding a  $T$  with fixed point close to our target, we find a  $T$  which sends the target close to itself.

# Polynomial ODEs

Consider autonomous, polynomial (in  $x$ ) vector fields

$$f(x) = \sum_{k=0}^N c_k x^k, \text{ for some } N > 0.$$

Then

$$(Tx)(t) = x_0 + \int_0^t \sum_{k=0}^N c_k (x(s))^k ds.$$

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$$\begin{aligned}\Delta^2 &= \int_I [x(t) - (Tx)(t)]^2 dt \\ &= \int_I \left[ x(t) - x_0 - \sum_{k=0}^N c_k g_k(t) \right]^2 dt,\end{aligned}$$

where  $g_k(t) = \int_0^t (x(s))^k ds$ ,  $k = 0, 1, 2, \dots$  (“integrated moments of  $x(t)$ ”)

## Imposing the stationarity conditions

$$\frac{\partial(\Delta^2)}{\partial x_0} = 0 \text{ and } \frac{\partial(\Delta^2)}{\partial c_k} = 0$$

gives

$$\begin{bmatrix} 1 & \langle g_0 \rangle & \dots & \langle g_N \rangle \\ \langle g_0 \rangle & \langle g_0 g_0 \rangle & \dots & \langle g_0 g_N \rangle \\ \langle g_1 \rangle & \langle g_1 g_0 \rangle & \dots & \langle g_1 g_N \rangle \\ \dots & \dots & \dots & \dots \\ \langle g_N \rangle & \langle g_N g_0 \rangle & \dots & \langle g_N g_N \rangle \end{bmatrix} \begin{bmatrix} x_0 \\ c_0 \\ c_1 \\ \dots \\ c_N \end{bmatrix} = \begin{bmatrix} \langle x \rangle \\ \langle x g_0 \rangle \\ \langle x g_1 \rangle \\ \dots \\ \langle x g_N \rangle \end{bmatrix}$$

where  $\langle f \rangle = \int_I f(t) dt$  and the **colored entries** appear only if we treat  $x_0$  as a free parameter.

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**BUT** if  $x(t)$  is a solution to (1) for  $t \in I$ ,  $f \in \mathcal{F}(D)$ , then given any  $\epsilon > 0 \exists$  an interval  $\bar{I} \subseteq I$  and a Picard operator  $T_\epsilon \in \Pi(\bar{I})$  such that  $\|x - T_\epsilon x\|_\infty < \epsilon$ , where the norm is computed over  $\bar{I}$ .

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We can **partition**  $I$  in the hope of doing better.

This work extends to systems in a straightforward way.

# Examples

1. Let  $x(t) = Ae^{Bt} + C$  be a target solution, where  $A, B, C \in \mathbb{R}$ . This is the solution to the linear ODE  $\dot{x}(t) = -BC + Bx$ , for which  $A$  plays the role of the arbitrary constant.

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Choose  $N = 1$  in our linear system and solve to get

$$x_0 = A + C, \quad c_0 = -BC, \quad c_1 = B,$$

agreeing with the above ODE (actually independent of  $I$  and  $N$ ).

2. Let  $x(t) = t^2$  be the target solution on the interval  $[0, 1]$ . Notice that  $\dot{x}(t) = 2t = 2\sqrt{x}$  is the exact ODE. Set  $N = 1$  in the linear system to get the linear IVP

$$\dot{x}(t) = \frac{5}{12} + \frac{35}{18}x, \quad x(0) = -\frac{1}{27},$$

with corresponding collage distance  $\|x - Tx\|_2 = 0.0124$ .

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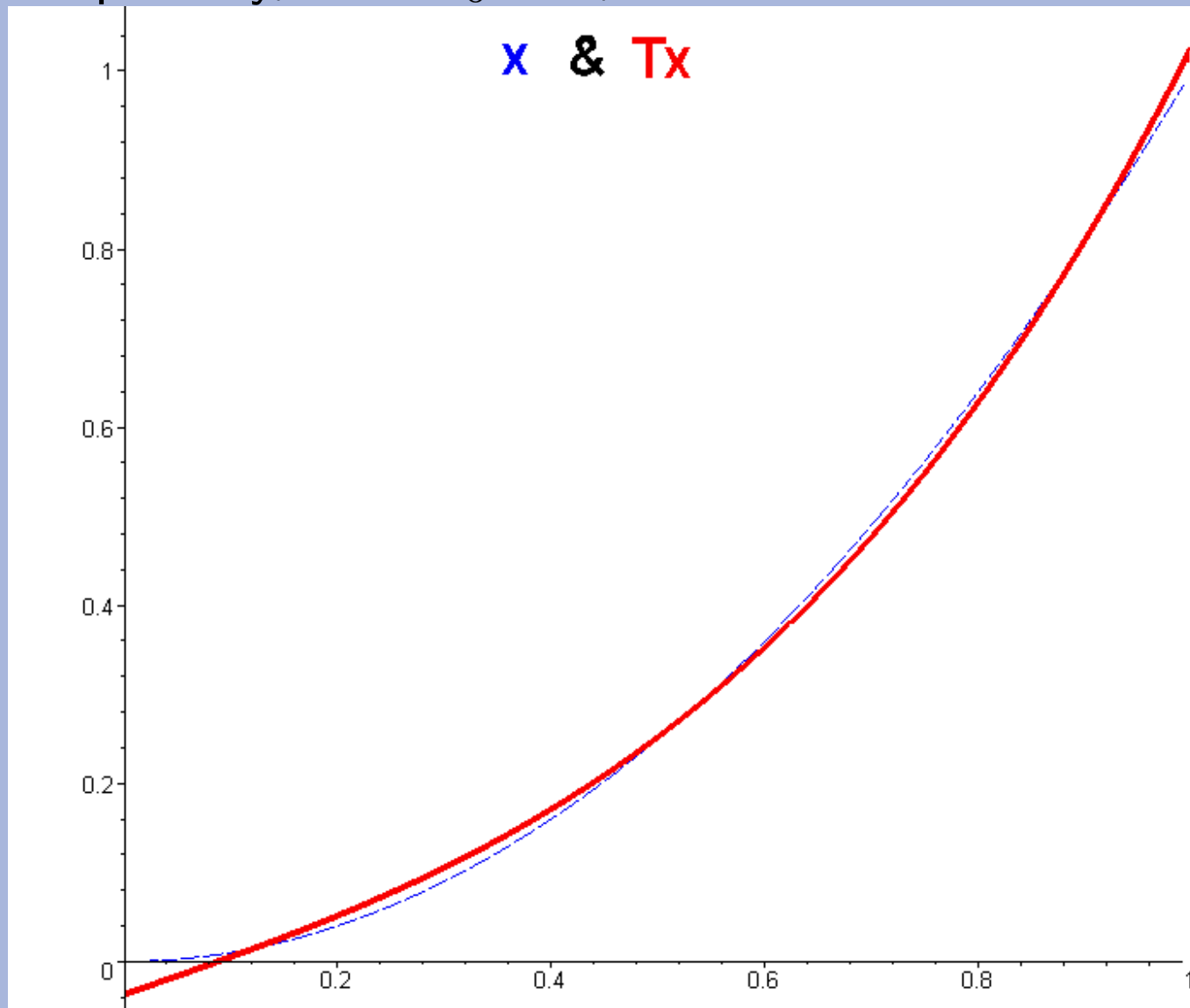
If we force the initial value to agree with the target curve ( $x(0) = 0$ ), the resulting linear IVP is

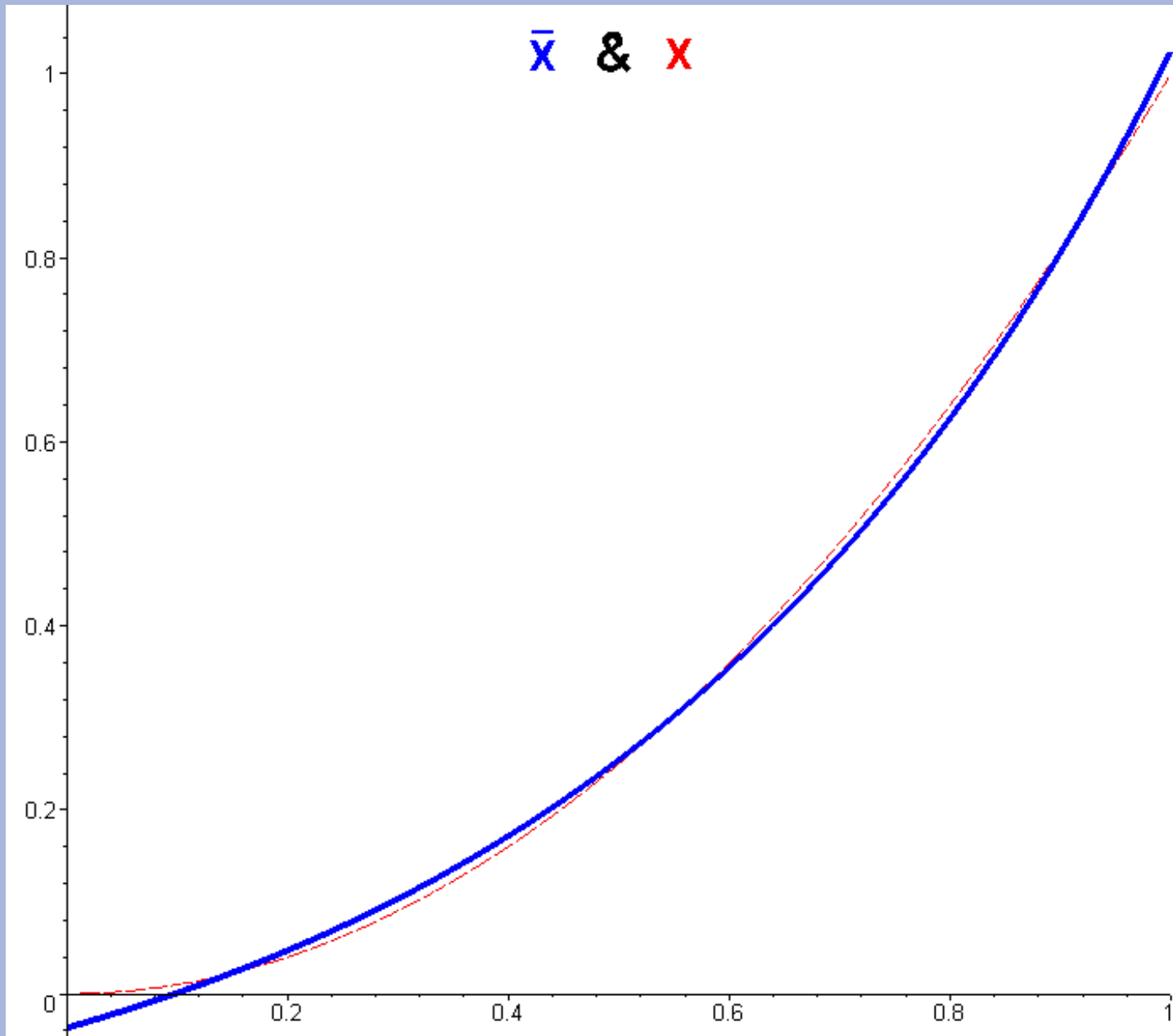
$$\dot{x}(t) = \frac{5}{16} + \frac{35}{16}x, \quad x(0) = 0,$$

with corresponding collage distance  $\|x - Tx\|_2 = 0.0186$ .

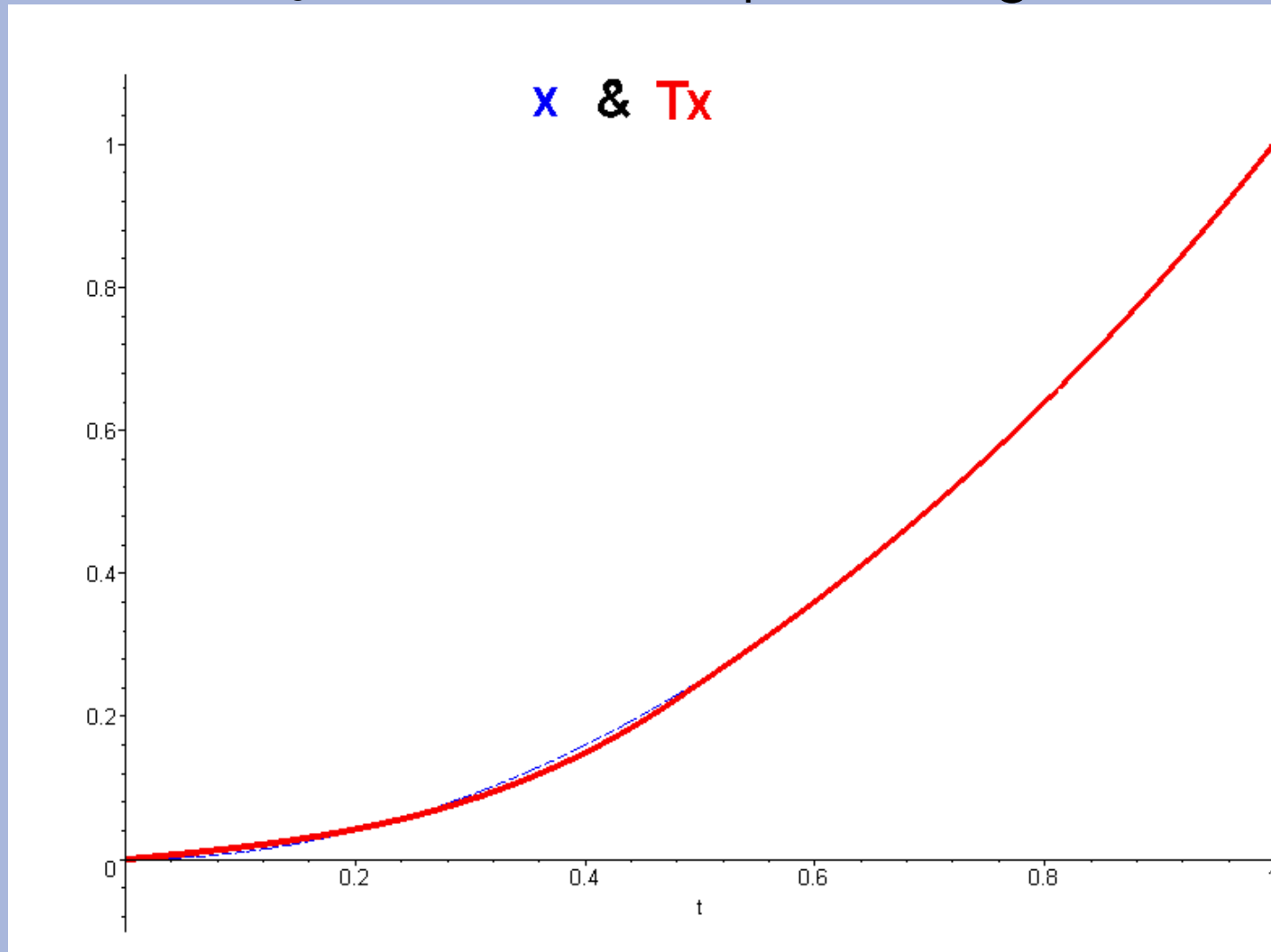
Graphically, with  $x_0$  free,

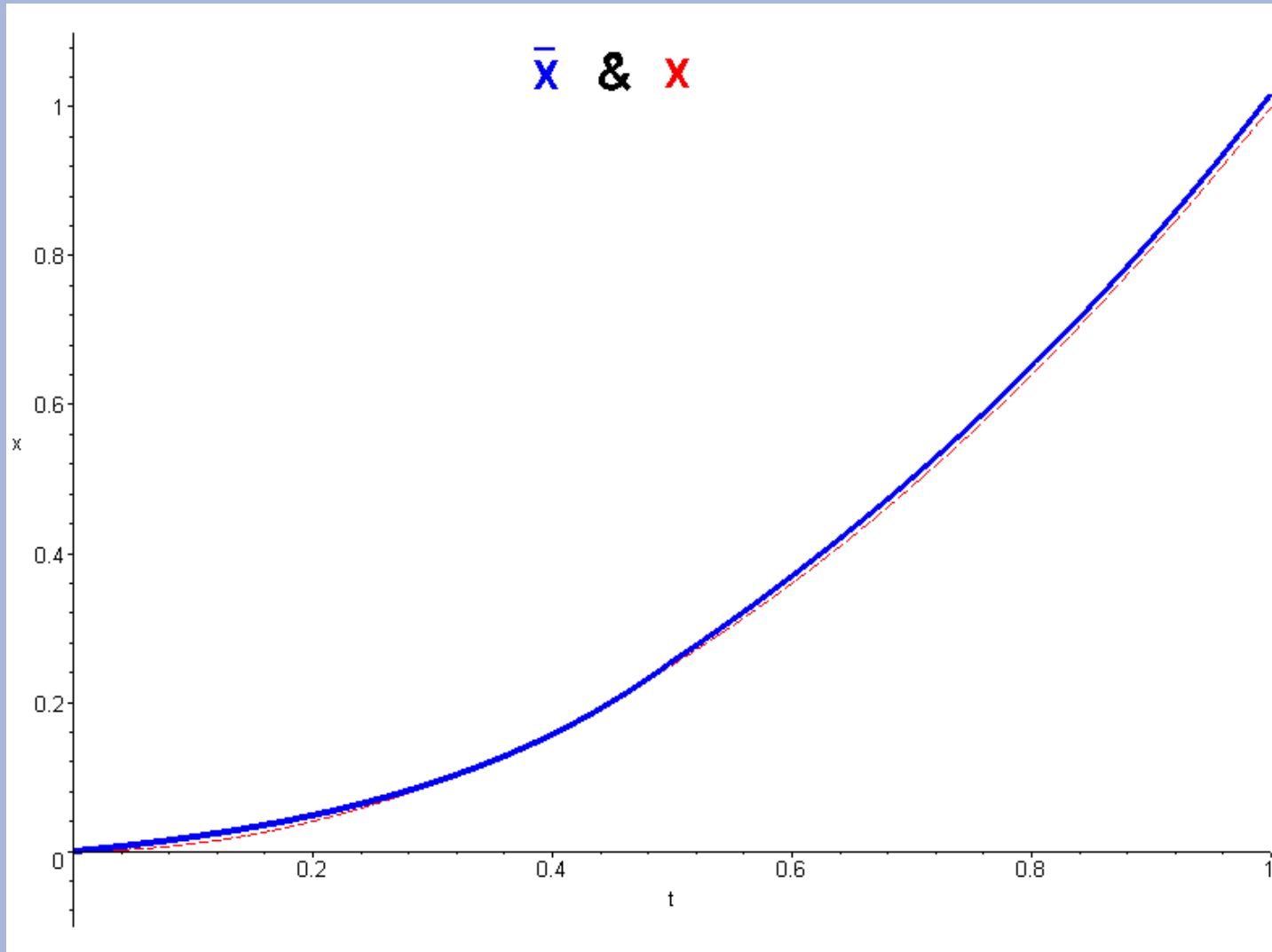
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And with  $x_0$  constrained to equal 0, we get





Of course, if we increase the degree of  $f$ , the collage and real errors decrease (we do not know whether we can decrease them to 0 without partitioning). We obtain:

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$f$ quadratic, $x_0$ constrained	$\frac{105}{512} + \frac{945}{256}x - \frac{1155}{512}x^2$	0	0.0070	0.0300

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$f$ quadratic, $x_0$ variable	$\frac{35}{128} + \frac{105}{32}x - \frac{231}{128}x^2$	$-\frac{1}{60}$	0.0047	0.0049

3. Consider  $x(t) = \frac{-125}{8}t^4 + \frac{1225}{36}t^3 - \frac{625}{24}t^2 + \frac{25}{3}t$ , with  $I = [0, 1]$ , and repeat the calculations of the previous example. This quartic has a local maximum at  $t = \frac{1}{3}$  and  $t = \frac{4}{5}$  and a local minimum  $t = \frac{1}{2}$ . The coefficients were chosen to scale  $x(t)$  for graphing on  $[0, 1]^2$ .

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Results:

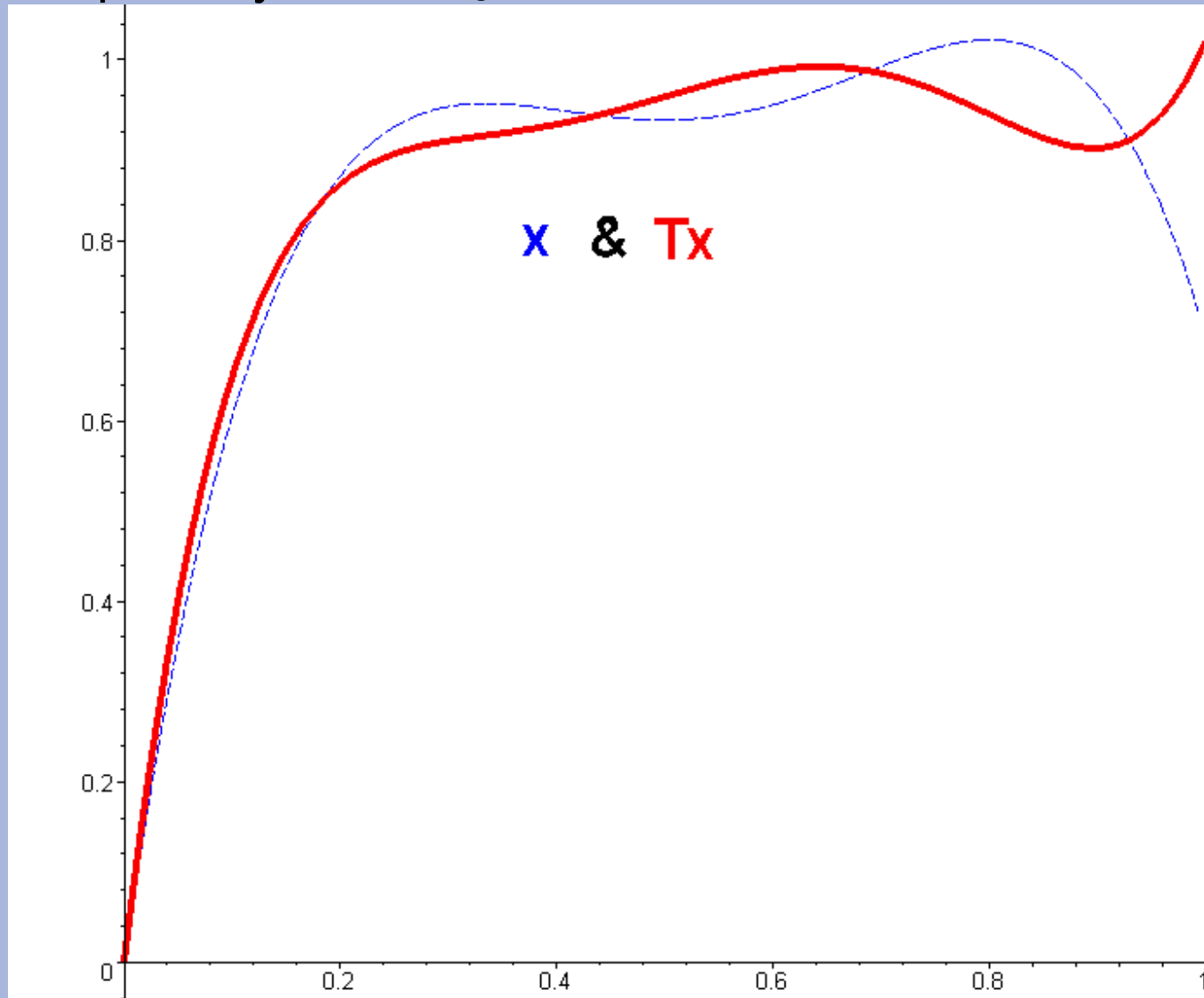
	$f$	IC	$\ x - Tx\ _2$	$\ x - \bar{x}\ _2$
$f$ linear $x_0$ constrained	$\frac{158165}{15844} - \frac{40887}{3961}x$	0	0.0608	0.0504
$f$ linear $x_0$ variable	$\frac{192815}{18444} - \frac{16632}{1537}x$	$-\frac{8425}{221328}$	0.0604	0.0497

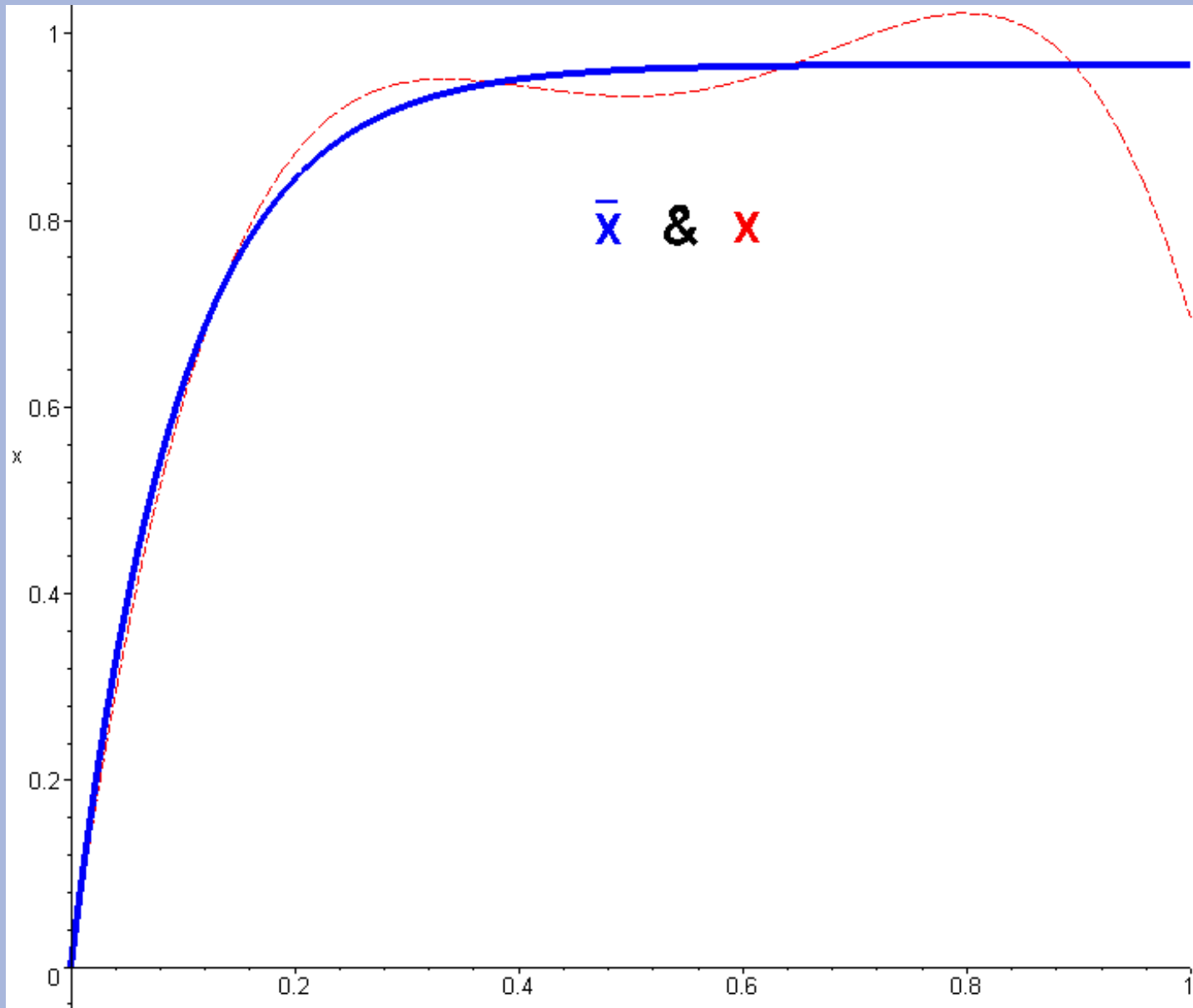
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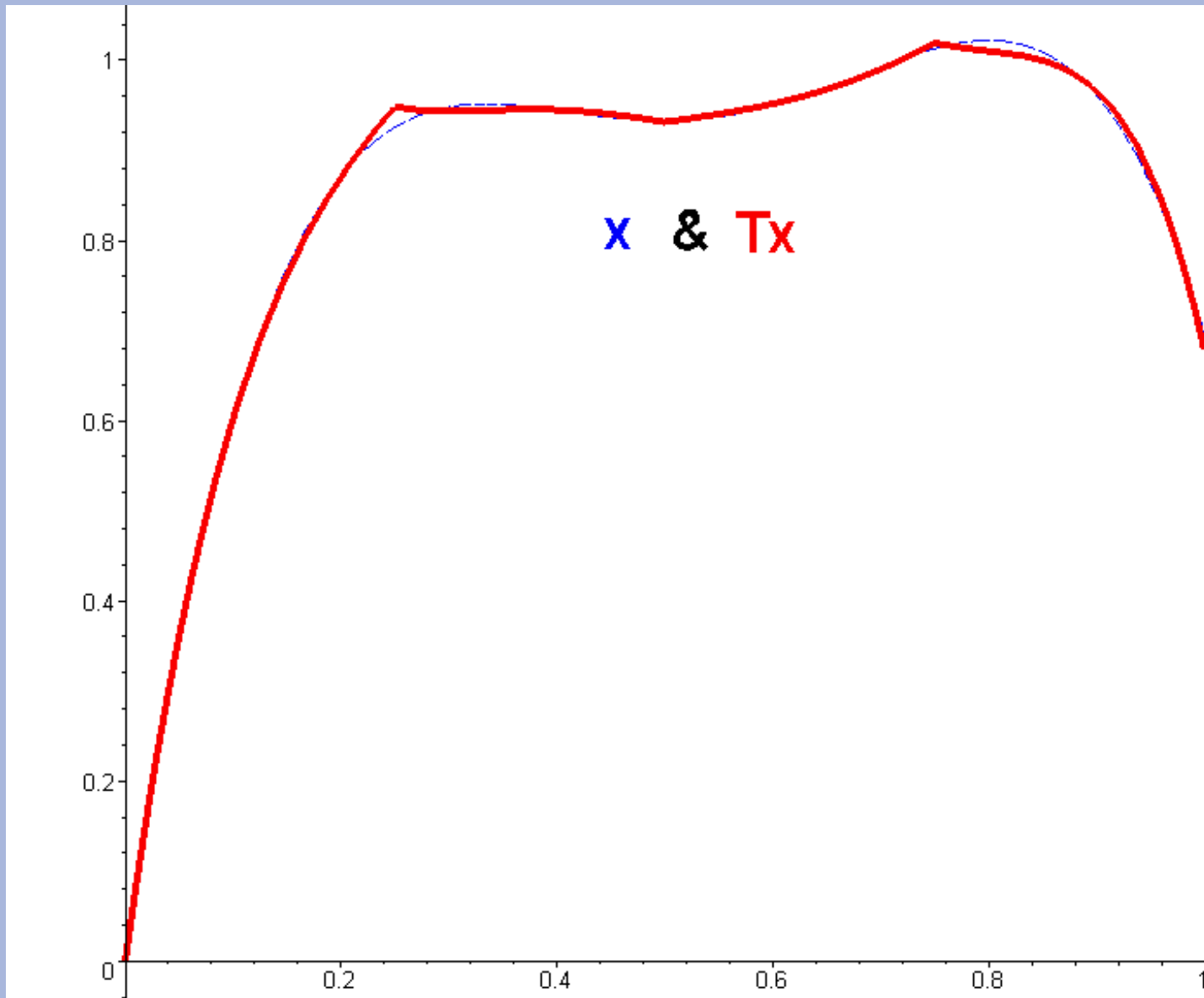
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$f$ quadratic $x_0$ constrained	$9.5235 - 8.6938x - 1.2020x^2$	0	0.0607	0.0497
$f$ quadratic $x_0$ variable	$11.0343 - 12.4563x + 1.0744x^2$	-0.0518	0.0603	0.0501

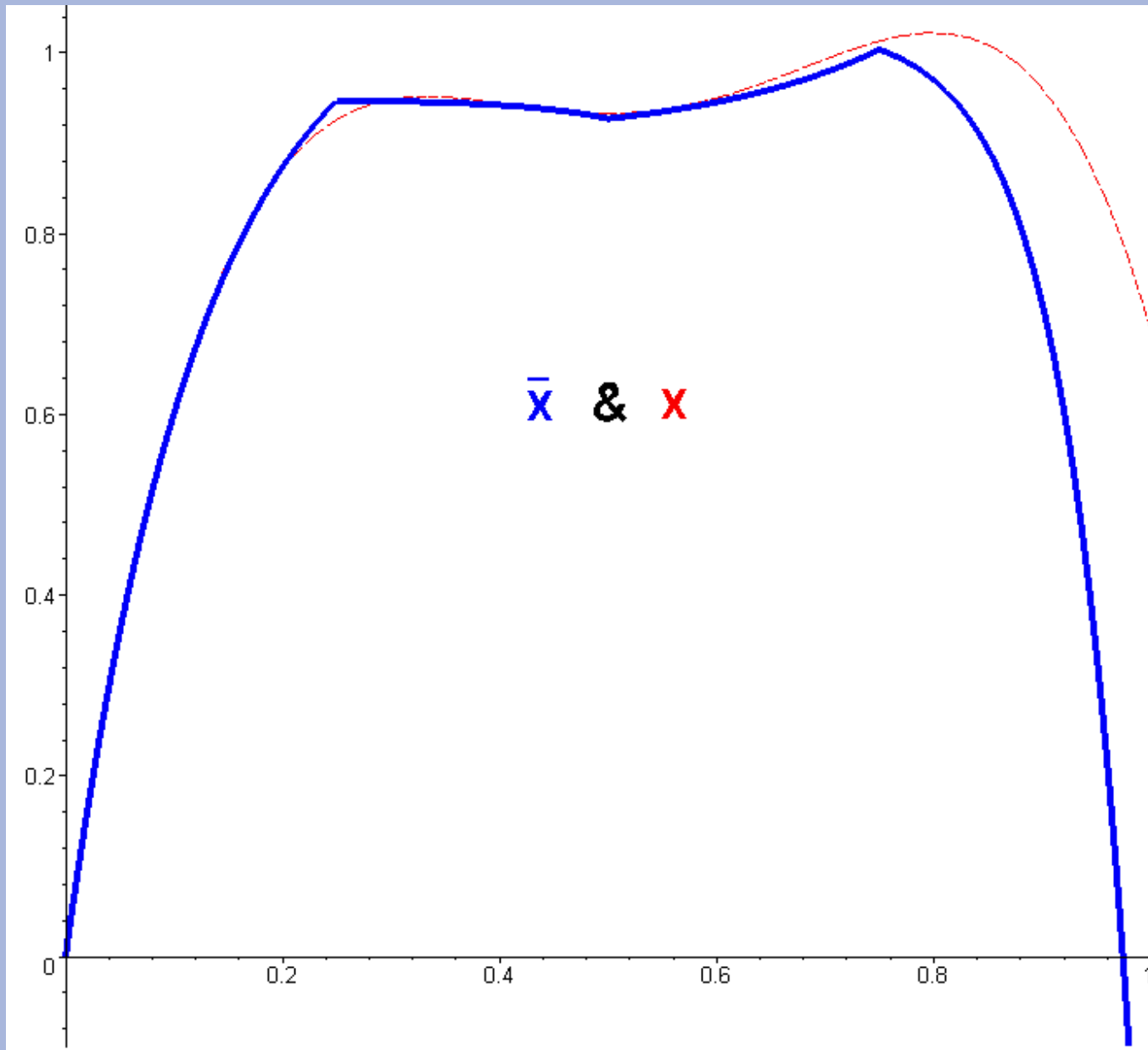
Graphically, with  $x_0$  free,





We might partition the interval  $[0, 1]$ , looking for a piecewise linear  $f$ . It is most effective to partition at the turning points of the target function. Graphs illustrate the improvement. Of course, we could increase the degree of  $f$  or partition further to improve results even more.





4. Consider the Lotka-Volterra system

$$\begin{aligned}\dot{x}(t) &= x - 2xy, & x(0) &= \frac{1}{3}, \\ \dot{y}(t) &= 2xy - y, & y(0) &= \frac{1}{3},\end{aligned}$$

the solution of which is a periodic cycle. We solve numerically, choose subsets of points  $(t_i, x(t_i))$  and  $(t_i, y(t_i))$  on the solution, and fit each set of points to a polynomial of degree ?, called  $x(t)$  and  $y(t)$ .

The results are summarized in the following table.

form of $f$ and $g$	$f$ and $g$	initial conditions	collage distances	actual $\mathcal{L}^2$ error
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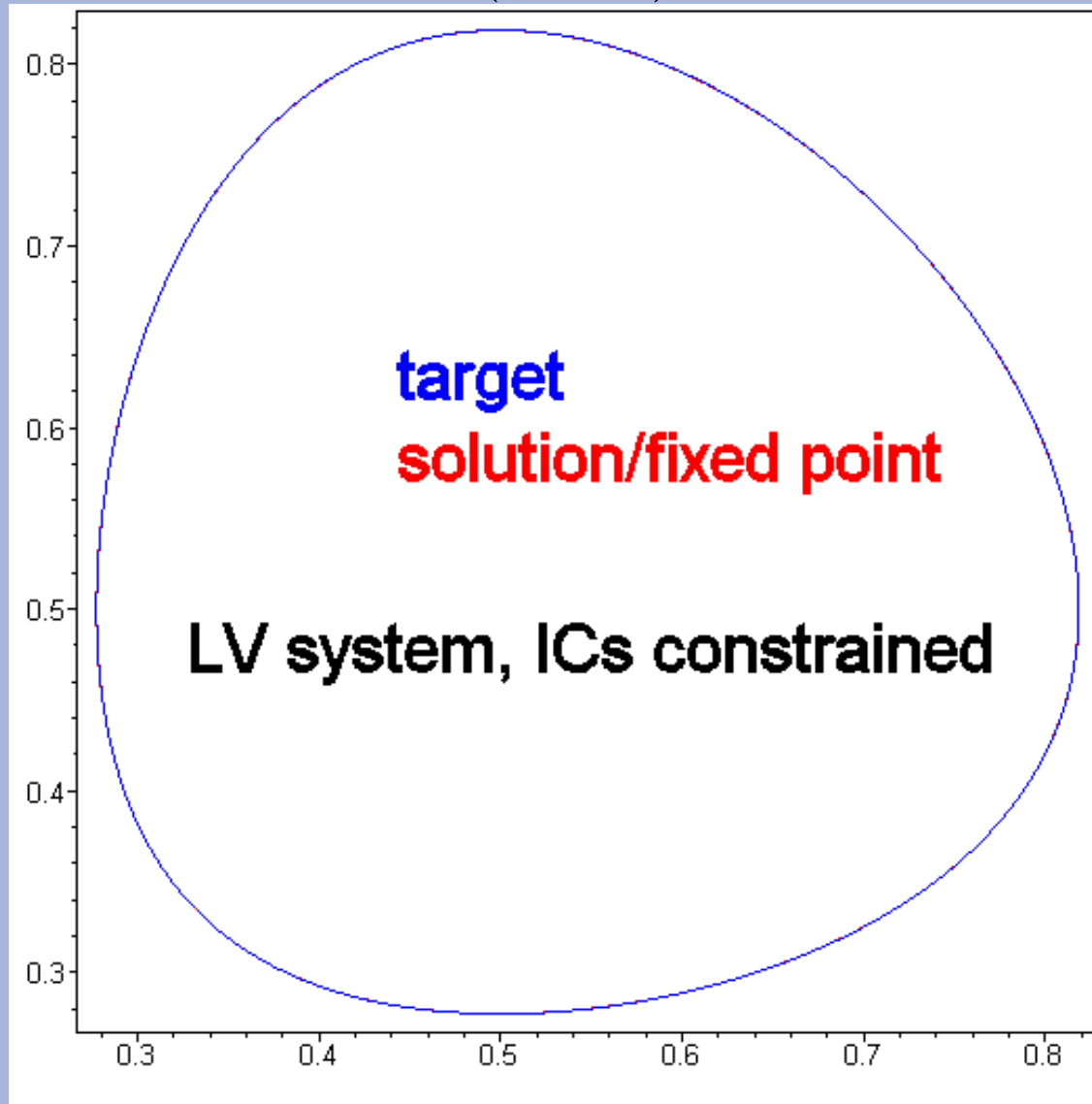
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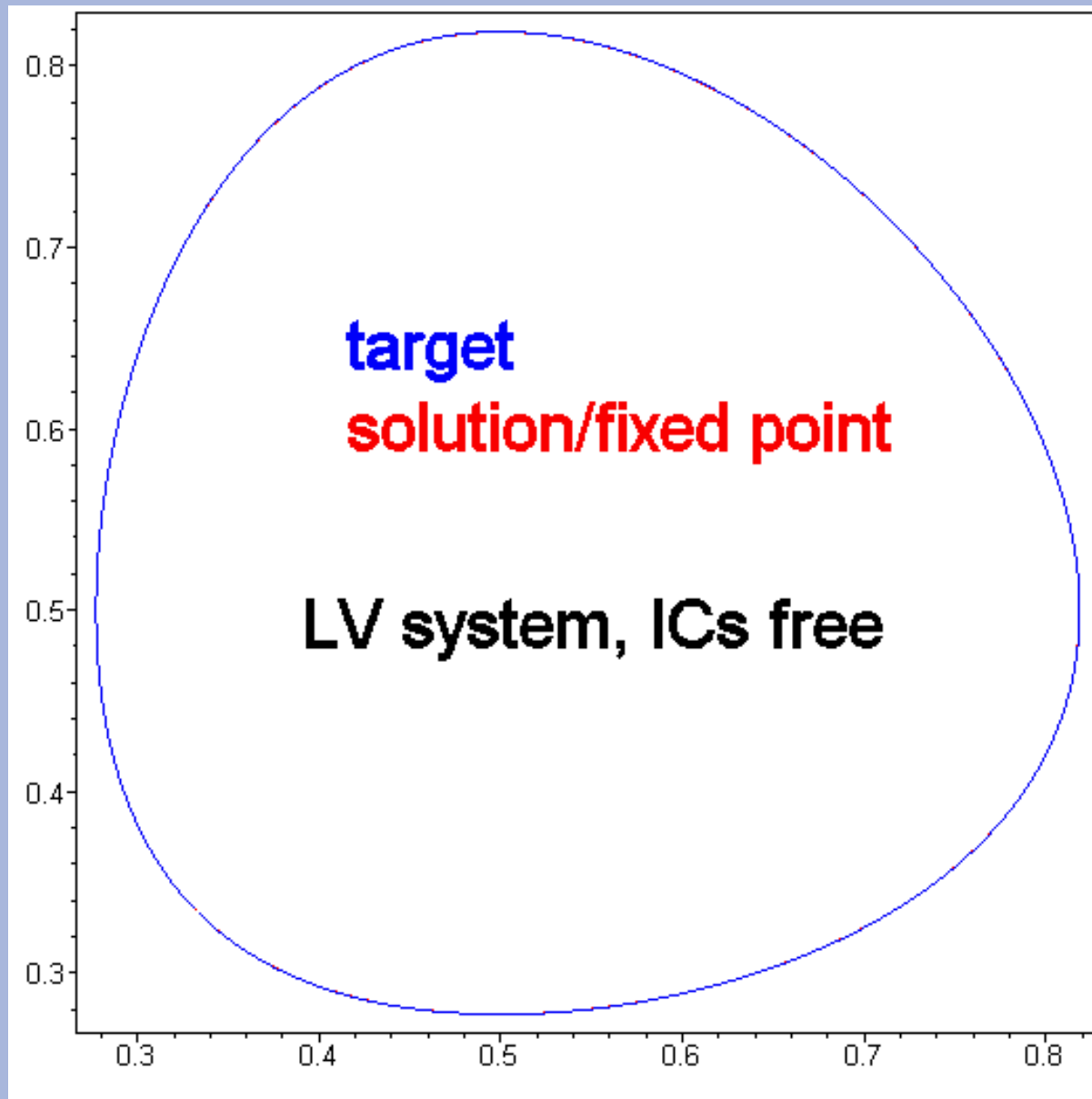
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And with  $(x_0, y_0)$  constrained to be  $(\frac{1}{3}, \frac{1}{3})$ ,

