Perturbation methods

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Additional Readings

- Holmes, M. H. Introduction to perturbation methods. (Springer, 2013).
- Van Dyke M. Perturbation methods in fluid mechanics. (Parabolic Press, 1975).
- Bender, C. M. Orszag, S. A. Advanced mathematical methods for scientists and engineers. (Springer, 1999).

A warm up example

Consider the position of a ball being thrown vertically. From newtons laws, the acceleration of the ball is given by

$$\frac{d^2x}{dt^2} = -\frac{gR^2}{x + R^2} \tag{1.1}$$

Where x is the vertical position, R is the radius of the earth, and g the gravitational constant.

Can we easily solve this problem?

A warm up example

Not easily solved:

$$\frac{d^2x}{dt^2} = -\frac{gR^2}{x + R^2}$$

But if I am throwing the ball from $x(0) = 0$ and $x'(0) = v_0$,

$x(t)$ is small compared to R.

We can then simplify the problem:

$$\frac{d^2x}{dt^2} = -g \tag{1.2}$$

A warm up example

Now,

$$\frac{d^2x}{dt^2} = -g$$

is easy to solve:

$$x(t) = -1/2gt^2 + v_0 t \tag{1.3}$$

- But how accurate is this solution?
- And is it based on solid mathematical footing?

Preliminaries

Theorem (Taylor's theorem)

Given a function $f(\epsilon)$, *suppose that* $f^{(n+1)}$ *is continuous for* $\epsilon_a < \epsilon < \epsilon_b$. *Assume* $\epsilon_0, \epsilon \in (\epsilon_a, \epsilon_b)$, *then*

$$f(\epsilon) = f(\epsilon_0) + (\epsilon - \epsilon_0)f'(\epsilon_0) + \cdots + \frac{1}{n!}(\epsilon - \epsilon_0)^n f^{(n)}(\epsilon) + R_{n+1} \tag{1.4}$$

R_{n+1} lets us estimate the error of an approximation

Preliminaries

Theorem (l'Hopitals rule)

Suppose $f(\epsilon)$ *and* $\phi(\epsilon)$ *are differentiable on* (ϵ_0, ϵ_b) *and* $\phi'(\epsilon) \neq 0$ *in this interval. If* $\lim_{\epsilon \to \epsilon_0} f(\epsilon) = \lim_{\epsilon \to \epsilon_0} g(\epsilon) = 0$ *or* $\pm\infty$ *and*

$$\lim_{\epsilon \to \epsilon_0} \frac{f'(\epsilon)}{\phi'(\epsilon)} = A$$

exists, then,

$$\lim_{\epsilon \to \epsilon_0} \frac{f(\epsilon)}{\phi(\epsilon)} = A$$

Order notation

Definition

$f = O(\phi)$, or ' f **is big Oh of** ϕ' as $\epsilon \to \epsilon_0$ if there are constants k and ϵ_1 so that

$$|f(\epsilon)| \leq k|\phi(\epsilon)| \text{ for } \epsilon_0 < \epsilon < \epsilon_1$$

If

$$\lim_{\epsilon \to \epsilon_0} \frac{f(\epsilon)}{\phi(\epsilon)} = L$$

where $-\infty < L < \infty$, then $f = O(\phi)$, or '**big Oh of** ϕ' as $\epsilon \to \epsilon_0$.

Order notation

Definition

$f = o(\phi)$, or ' f **is little Oh of** ϕ' as $\epsilon \to \epsilon_0$ if for every positive δ there is an ϵ_2 so that

$$|f(\epsilon)| \leq \delta |\phi(\epsilon)| \text{ for } \epsilon_0 < \epsilon < \epsilon_2$$

If

$$\lim_{\epsilon \to \epsilon_0} \frac{f(\epsilon)}{\phi(\epsilon)} = 0$$

then $f = o(\phi)$, or '**little Oh of** ϕ' as $\epsilon \to \epsilon_0$.

Example

Let $f(\epsilon) = sin(\epsilon)$ and $\phi = \epsilon$. Is f 'big Oh' or 'little Oh' of ϵ, for small values of ϵ?

Applying Taylor's theorem, $f = \epsilon - \frac{1}{2}\epsilon^2 sin(\xi)$ or

$f = \epsilon - \frac{\epsilon^3}{3!} + \frac{\epsilon^5}{5!} + \dots$.

Either way, $\lim_{\epsilon \to 0} f/\phi = 1$.

So f is $O(\epsilon)$, or big Oh of ϵ.

Example

Let $f = e^{-\frac{1}{\epsilon}}$ and $\phi = \epsilon^{\alpha}$. For what values of α is $f = o(\phi)$?

We require $\lim_{\epsilon \to 0} \frac{e^{-\frac{1}{\epsilon}}}{\epsilon^{\alpha}} = 0$.

First, set $\delta = 1/\epsilon$. Then our limit is equivalent to:

$$\lim_{\delta \to \infty} \frac{e^{-\delta}}{\delta^{-\alpha}} = \lim_{\delta \to \infty} \frac{\delta^{\alpha}}{e^{\delta}}$$

Since it is of the form $\frac{\infty}{\infty}$ we can apply l'Hopitals rule several times.

Example cont.

We have:

$$\lim_{\epsilon \to 0} \frac{e^{-\frac{1}{\epsilon}}}{\epsilon^{\alpha}} = \lim_{\delta \to \infty} \frac{e^{-\delta}}{\delta^{-\alpha}} = \lim_{\delta \to \infty} \frac{\delta^{\alpha}}{e^{\delta}} \overset{L.H.}{=} \lim_{\delta \to \infty} \frac{\alpha \delta^{\alpha-1}}{e^{\delta}} \underbrace{\overset{L.H.}{=} \ldots \overset{L.H.}{=} 0}_{\lceil \alpha \rceil \text{ times}}$$

We apply L.H. $\lceil \alpha \rceil$ many times if $\alpha > 0$. Eventually the exponent in the numerator will be ≤ 0.

So for any value of α, $e^{-1/\epsilon} = o(\epsilon^{\alpha})$.

Asymptotic approximation

Definition

We say that $\phi(\epsilon)$ is an asymptotic approximation of $f(\epsilon)$ as $\epsilon \to \epsilon_0$ whenever $f = \phi + o(\phi)$. We denote this by writing $f \sim \phi$.

Example

Let $f = \epsilon^2 + \epsilon^5$. Are $\phi_1 = \epsilon^2$, and $\phi_2 = 2/3\epsilon^2$ asymptotic approximations for small ϵ?

Example cont.

Let $f = \epsilon^2 + \epsilon^5$. Are $\phi_1 = \epsilon^2$, and $\phi_2 = 2/3\epsilon^2$ asymptotic approximations?

- ϕ_1 is an asymptotic approximation as $\lim_{\epsilon \to 0} \frac{\epsilon^5}{\epsilon^2} = 0$.
- ϕ_2 is not. Writing $f = \phi_2 + 1/3\epsilon^2 + \epsilon^5$ We see that $\lim_{\epsilon \to 0} \frac{1/3\epsilon^2 + \epsilon^5}{2/3\epsilon^2} \neq 0$. I.E. $1/3\epsilon^2 + \epsilon^5$ is not $o(2/3\epsilon^2)$.

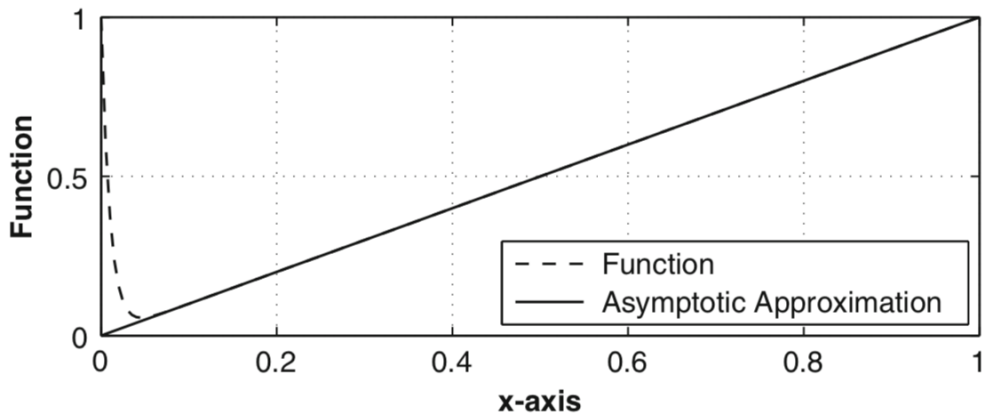
The main idea is that the **error term needs to have a higher order than the approximation term**.

A problem with asymptotic approximations

Unfortunately, asymptotic approximations say very little about accuracy when compared to actual values.

Example

Look at $f(x) = x + e^{-x/\epsilon}$ for small ϵ. It is easy to verify $f \sim x$, but the approximation is bad near zero



Asymptotic expansion

One way to fix these bad approximations, or at least measure the error is an asymptotic expansion.

Definition

- The functions $\phi_1(\epsilon), \phi_2(\epsilon), \ldots,$ form an **asymptotic sequence** as $\epsilon \to \epsilon_0$ if and only if $\phi_{m+1} = o(\phi_m)$ as $\epsilon \to \epsilon_0$ for all m.

Asymptotic expansion

- If $\phi_1(\epsilon), \phi_2(\epsilon), \ldots,$ is an asymptotic sequence, then $f(\epsilon)$ has an **asymptotic expansion** to n terms with respect to this sequence, if and only if

$$f = \sum_{k=1}^{m} a_k \phi_k + o(\phi_m) \text{ for } m = 1, 2, \ldots, n \text{ as } \epsilon \to \epsilon_0, \tag{3.1}$$

where a_k are independent of ϵ. We write

$$f \sim a_1\phi_1(\epsilon) + a_2\phi_2(\epsilon) + \cdots + a_n\phi_n(\epsilon) \tag{3.2}$$

and ϕ_k are referred to as gauge functions.

Gauge functions

Since asymptotic expansions are not unique, gauge functions can be prescribed or determined from Taylor expansions, or by "educated guess".

Example

$$f(\epsilon) = \frac{1}{\epsilon} cos(\epsilon)$$

$$= \frac{1}{\epsilon} \underbrace{(1 - \frac{1}{2}\epsilon^2 + \dots)}_{\text{Taylor series}}$$

$$f(\epsilon) \sim \frac{1}{\epsilon} - \frac{1}{2}\epsilon.$$

Gauge functions

Example

Suppose $\phi_1, \phi_2, \ldots$ are given.

By definition $f = a_1\phi_1 + o(\phi_1)$ as $\epsilon \to \epsilon_0$. So

$a_1 = f/\phi_1 - o(\phi_1)/\phi_1$ as $\epsilon \to \epsilon_0$. Thus,

$$a_1 = \lim_{\epsilon \to \epsilon_0} \frac{f}{\phi_1}.$$

Continuing, $f = a_1\phi_1 + a_2\phi_2 + o(\phi_2)$ as $\epsilon \to \epsilon_0$. i.e.

$$a_2 = \lim_{\epsilon \to \epsilon_0} \frac{f - a_1\phi_1}{\phi_2}.$$

and so on...

Asymptotic expansion

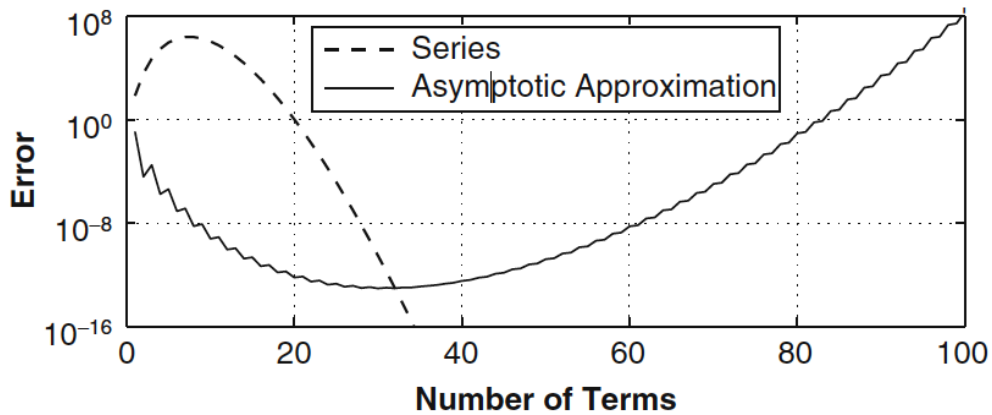
Look at the Bessel function

$$J_0(z) = \sum_{k=0}^{\infty} \frac{(-1)^k z^{2k}}{2^{2k}(k!)^2}. \tag{3.3}$$

Without getting into details, J_0 is a convergent series.

We can write $f(\epsilon) = J_0(1/\epsilon) \sim \sum_{k=0}^{N} a_k \phi_k(\epsilon)$, but the asymptotic expansion is divergent as $N \to \infty$.

Continued



The asymptotic sequence is designed to give a good approximation of f for $\epsilon \to 0$ (for a fixed N), whereas the convergent series gives good approximations as $N \to \infty$ (for a fixed ϵ).

Manipulations of Asymptotic expansions

Its not obvious that

$$f(x,\epsilon) \sim \phi_1(x,\epsilon) + \phi_2(x,\epsilon) \text{ as } \epsilon \to \epsilon_0$$

implies that

$$\frac{d}{dx} f(x,\epsilon) \sim \frac{d}{dx}\phi_1(x,\epsilon) + \frac{d}{dx}\phi_2(x,\epsilon) \text{ as } \epsilon \to \epsilon_0$$

Why? We are never guaranteed that the derivatives of the gauge functions are also an asymptotic sequence..

Manipulations of Asymptotic expansions

Luckily, if

$$f(x,\epsilon) \sim a_1(x)\phi_1(\epsilon) + a_2(x)\phi_2(\epsilon) \text{ as } \epsilon \to \epsilon_0$$

and if

$$\frac{d}{dx} f(x,\epsilon) \sim b_1(x)\phi_1(\epsilon) + b_2(x)\phi_2(\epsilon) \text{ as } \epsilon \to \epsilon_0$$

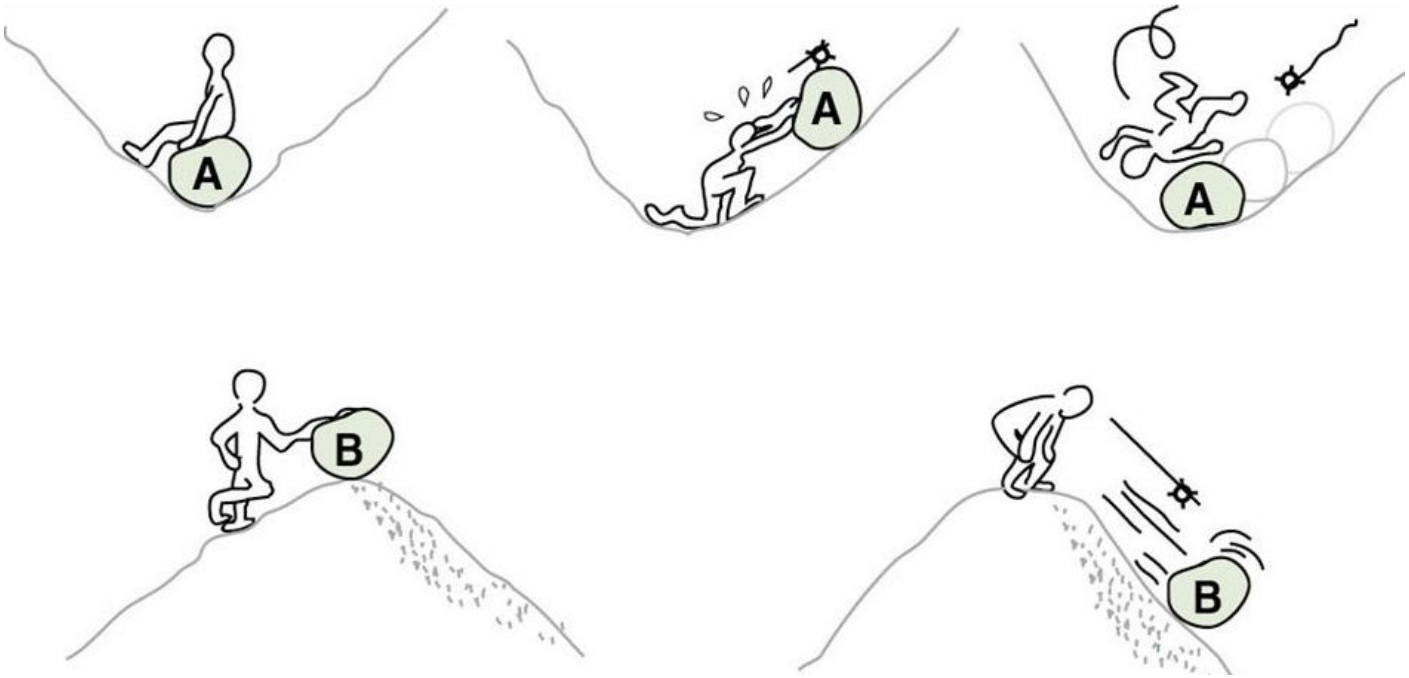
then

$$b_k = \frac{d}{dx} a_k.$$

Perturbations

Definition (Perturbation)

A (small) deviation to the theoretical motion, or structure of system.



Perturbations

Definition

- A **regular perturbation** problem is a problem, whose solution can be well approximated by setting the perturbation parameter to zero.
- A **singular perturbation** problem is a problem, whose solution can **not** be well approximated by setting the perturbation parameter to zero.

Example: Regular perturbation

Consider the solution to $x^2 + 2\epsilon x - 1 = 0$, where ϵ is a small perturbation parameter.

Setting $\epsilon = 0$ gives an approximate solution of

$$x \approx 1, -1.$$

Example: $x^2 + 2\epsilon x - 1 = 0$

Apply an asymptotic expansion on x. i.e.

$x \sim x_0\epsilon^\alpha + x_1\epsilon^\beta + x_2\epsilon^\gamma + \ldots$, ($\alpha < \beta < \gamma$ to ensure asymptotic sequence). We arrive at:

$$\epsilon^{2\alpha}x_0^2 + 2\epsilon^{\alpha+\beta}x_0x_1 + \cdots + 2\epsilon(\epsilon^\alpha x_0 + \epsilon^\beta x_1 + \ldots) - 1 = 0.$$

starting at the lowest exponent we need to cancel terms.

Either $\alpha = -1$ or 0. We take $\alpha = 0$.

$O(1)$: $\quad x_0^2 - 1 = 0 \rightarrow x_0 = \pm 1$.

Example: $x^2 + 2\epsilon x - 1 = 0$

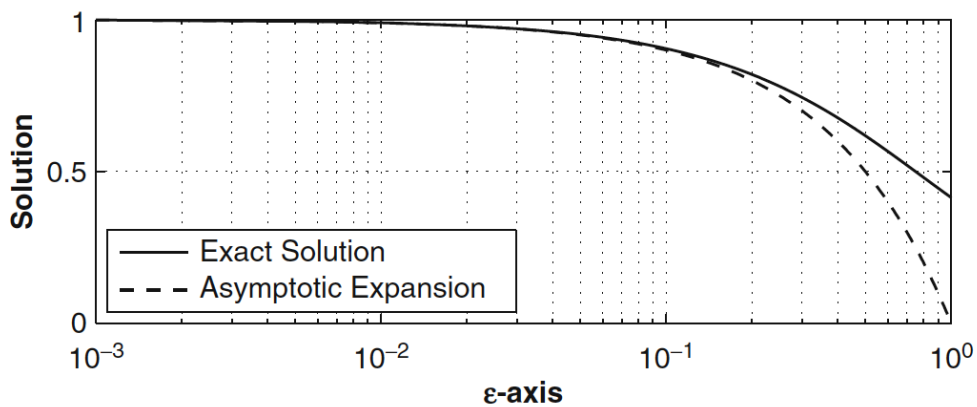
With $\alpha = 0$, and $x_0 = \pm 1$ we solve:

$$\cancel{x_0^2} + 2\epsilon^\beta x_0 x_1 + \cdots + 2\epsilon(x_0 + \epsilon^\beta x_1 + \dots) - \cancel{1} = 0.$$

Now we must balance the next order terms, which is $O(\epsilon)$, hence we must choose $\beta = 1$.

$O(\epsilon)$: $\quad 2x_0x_1 + 2x_0 = 0 \to x_1 = -1.$

So the solution is $x \sim \pm 1 - \epsilon$.



Example: singular perturbation

Consider the solutions to $\epsilon x^2 + 2x - 1 = 0$.

Setting $\epsilon = 0$ gives the solution $x = 1/2$

But this is a quadratic, so we should have two solutions?

Again, we apply the asymptotic expansion

$$x \sim x_0 \epsilon^{\alpha} + x_1 \epsilon^{\beta} + x_2 \epsilon^{\gamma} + \ldots,$$

with $\alpha < \beta < \gamma$.

Example: $\epsilon x^2 + 2x - 1 = 0$

After substitution:

$$\underbrace{\epsilon(\epsilon^{2\alpha}x_0^2 + 2\epsilon^{\alpha+\beta}x_0x_1 + \dots)}_{①} + \underbrace{2(\epsilon^{\alpha}x_0 + \epsilon^{\beta}x_1 + \dots)}_{②} - \underbrace{1}_{③} = 0.$$

How do we balance orders?

(i) ③$\sim$ ② and ① is higher order

(ii) ③$\sim$ ① and ② is higher order

(iii) ②$\sim$ ① and ③ is higher order

Example: $\epsilon x^2 + 2x - 1 = 0$ Case (i)

(3) $\sim$ (2) and (1) is higher order

$$\underbrace{\epsilon(\epsilon^{2\alpha}x_0^2 + 2\epsilon^{\alpha+\beta}x_0x_1 + \dots)}_{(1)} + \underbrace{2(\epsilon^{\alpha}x_0 + \epsilon^{\beta}x_1 + \dots)}_{(2)} - \underbrace{1}_{(3)} = 0.$$

$\alpha = 0$ is required.

$O(1)$: $\quad x_0 = 1/2.$

To balance the next order we need $\beta = 1$

$O(\epsilon)$: $\quad x_0^2 + 2x_1 = 0 \to x_1 = -1/8$

But this still doesn't give us the second solution.

Example: $\epsilon x^2 + 2x - 1 = 0$ Case (ii)

③$\sim$ ① and ② is higher order

$$\underbrace{\epsilon(\epsilon^{2\alpha}x_0^2 + 2\epsilon^{\alpha+\beta}x_0x_1 + \dots)}_{①} + \underbrace{2(\epsilon^{\alpha}x_0 + \epsilon^{\beta}x_1 + \dots)}_{②} - \underbrace{1}_{③} = 0.$$

$1 + 2\alpha = 0$ is required, i.e. $\alpha = -1/2$.

This means that ②$\sim O(\epsilon^{-1/2})$ which is lower order than ①,③.

A contradiction of our assumption, and it would be impossible to balance the lowest order.

Example: $\epsilon x^2 + 2x - 1 = 0$ Case (iii)

(2) $\sim$ (1) and (3) is higher order

$$\underbrace{\epsilon(\epsilon^{2\alpha}x_0^2 + 2\epsilon^{\alpha+\beta}x_0x_1 + \dots)}_{(1)} + \underbrace{2(\epsilon^{\alpha}x_0 + \epsilon^{\beta}x_1 + \dots)}_{(2)} - \underbrace{1}_{(3)} = 0.$$

$1 + 2\alpha = \alpha$ is required, i.e. $\alpha = -1$. The problem becomes:

$$(\epsilon^{-1}x_0^2 + 2\epsilon^{\beta}x_0x_1 + \dots) + 2(\epsilon^{-1}x_0 + \epsilon^{\beta}x_1 + \dots) - 1 = 0.$$

To balance the $O(1)$ term, (3), it is clear we require $\beta = 0$

Example: $\epsilon x^2 + 2x - 1 = 0$ Case (iii)

$$(\epsilon^{-1}x_0^2 + 2x_0x_1 + \dots) + 2(\epsilon^{-1}x_0 + x_1 + \dots) - 1 = 0.$$

$O(\frac{1}{\epsilon})$: $\quad x_0^2 + 2x_0 = 0 \rightarrow \mathbf{x_0 = 0, -2}$

$O(1)$: $\quad 2x_0x_1 + 2x_1 - 1 = 0 \rightarrow$ for $x_0 = -2$, $x_1 = -\frac{1}{2}$. For $x_0 = 0$, $x_1 = \frac{1}{2}$. Our two asymptotic approximations are:

$x \sim \epsilon^{-1}x_0 + x_1$

$x \sim \frac{1}{2}$

$x \sim -\frac{2}{\epsilon} - \frac{1}{2}$

Boundary layer problems

Consider the forces:

- spring $-kx$
- friction or drag $-bv$
- weight/normal force

Then, by Newtons laws:

$$F = ma = -kx - bv$$

$$mx'' + bx' + kx = 0$$

Small mass damped oscillator

What if the mass on the end of the spring is small?

Also, suppose we can only view the position of the mass instantaneously every second?

Our problem then becomes:

$$\epsilon x'' + 2x' + 2x = 0 \tag{5.1}$$

$$x(0) = 0 \quad x(1) = 1 \tag{5.2}$$

Lets approximate this solution!

Outer Solution

As discussed we begin by applying an asymptotic expansion

$$x(t) = x_0(t) + \epsilon x_1(t) + \dots$$

Leading to:

$$\epsilon(x_0'' + \epsilon x_1'' + \dots) + 2(x_0' + \epsilon x_1' + \dots) + 2(x_0 + \epsilon x_1 + \dots) = 0$$

Balancing:

$$O(1): \quad x_0' + x_0 = 0 \rightarrow x_0(t) = ae^{-t}$$

Outer Solution

Now, we have that $x_0(t) = ae^{-t}$. However we have two boundary conditions and only one constant.

This means that this solution will do a poor job approximating near one of the boundary conditions.

We assume that there is a boundary layer, at either $t = 0$ or $t = 1$, where we must use a different approximation.

Boundary Layer

Intuitively we can assume the boundary layer is close to $t = 0$.

We introduce a *boundary layer coordinate* and *solution:*

$$\bar{t} = \frac{t}{\epsilon^\alpha}, \qquad X(\bar{t}) = x(\epsilon^\alpha \bar{t})$$

Where α will be determined when balancing orders.

Now from chain rule:

$$\frac{d}{dt} = \frac{d\bar{t}}{dt}\frac{d}{d\bar{t}} = \frac{1}{\epsilon^\alpha}\frac{d}{d\bar{t}}$$

Boundary Layer

Now, our problem becomes:

$$\epsilon^{1-2\alpha}\frac{d^2X}{d\bar{t}^2} + 2\epsilon^{-\alpha}\frac{dX}{d\bar{t}} + 2X = 0,$$

$$X(0) = 0$$

Note, only the $t = 0$ B.C. applies here. As $\bar{t} = \frac{t}{\epsilon^\alpha}$ blows up as t moves away from 0 and $\epsilon \to 0$.

Inner Solution

Again, we apply the asymptotic expansion:

$$X(\bar{t}) = X_0(\bar{t}) + \epsilon^{\gamma} X_1(\bar{t}) + \dots$$

After substitution

$$\underbrace{\epsilon^{1-2\alpha} \frac{d^2}{d\bar{t}^2}(X_0 + \dots)}_{①} + \underbrace{2\epsilon^{-\alpha} \frac{d}{d\bar{t}}(X_0 + \dots)}_{②} + \underbrace{2(X_0 + \dots)}_{③} = 0,$$

(i) ③ $\sim$ ② and ① is higher order - won't consider $\frac{d^2 Y}{d\bar{t}^2}$

(ii) ③ $\sim$ ① and ② is higher order - leads to a contradiction

(iii) ② $\sim$ ① and ③ is higher order - needs $\alpha = 1$ but works!

Inner Solution

$$\epsilon^{-1}\frac{d^2}{d\bar{t}^2}(X_0 + \dots) + 2\epsilon^{-1}\frac{d}{d\bar{t}}(X_0 + \dots) + 2(X_0 + \dots) = 0,$$

$$O(\tfrac{1}{\epsilon}): \quad X_0'' + 2X_0' = 0,\ X_0(0) = 0.$$

$$\rightarrow X_0(\bar{t}) = A(1 - e^{-2\bar{t}}),$$

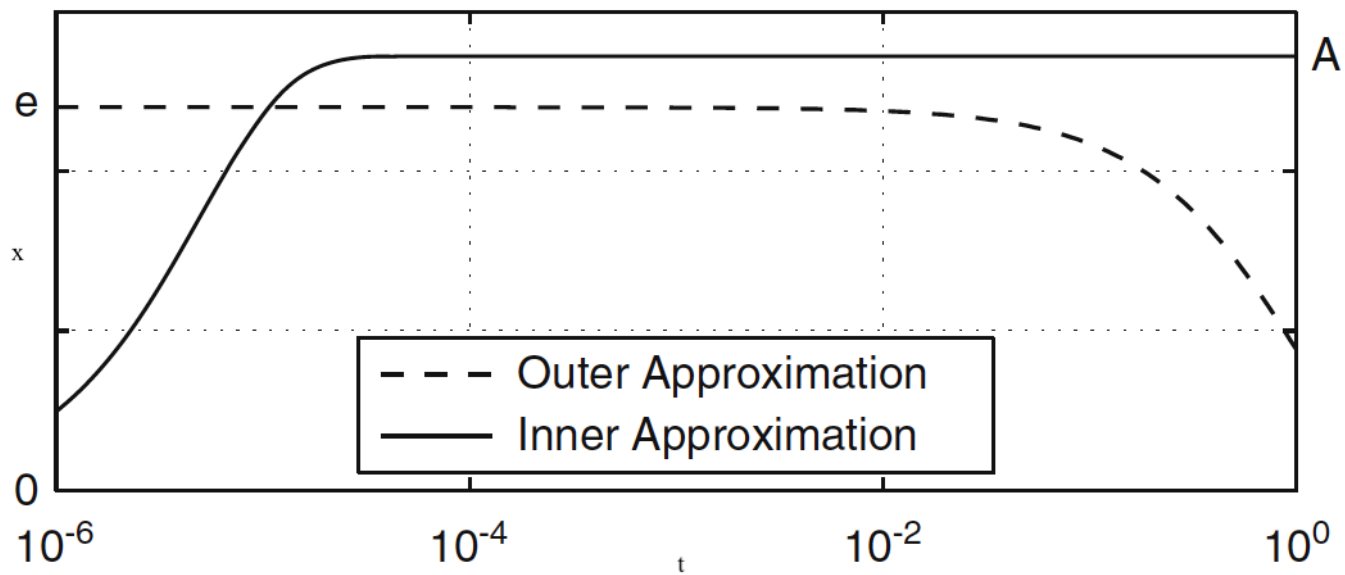
where A is an arbitrary constant that will be solved for later.

Quick recap:

So far we have computed the outer solution: $x_0(t) = ae^{1-t}$.

We can now conclude that the outer solution should match up the B.C. at $t = 1$. Thus $x_0(t) = e^{1-t}$.

The inner solution is $X_0(\bar{t}) = A(1 - e^{-2\bar{t}})$ with unknown A

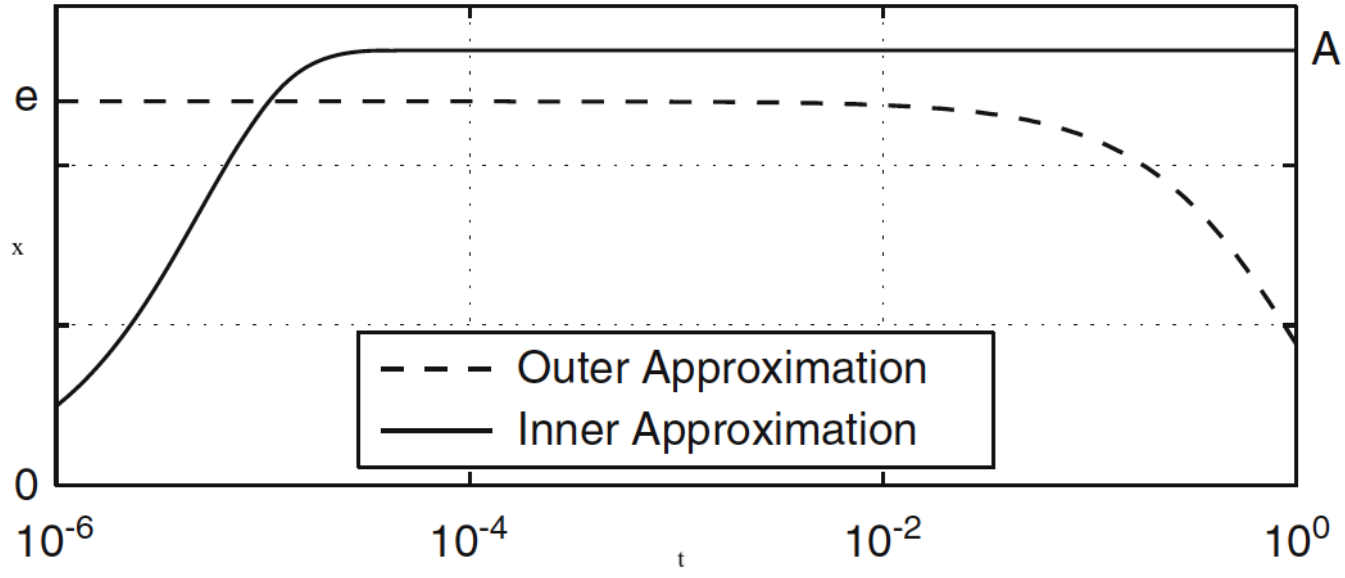


Matching

Note: The inner and outer solutions are meant to be approximations of the same solution.

They are just only accurate near their respective boundary.

Well, if they approximate the same solution, there should be a transition region where they are the same.



Matching

That is, as the inner solution leaves the boundary layer, $(\bar{t} \to \infty)$, the inner solution should match with outer solution as the outer enters the boundary layer $(t \to 0)$.

In other words:

$$X_0(\infty) = \lim_{\bar{t}\to\infty} X_0 = \lim_{t\to 0} x_0 = x_0(0^+)$$

$$\lim_{\bar{t}\to\infty} A(1 - e^{-2\bar{t}}) = \lim_{t\to 0} e^{1-t}$$

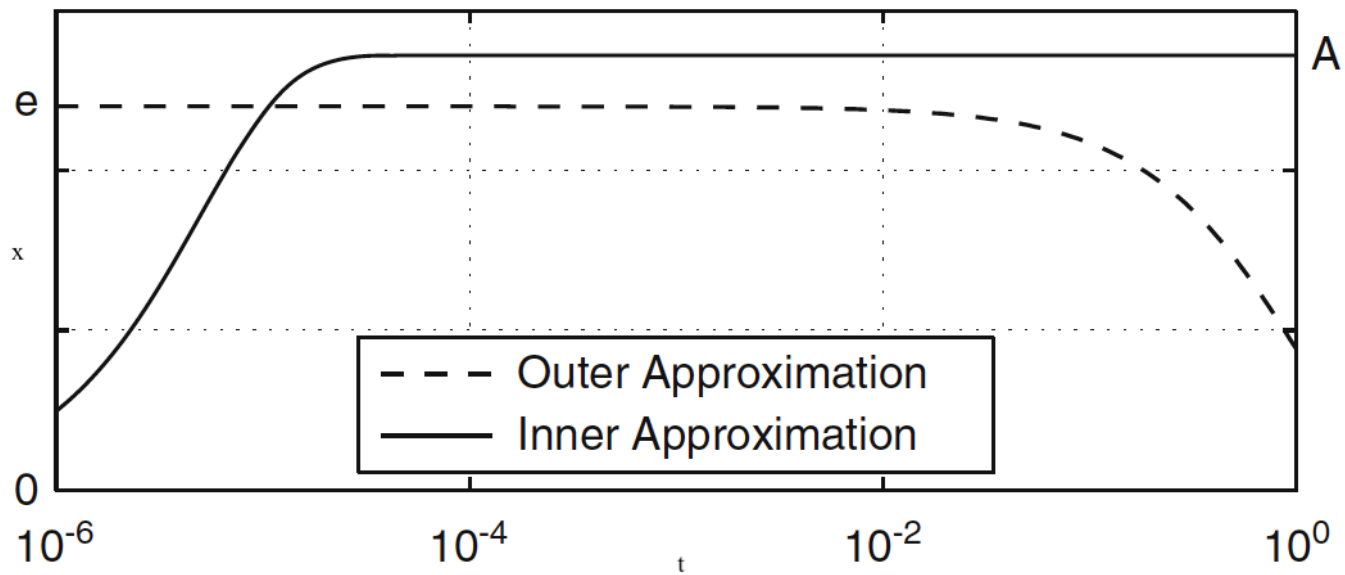
$$\implies A = e$$

Composite expansion

We now have an outer solution: $x_0(t) = e^{1-t}$. That only works away from $t = 0$.

and an inner solution, $X_0(\bar{t}) = e - e^{1-2\bar{t}}$, that only works near $t = 0$.

Can we construct a solution that is valid everywhere?

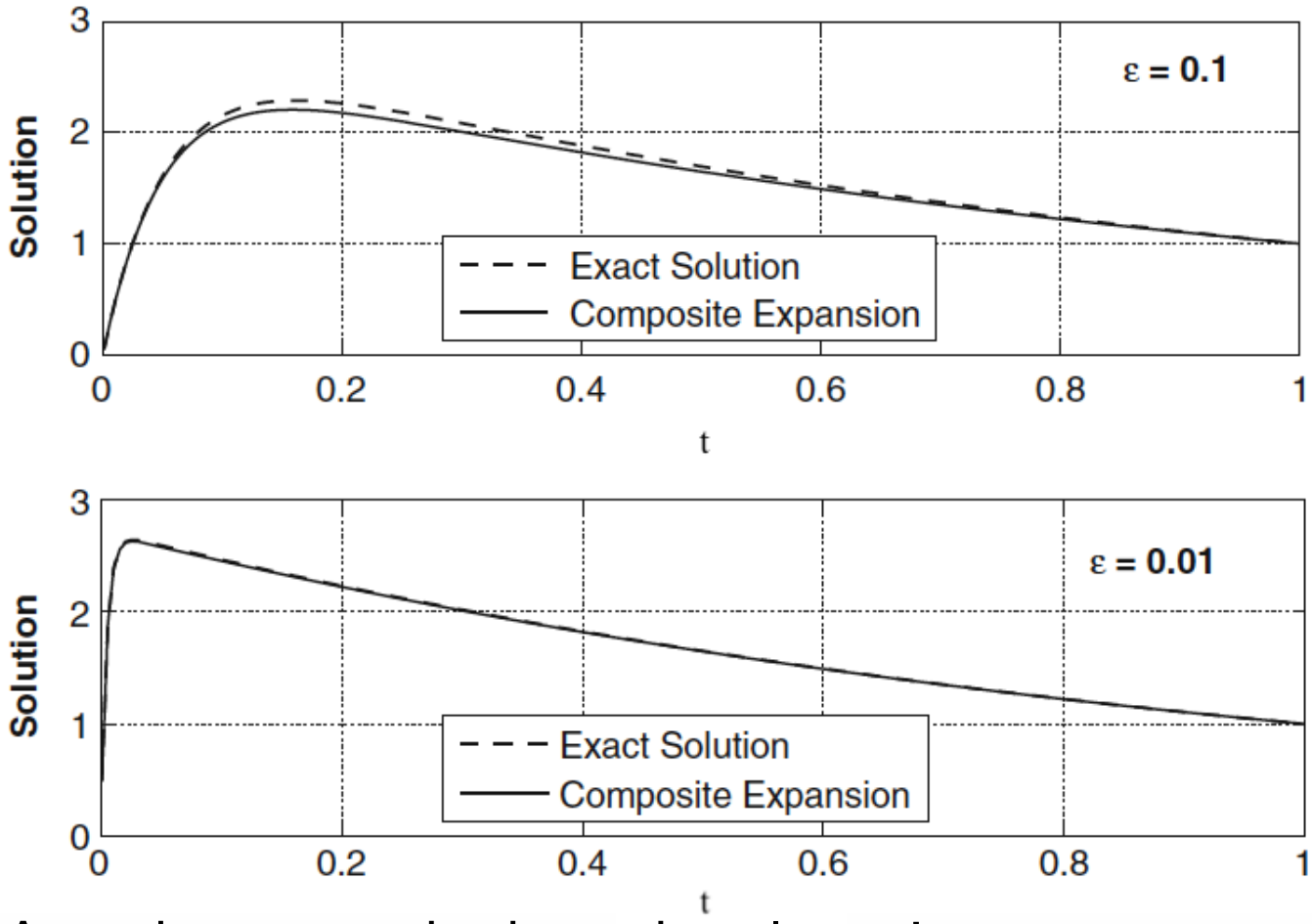


Composite expansion

By the matching condition, we note that the solutions overlap in the transition region ($X_0(\infty) = x_0(0^+)$), and that they are constant away from their valid approximation intervals. Thus we can add the solutions together and subtract the overlap.

$$\begin{aligned} x \sim & X_0(\bar{t}) + x_0(t) - X_0(\infty) \\ = & (e - e^{1-2\bar{t}}) + e^{1-t} - e \\ = & e^{1-t} - e^{1-2\frac{t}{\epsilon}} \end{aligned}$$

Comparing solutions



Note: As ϵ decreases the boundary layer is more pronounced, and the approximation is better.

Motivation

Question:

- How is this method applied in science?

Answer:

- A classical example is with the Michaelis-Menton approximation for am enzyme reaction.

  Or predator-prey models with a small predator conversion efficiency.

Enzyme reaction

Consider the chemical reaction:

$$\mathrm{S} + \mathrm{E} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \mathrm{C} \xrightarrow{k_2} \mathrm{E} + \mathrm{P}$$

Denote $s = [S]$, $e = [E]$, $c = [C]$, and $p = [P]$.

Deriving the Michaelis-Menton equations

$$S + E \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C \xrightarrow{k_2} E + P$$

- We start with the Law of Mass Action.
- Assume $e + c = r$ is constant. Then we don't need the equation for e .
- Initially $c(0) \approx 0$, so $e(0) = r$.
- Note that the equation for p is decoupled, so we leave it out.

Deriving the Michaelis-Menton equations

We derive the ODE system for S and C.

$$\mathrm{S} + \mathrm{E} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \mathrm{C} \xrightarrow{k_2} \mathrm{E} + \mathrm{P}$$

$$\begin{aligned} \frac{ds}{dt} &= -k_1 es + k_{-1} c \\ \frac{dc}{dt} &= k_1 es - k_{-1} c - k_2 c \end{aligned}$$

subject to $s(0) = s_0$, $c(0) = 0$ and $r = e(0)$.

Non-Dimensionalization

It is often very useful to non-dimensionalize a model before performing any analysis. The benefits include:

- All state variables are comparable in magnitude.
- Reduces the number of parameters
- Do not have to worry about units.
- Readily show where and how a perturbation parameter arises.
- Easily transfers to the original "real" system.

Introducing the following dimensionless variables and parameters and using $e + c = r$

$$u = \frac{s}{s_0} \qquad v = \frac{c}{r} \qquad \tau = k_1 r t$$
$$\alpha = \frac{k_{-1}}{k_1 s_0} \quad \kappa = \frac{k_{-1} + k_2}{k_1 s_0} = \frac{K_n}{s_o} \quad \epsilon = \frac{r}{s_0}$$

leads to

$$\frac{du}{d\tau} = -u + uv + \alpha v \tag{6.1}$$
$$\frac{dv}{d\tau} = \frac{1}{\epsilon}(u - uv - \kappa v). \tag{6.2}$$

subject to $u(0) = 1$, $v(0) = 0$.

Its reasonable to assume $0 < \epsilon = \frac{r}{s_0} = \frac{e_0}{s_0} \ll 1$.

Now, rewriting (6.2) as:

$$\epsilon \frac{dv}{d\tau} = u - uv - \kappa v \tag{6.3}$$

- apply the quasi-steady-state assumption
- set $\epsilon = 0$

This leads to

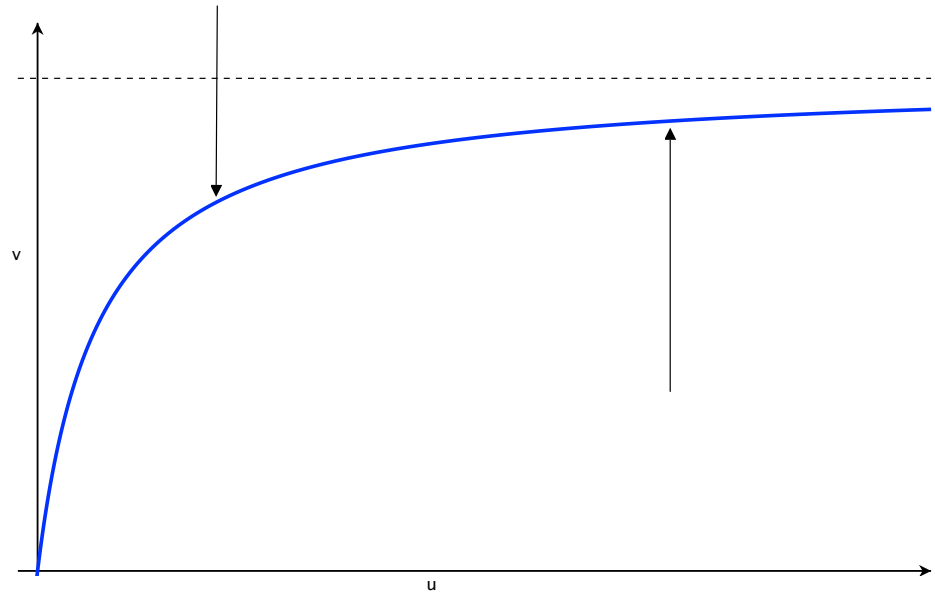
$$v = \frac{u}{\kappa + u}.$$

Now we aim to work through the slow manifold analysis and perturbation analysis of the full 2-D model for u and v.

Slow Manifold Analysis

- The $\frac{1}{\epsilon}$ in the $\frac{dv}{d\tau}$ equation implies that v is a fast variable, or the inner variable.
- That is, if v is not near the set $u - uv - \kappa v = 0$, then v will be changing fast.
- The curve, or set $u - uv - \kappa v = 0$ (or $v = \frac{u}{\kappa + u}$) is called the **slow manifold.**

We plot the slow manifold in phase space



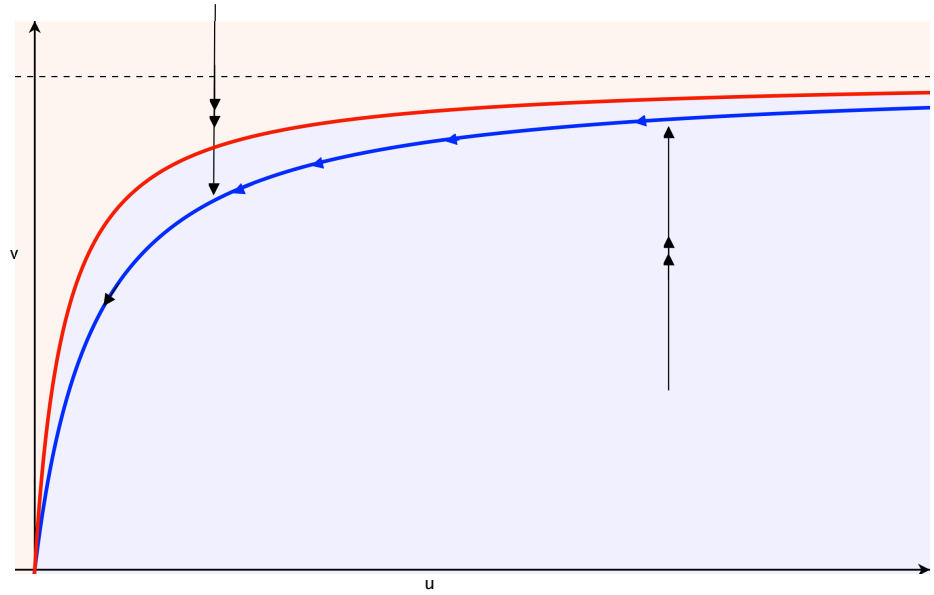
- $v = \frac{u}{\kappa+u}$ in blue
- black lines show the direction of the flow away from the slow manifold.

Question:

- What is the direction of movement near/on the slow manifold?

Well, intuitively we can argue the movement is towards the origin. Why is this?

Alternatively, we can consider the sign of $\frac{du}{d\tau}$.



- red curve is $\dfrac{du}{d\tau} = 0$.
- blue curve is the slow manifold.
- The red and blue shaded region show where the derivative is positive and negative respectfully.
- The slow manifold lies below the u nullcline implying $\dfrac{du}{d\tau}$

Perturbation analysis

Start again with the non-dimensional system:

$$\frac{du}{d\tau} = -u + uv + \alpha v \tag{6.4}$$

$$\epsilon\frac{dv}{d\tau} = u - uv - \kappa v. \tag{6.5}$$

$$u(0) = 1 \quad v(0) = 0 \tag{6.6}$$

This is a singular perturbation problem. Why?

We aim to construct inner and outer solutions.

- These terms come from boundary layer problems and the inner solution refers to the dynamics near the boundary.
- The outer solution refers to the dynamics significantly far enough away from the boundary

In our case

- Inner solution is for small time
- Outer is for large enough time.

Outer Solution

We apply an asymptotic expansion:

$$u(\tau) = u_0(\tau) + \epsilon u_1(\tau) + \epsilon^2 u_2(\tau) + \cdots \tag{6.7}$$

$$v(\tau) = v_0(\tau) + \epsilon v_1(\tau) + \epsilon^2 v_2(\tau) + \cdots \tag{6.8}$$

These do not necessarily converge as $n \to \infty$. The series aims to make a statement about $\epsilon \to 0$. We don't really care about $n \to \infty$. See Holmes (2013) for details.

We substitute the expansions into the system, collect like terms and simplify. The leading order problem, for the outer solution, is given by

$$\mathcal{O}(1): \quad \frac{du_0}{d\tau} = -u_0 + u_0 v_0 + \alpha v_0$$

$$0 = u_0 - u_0 v_0 - \kappa v_0.$$

$$u_0(0) = 1 \quad v_0(0) = 0.$$

This is a differential-algebraic system.

We solve the algebraic equation:

$$v_0(\tau) = \frac{u_0(\tau)}{\kappa + u_0(\tau)}, \tag{6.9}$$

which allows us to write the first equation as:

$$\frac{du_0}{d\tau} = \frac{-(\kappa - \alpha)u_0}{\kappa + u_0}, \tag{6.10}$$

which furthermore can be solved;

$$u_0(\tau) + \kappa \ln u_0(\tau) = A - (\kappa - \alpha)\tau, \tag{6.11}$$

Where A is a constant of integration, that upon imposing the initial condition $u_0(0) = 1$ gives $A = 1$.

Remark

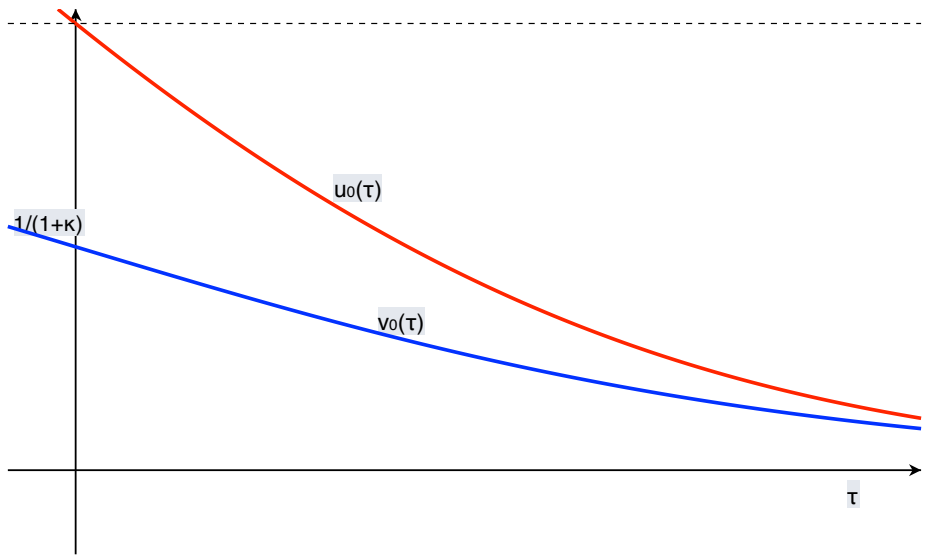
A note about the initial conditions of the outer solution.

- The initial conditions for the full model may not always be satisfied by the outer solution. Can you say why this might be? For example, the initial condition $v(0) = 0$ can not be satisfied by $v_0(\tau)$.
- We will see later that this is not an issue, because technically the initial conditions only need to be satisfied by the inner solution and later matched to the outer solution.

So our outer solution is given by

$$u_0(\tau) + \kappa \ln u_0(\tau) = 1 - (\kappa - \alpha)\tau \tag{6.12}$$

$$v_0(\tau) = \frac{u_0(\tau)}{\kappa + u_0(\tau)} \tag{6.13}$$



- The red curve shows u_0,
- The blue curve shows v_0

Question:

- What assumptions were made when constructing the outer problem?
- We neglected the $\epsilon \frac{dv}{d\tau}$ term
- Essentially implying $\epsilon \frac{dv}{d\tau} = \mathcal{O}(\epsilon)$.
- Which is only true when $\frac{dv}{d\tau} = \mathcal{O}(1)$.

These assumptions are only valid when the reaction is well underway.

Question:

- How do we handle what happens for $\tau \ll 1$?

We introduce a new timescale, one that lets us take a closer look at the neighbourhood near $\tau = 0$.

Inner Solution

Let the new timescale be $\sigma = \delta(\epsilon)\tau$, were $\delta(\epsilon)$ is to be determined.

- We want σ to be $\mathcal{O}(1)$ when $\tau = \mathcal{O}(\epsilon)$

We introduce the fast, or inner, variables;

$$u(\tau;\epsilon) = U(\sigma;\epsilon) \quad v(\tau;\epsilon) = V(\sigma;\epsilon) \tag{6.14}$$

subject to initial conditions $U(0) = 1,\ V(0) = 0$.

Apply the asymptotic expansion:

$$U(\sigma;\epsilon) = U_0 + \epsilon U_1 + \epsilon^2 U_2 + \cdots \tag{6.15}$$

$$V(\sigma;\epsilon) = V_0 + \epsilon V_1 + \epsilon^2 V_2 + \cdots \tag{6.16}$$

and by chain rule,

$$\frac{dv}{d\tau} = \delta(\epsilon)\frac{dV}{d\sigma}, \tag{6.17}$$

the fast system is given by

$$\frac{dU}{d\sigma} = \frac{1}{\delta(\epsilon)}(-U + (U+\alpha)V) \tag{6.18}$$

$$\delta(\epsilon)\epsilon\frac{dV}{d\sigma} = U - (U+\kappa)V \tag{6.19}$$

We chose $\delta(\epsilon) = \frac{1}{\epsilon}$ so that we retain the $\frac{dV}{d\sigma}$ term at leading order. In other words, we force a regular perturbation. Substitution of the asymptotic expansion, simplifying etc. the leading order problem is given by:

$$\mathcal{O}(1): \quad \frac{dU_0}{d\sigma} = 0 \tag{6.20}$$

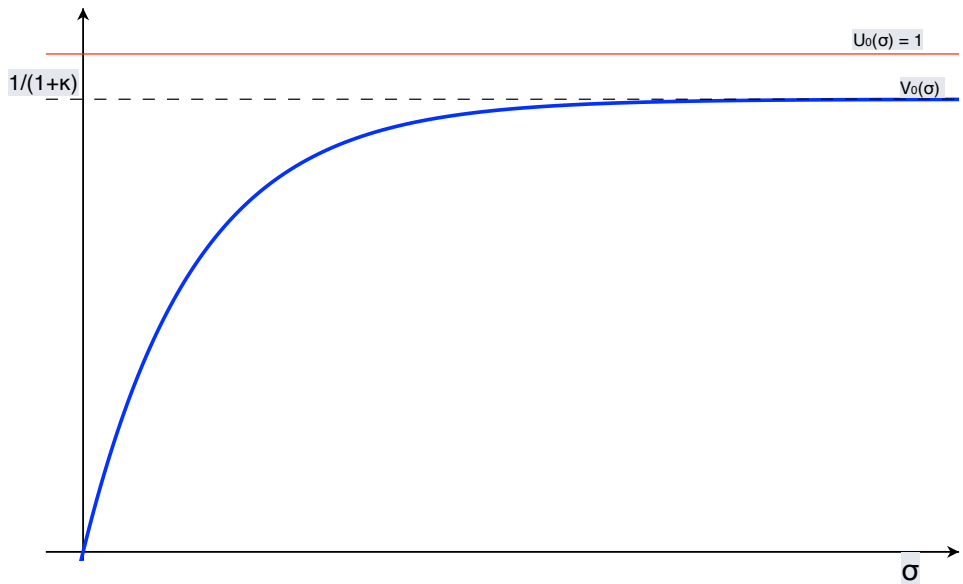
$$\frac{dV_0}{d\sigma} = U_0 - (U_0 + \kappa)V_0 \tag{6.21}$$

$$U_0(0) = 1 \quad V_0(0) = 0 \tag{6.22}$$

Which has the solution:

$$U_0(\sigma) = 1 \tag{6.23}$$

$$V_0(\sigma) = \frac{1}{1+\kappa}(1 - e^{-(1+\kappa)\sigma}) \tag{6.24}$$



- The red curve shows U_0,
- The blue curve shows V_0

- Here, the inner solution can satisfy the initial conditions, however for large values of σ a contradiction arises.
- That is, the complex and substrate both should tend to zero in the reaction. Conveniently, the outer solution tends to zero.

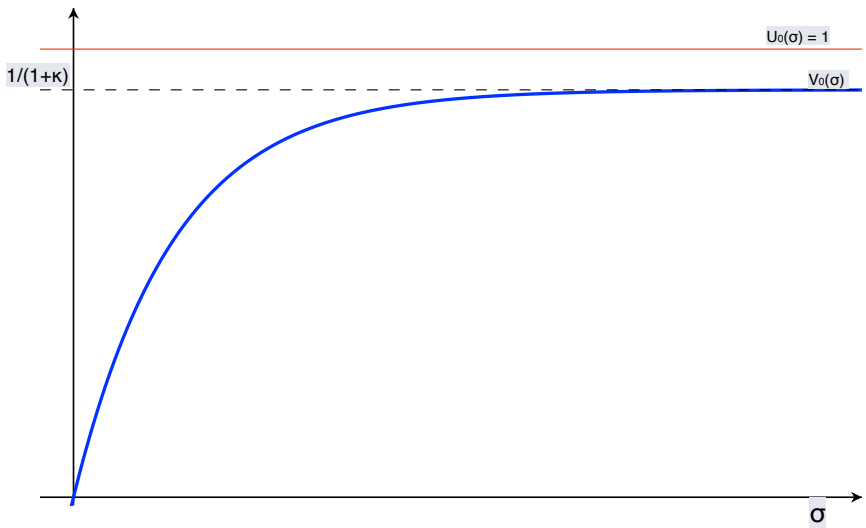
Question:

- How do we link the inner and outer solutions?

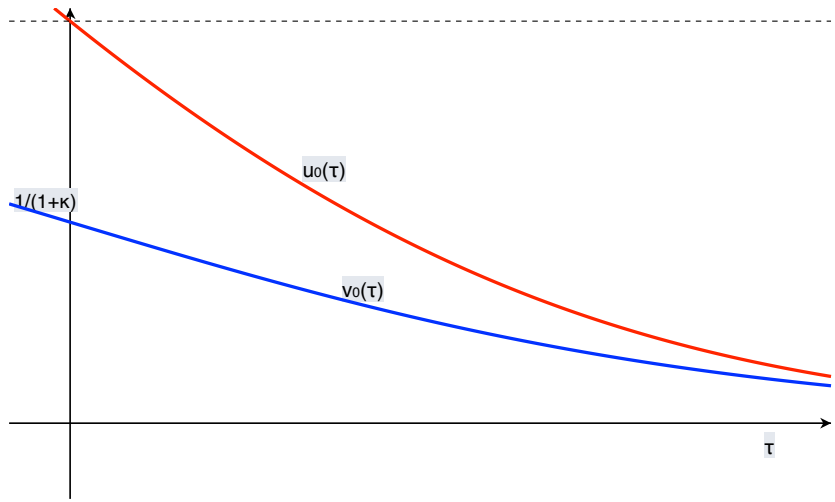
We use the asymptotic matching condition. We essentially glue the solutions together to come up with a uniform (for all time) solution, still of the first order.

We currently have:

inner solution



outer solution



We need to "match" these solutions.

The matching process comes from the dynamics, which are as follows:

- We start on the inner solution
- Eventually, the inner solution will become invalid
- But the outer solution will eventually become valid.
- The dynamics "transition" from inner to outer over some transitional layer.

We want the inner and outer solutions to match-up and transition nicely.

That is, for the matching we require;

$$\lim_{\sigma\to\infty} U_0(\sigma) = \lim_{\tau\to 0} u_0(\sigma) = u_{m0} \tag{6.25}$$

$$\lim_{\sigma\to\infty} V_0(\sigma) = \lim_{\tau\to 0} v_0(\sigma) = v_{m0} \tag{6.26}$$

In our example, this condition is satisfied naturally, and

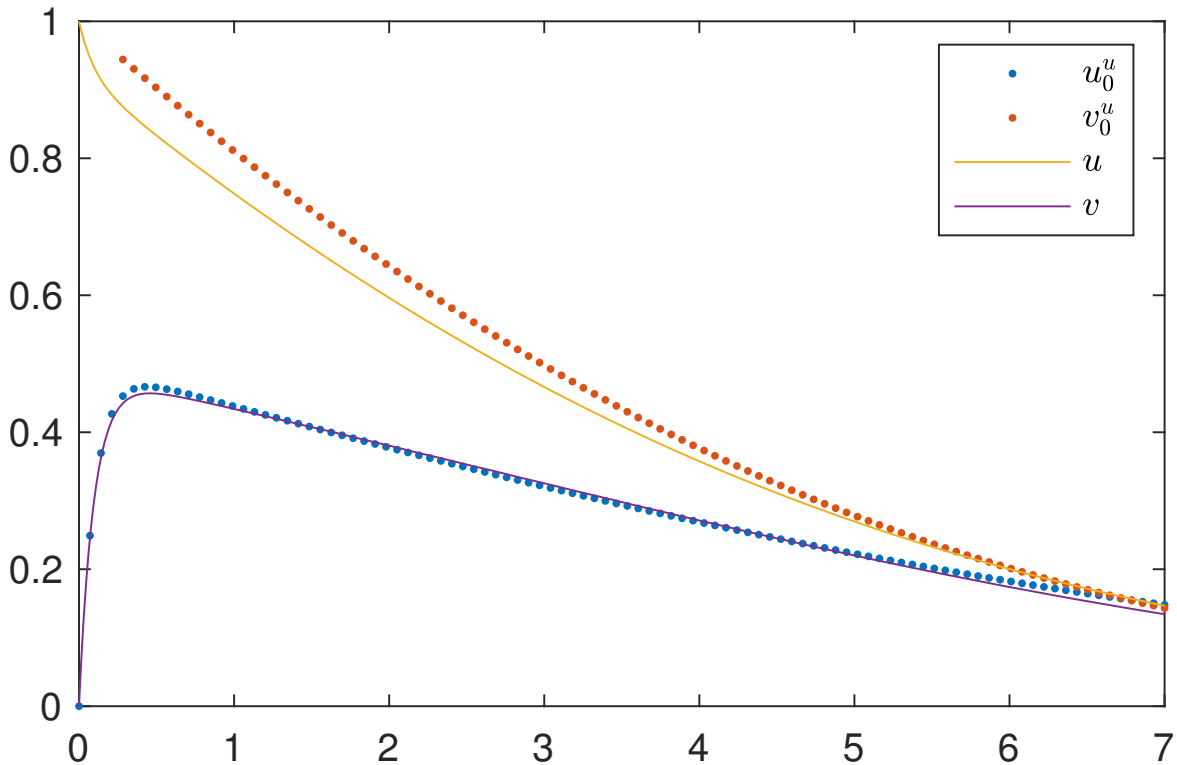
$$\lim_{\sigma\to\infty} U_0(\sigma) = \lim_{\tau\to 0} u_0(\sigma) = u_{m0} = 1, \tag{6.27}$$

$$\lim_{\sigma\to\infty} V_0(\sigma) = \lim_{\tau\to 0} v_0(\sigma) = v_{m0} = \frac{1}{\kappa+1}. \tag{6.28}$$

We can finally construct an uniform first order approximation given by;

$$u_0^u(\tau) = u_0(\tau) + U_0(\tau/\epsilon) - u_{m0}$$

$$v_0^u(\tau) = v_0(\tau) + V_0(\tau/\epsilon) - v_{m0}$$



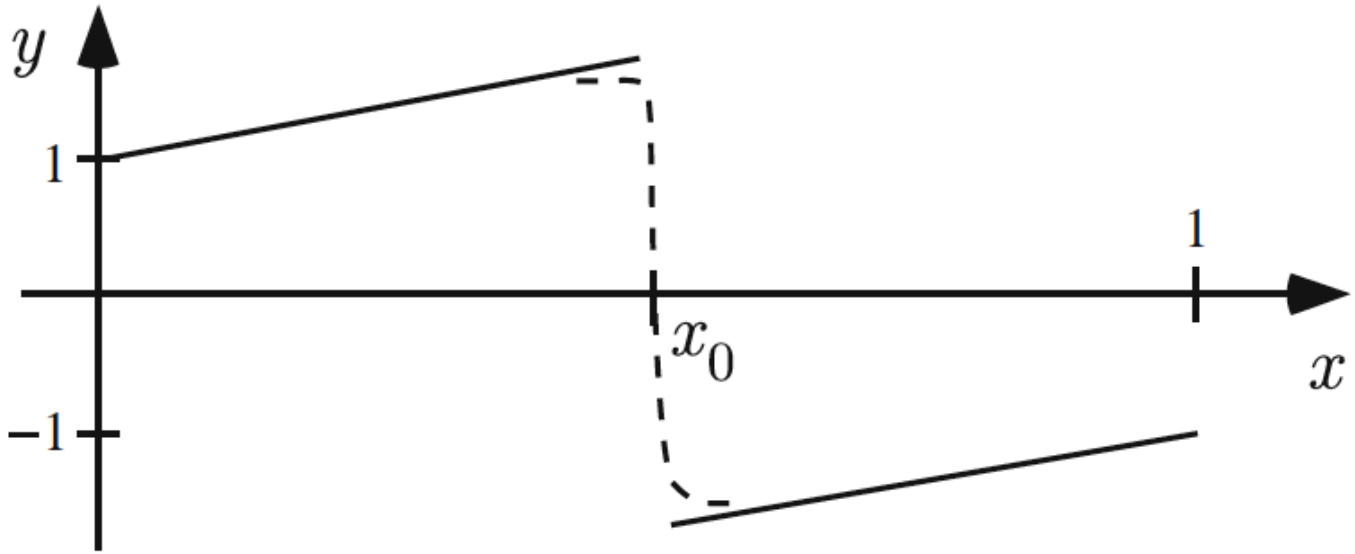
Other methods in Perturbation theory:

- Interior layers
- Multiple scales
- WKB method

Interior layer

This methods is similar to that of the boundary layer examples.

- Has two outer solutions (left and right of interior layer)
- Interior layer coordinate $\bar{x} = \frac{x - x_0}{\epsilon^\alpha}$ with corresponding interior solution.



A problem can contain any combination of boundary layers

Multiple Scales

In the method of matched asymptotic expansion we applied the expansion of our desired solution as:

$$y(t) = a_0(\epsilon)x_0(t) + a_1(\epsilon)x_1(t) + \dots$$

where $a_0(\epsilon), a_1(\epsilon), \dots$ is an asymptotic sequence.

In the method of multiple scales we assume there are multiple scales of the independent variable. i.e. $t_1 = t$ and $t_2 = \frac{t}{\epsilon^\alpha}$

Multiple scales

In doing this, we have that

$$\frac{d}{dt} \to \frac{dt_1}{dt}\frac{\partial}{t_1} + \frac{dt_2}{dt}\frac{\partial}{_2} = \frac{\partial}{\partial t_1} + \epsilon^{\alpha}\frac{\partial}{\partial t_2}$$

and we would now use the expansion:

$$y(t) \sim y_0(t_1, t_2) + \epsilon y_1(t_1, t_2) + \dots$$

and solving for y_0 proceeds similarly to previous methods.

This methods makes it easier to avoid secular terms. i.e. when the terms eventually are comparable. E.g.

$y \sim \sin(t) + \epsilon t \sin(t)$

WKB method

The WKB method, like other methods, seeks to approximate the solution $y(t)$. However, here, we assume that the solution depends on the fast variation in an exponential fashion. The expansion takes the form:

$$y(t) \sim e^{\frac{\theta(t)}{\epsilon^\alpha}} (y_0(t) + \epsilon^\alpha y_1(t) + \dots)$$

Actually, in many cases the WKB method can be easier to use, although the assumptions are limiting.

Thank you!

Contact me!

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