Math 515
Essential Perturbation Theory and Asymptotic Analysis
Chapter 01

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Chapter 01, Part 2 of 2
Motivating Themes

A Regular Perturbation Initial Value Problem

Projectile Motion Near the Surface of the Earth

The force due to gravity, F, exerted on a small, dense ball of mass m near the surface of the Earth is given by the relation

$$F = -\frac{GmM}{(R+x)^2},$$

where G is the gravitational constant, M is the mass of the Earth in kilograms, R is the radius of the Earth in meters, and x is the height above the surface of the Earth in meters. We will assume for simplicity that the ball moves only in the radial direction, outward from the center of the Earth. Newton's second law of motion reads $F = ma$, where a is the acceleration of the ball in the radial direction, and implies that

$$\frac{\mathrm{d}^2 x}{\mathrm{d}t^2}(t) = a(t) = -\frac{GM}{(R+x(t))^2},$$

where t is measured in seconds. Let as assume that the ball is launched with an initial height of zero and an initial velocity of v_o, in other words,

$$x(0) = 0 \quad \text{and} \quad \frac{\mathrm{d}x}{\mathrm{d}t}(0) = v_o.$$

Non-Dimensionalization

Let us define $\tau := t/t_\star$ and $y(\tau) := x(\tau t_\star)/x_\star$, where $x_\star$ is a positive characteristic height above the Earth (in meters) and $t_\star$ is a positive characteristic time for the problem (measured in seconds). Then

$$\frac{\mathrm{d}x}{\mathrm{d}t}(t) = \frac{\mathrm{d}\tau}{\mathrm{d}t}\frac{\mathrm{d}x}{\mathrm{d}\tau}(\tau t_\star) = \frac{x_\star}{t_\star}\frac{\mathrm{d}y}{\mathrm{d}\tau}(\tau),$$

and, likewise

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2}(t) = \frac{x_\star}{t_\star^2}\frac{\mathrm{d}^2y}{\mathrm{d}\tau^2}(\tau).$$

Therefore,

$$\frac{\mathrm{d}^2y}{\mathrm{d}\tau^2}(\tau) = -\frac{\frac{GM}{R^2}\frac{t_\star^2}{x_\star}}{\left(1+\varepsilon y(\tau)\right)^2},$$

where $\varepsilon := \frac{x_\star}{R}$. We will choose the characteristic height and time so that

$$\frac{GM}{R^2}\frac{t_\star^2}{x_\star} = 1. \tag{1}$$

Non-Dimensionalization

Consider the initial velocity. We transform that condition, using our change of variables, to

$$v_o = \frac{\mathrm{d}x}{\mathrm{d}t}(0) = \frac{x_\star}{t_\star}\frac{\mathrm{d}y}{\mathrm{d}\tau}(0).$$

In other words,

$$\frac{\mathrm{d}y}{\mathrm{d}\tau}(0) = \frac{v_o t_\star}{x_\star}.$$

To complete our non-dimensionalization process, we require

$$\frac{v_o t_\star}{x_\star} = 1. \tag{2}$$

Solving Equations (1) and (2), we have

$$x_\star = \frac{R^2 v_o^2}{GM} \quad \text{and} \quad t_\star = \frac{R^2 v_o}{GM}.$$

A Regular Perturbation Problem

To sum up, the non-dimensionalized problem is given by

$$\frac{\mathrm{d}^2 y}{\mathrm{d}t^2}(t) = -\frac{1}{(1+\varepsilon y(t))^2}, \quad y(0) = 0, \quad y'(0) = 1, \tag{3}$$

where $\varepsilon > 0$ is a (typically small) dimensionless parameter. We expect the problem to be regular, in the sense that, when $\varepsilon = 0$, the problem maintains its essential structure. In particular, it is still second order. The model conforms to our grade school notion that the acceleration due to gravity in a layer very near to the surface of the Earth is very nearly constant. In this case, the acceleration is just normalized to -1 as $\varepsilon \searrow 0$.

A Perturbative Solution Approach

As the product of y and ε becomes non-negligible, because the non-dimensional height y is becoming large, we expect the motion to deviate from the usual parabolic trajectory.

Naturally, in this course we want to compute analytical approximations that are valid for small, but non-zero, values of ε, without numerical approximation. Let us suppose that

$$y(t) = y_0(t) + \varepsilon y_1(t) + \varepsilon^2 y_2(t) + \cdots .$$

Plugging this into the differential equation and boundary conditions and equating terms, we have, for the leading order and first order equations,

$$\begin{aligned} \varepsilon^0 : &\quad y_0''(t) = -1, \quad y_0(0) = 0, \quad y_0'(0) = 1, \\ \varepsilon^1 : &\quad y_1''(t) = 2y_0(t), \quad y_1(0) = 0, \quad y_1'(0) = 0. \end{aligned}$$

Asymptotic Expansion

Considering

$$\begin{aligned} \varepsilon^0 :& \quad y_0''(t) = -1, \quad y_0(0) = 0, \quad y_0'(0) = 1, \\ \varepsilon^1 :& \quad y_1''(t) = 2y_0(t), \quad y_1(0) = 0, \quad y_1'(0) = 0, \\ \varepsilon^2 :& \quad y_2''(t) = 2y_1(t) - 3y_0^2(t), \quad y_2(0) = 0, \quad y_2'(0) = 0. \end{aligned}$$

The leading-order solution, y_0, is

$$y_0(t) = -\frac{1}{2}t^2 + t,$$

and the first-order correction, y_1, is given by

$$y_1(t) = \frac{1}{3}t^3 - \frac{1}{12}t^4.$$

The second-order correction, y_2, is

$$y_2(t) = \frac{1}{360}(-90t^4 + 66t^5 - 11t^6).$$

Thus,

$$y(t) = -\frac{1}{2}t^2 + t + \left(\frac{1}{3}t^3 - \frac{1}{12}t^4\right)\varepsilon + \frac{1}{360}(-90t^4 + 66t^5 - 11t^6)\varepsilon^2 + \cdots .$$

Composite Approximations

So, to a good approximation, valid when we believe that the ε^2 term, and, of course, all higher-order terms, are negligible, we have the following approximate solution to our problem:

$$y_{\mathrm{c},1}(t,\varepsilon) = -\frac{1}{2}t^2 + t + \left(\frac{1}{3}t^3 - \frac{1}{12}t^4\right)\varepsilon, \tag{4}$$

which we call the **first-order composite solution**. Keeping the first three terms of our expansion yields the **second-order composition solution**

$$\begin{aligned} y_{\mathrm{c},2}(t,\varepsilon) = -\frac{1}{2}t^2 + t + \left(\frac{1}{3}t^3 - \frac{1}{12}t^4\right)\varepsilon \\ + \frac{1}{360}(-90t^4 + 66t^5 - 11t^6)\varepsilon^2. \end{aligned} \tag{5}$$

See the figure on the next slide.

Approximate Trajectories

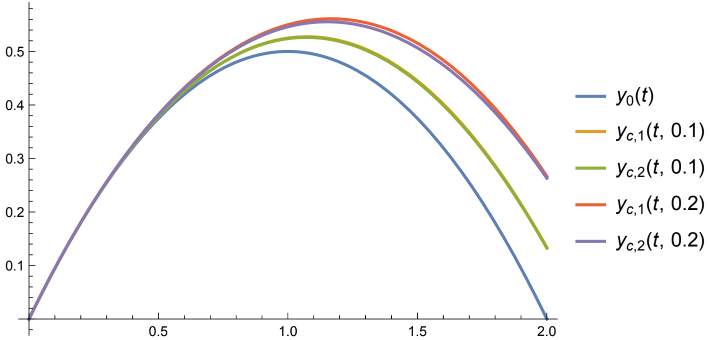

Figure: Plots of the approximate projectile motions $y_0(t)$, $y_{c,1}(t,\varepsilon)$, and $y_{c,1}(t,\varepsilon)$, for the values $\varepsilon = 0.1$ and $\varepsilon = 0.2$. Observe that the approximate solutions, $y_{c,1}(t,\varepsilon)$ and $y_{c,1}(t,\varepsilon)$, predict that the projectile will fly higher than what is predicted by the model with a uniform, constant gravitational field, since the force of gravity weakens with distance.

Singular Perturbations and Boundary Layers

A Linear Singular Perturbation Boundary Value Problem

Let us consider the following problem: for any $\varepsilon > 0$, suppose that $u : [0,1] \to \mathbb{R}$ satisfies

$$\varepsilon \frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + (1+\varepsilon) y'(x) + y(x) = 0, \quad y(0) = 0, \quad y(1) = 1. \tag{6}$$

We are interested in solution to this problem for small values of ε. This is a singular perturbation problem because, when $\varepsilon = 0$, the problem reduces to the first-order ODE problem

$$y'(x) + y(x) = 0, \quad y(0) = 0, \quad y(1) = 1, \tag{7}$$

which has no solution.

A Linear Singularly Perturbed BVP

The difficulty with the problem

$$y'(x) + y(x) = 0, \quad y(0) = 0, \quad y(1) = 1, \tag{8}$$

is that a general solution to the first-order ordinary differential equation above, namely,

$$y(x) = Ce^{-x},$$

cannot satisfy both boundary conditions. But, for the case for which $\varepsilon > 0$, we are lucky. We can find the exact solution to this linear boundary value problem (BVP) easily. In particular, for any $\varepsilon > 0$,

$$y(x) = y(x, \varepsilon) := \frac{e^{-x} - e^{-x/\varepsilon}}{e^{-1} - e^{-1/\varepsilon}}. \tag{9}$$

Plots of the solution are shown on the next slide.

Boundary Layers

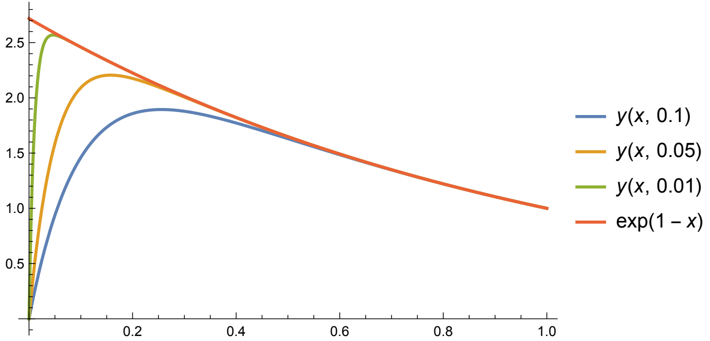

Figure: Plots of the solution $y(x) = y(x, \varepsilon)$, for the values $\varepsilon = 0.1$ (blue), $\varepsilon = 0.05$ (orange), and $\varepsilon = 0.01$ (green). The red line is the leading-order outer solution, $y_0(x) = e^{1-x}$.

Boundary Layers

The solution describe what is known as a **boundary layer** at $x = 0$, that is, a rapid transition in the function from one value or functional form to another value or functional form. For small values of $\varepsilon > 0$, as $x \searrow 0$, the solution rapidly transitions from the functional form e^{1-x} to the value zero.

Also observe that

$$y'(0, \varepsilon) \nearrow \infty, \quad \text{as} \quad \varepsilon \searrow 0.$$

In the usual parlance of analysis, we say that the sequence of solution functions, $\{y(\,\cdot\,, \varepsilon)\}_{\varepsilon>0}$ does not converge uniformly as $\varepsilon \searrow 0$.

Now, let us pretend that we do not know this true solution. Let us pretend that the only thing we know about the problem is that the boundary layer will occur at $x = 0$. We start by constructing a solution away from the boundary layer, the part called the **outer solution**.

Outer Solution

For the outer solution, we begin by assuming that, away from the boundary layer, our solution can be expanded as the series

$$y_{\text{out}}(x,\varepsilon) = y_0(x) + y_1(x)\varepsilon + y_2(x)\varepsilon^2 + \cdots . \tag{10}$$

Inserting this expansion into the equation

$$\varepsilon \frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + (1+\varepsilon)y'(x) + y(x) = 0 \tag{11}$$

we obtain

$$\begin{aligned} 0 = {} & y_0''(x)\varepsilon + y_1''(x)\varepsilon^2 + y_2''(x)\varepsilon^3 + \cdots \\ & + y_0'(x) + y_1'(x)\varepsilon + y_2'(x)\varepsilon^2 + \cdots \\ & + y_0'(x)\varepsilon + y_1'(x)\varepsilon^2 + y_2'(x)\varepsilon^3 + \cdots \\ & + y_0(x) + y_1(x)\varepsilon + y_2(x)\varepsilon^2 + \cdots . \end{aligned}$$

Outer Solution

Equating like powers of ε, we obtain a recursive sequence of equations:

$$\begin{aligned}
\varepsilon^0 : &\quad y_0'(x) + y_0(x) = 0, \\
\varepsilon^1 : &\quad y_1'(x) + y_1(x) = -(y_0'(x) + y_0(x))', \\
\varepsilon^2 : &\quad y_2'(x) + y_2(x) = -(y_1'(x) + y_1(x))', \\
&\vdots
\end{aligned}$$

The boundary conditions can be found via

$$1 = y_{\mathrm{out}}(1, \varepsilon) = y_0(1) + y_1(1)\varepsilon + y_2(1)\varepsilon^2 + \cdots ,$$

and equating like powers of ε., which yields

$$\begin{aligned}
\varepsilon^0 : &\quad y_0(1) = 1, \\
\varepsilon^1 : &\quad y_1(1) = 0, \\
\varepsilon^2 : &\quad y_2(1) = 0, \\
&\vdots
\end{aligned}$$

Outer Solution

The leading-order outer solution is

$$y_0(x) = e^{1-x}.$$

It satisfies the boundary condition at $x = 1$, as designed, but not at $x = 0$. The first-order solution is

$$y_1(x) = 0, \quad \forall\, x \in (0, 1].$$

In fact, for all $n \in \mathbb{N}$,

$$y_n(x) = 0, \quad \forall\, x \in (0, 1].$$

The outer solution is precisely

$$y_{\mathrm{out}}(x, \varepsilon) = e^{1-x}. \tag{12}$$

Inner Solution: The Stretched Variable

Now we want to construct the inner solution, that part of the solution that is valid in the boundary layer near $x = 0$. Before we begin, we need to determine the boundary layer thickness and the structure of the inner problem. We introduce a change of variables and use the method of dominant balance. Specifically, suppose that $z = \varepsilon^{\alpha} x$, which is called the **stretched variable**. Set $Y(z) := y(\varepsilon^{-\alpha} z) = y(x)$. Then,

$$\frac{\mathrm{d}y}{\mathrm{d}x}(x) = \frac{\mathrm{d}z}{\mathrm{d}x}\frac{\mathrm{d}Y}{\mathrm{d}z}(z) = \varepsilon^{\alpha}\frac{\mathrm{d}Y}{\mathrm{d}z}(z).$$

and

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2}(x) = \varepsilon^{2\alpha}\frac{\mathrm{d}^2 Y}{\mathrm{d}z^2}(z).$$

It follows that

$$\varepsilon^{1+2\alpha}\frac{\mathrm{d}^2 Y}{\mathrm{d}z^2}(z) + \varepsilon^{1+\alpha}\frac{\mathrm{d}Y}{\mathrm{d}z}(z) + \varepsilon^{\alpha}\frac{\mathrm{d}Y}{\mathrm{d}z}(z) + Y(z) = 0.$$

We assume that the function and all of its derivatives are of order $\varepsilon^0 = 1$ in the boundary layer, once the appropriate stretched variable is determined, that is, once α is determined.

Inner Solution: Dominant Balance

To find the value of α, we use the principle of dominant balance: (i) the coefficient of the first term balances with that of another term with respect to their powers of ε, and (ii) these two terms dominate all other terms in the limit $\varepsilon \searrow 0$. The options are as follows:

1. Terms 1 and 2 balance. In this case, $\varepsilon^{1+2\alpha} = \varepsilon^{1+\alpha}$, which implies that $\alpha = 0$. This is not a possibility, since $\varepsilon \not\gg \varepsilon^0$, as $\varepsilon \searrow 0$.
2. Terms 1 and 3 balance. In this case, $\alpha = -1$. Terms 1 and 3 are of order ε^{-1}. Terms 2 and 4 are both of order $\varepsilon^0 = 1$. This does satisfy dominant balance, since $\varepsilon^{-1} \gg \varepsilon^0 = 1$, as $\varepsilon \searrow 0$. ✓
3. Terms 1 and 4 balance. In this case, $\alpha = -1/2$ and terms 1 and 4 are of order $\varepsilon^0 = 1$. Term 2 is of order $\varepsilon^{1/2}$, and term 3 is of order $\varepsilon^{-1/2}$. This is not a possibility, since $\varepsilon^0 \not\gg \varepsilon^{-1/2}$, as $\varepsilon \searrow 0$.

Inner Solution: The Stretched Problem

Thus, using option 2, $z = \frac{x}{\varepsilon}$ and the inner equation is

$$\frac{1}{\varepsilon}\frac{\mathrm{d}^2 Y}{\mathrm{d}z^2}(z) + \frac{\mathrm{d}Y}{\mathrm{d}z}(z) + \frac{1}{\varepsilon}\frac{\mathrm{d}Y}{\mathrm{d}z}(z) + Y(z) = 0, \tag{13}$$

or, equivalently,

$$\frac{\mathrm{d}^2 Y}{\mathrm{d}z^2}(z) + (1+\varepsilon)\frac{\mathrm{d}Y}{\mathrm{d}z}(z) + \varepsilon Y(z) = 0, \tag{14}$$

Inner Solution: Leading-Order Approximation

As with the outer solution, we look for a solution of the form

$$Y_{\mathrm{in}}(z,\varepsilon) = Y_0(z) + Y_1(z)\varepsilon + Y_2(z)\varepsilon^2 + \cdots . \tag{15}$$

Plugging this into the inner equation (14), we have

$$\begin{aligned} 0 = {} & Y_0''(z) + Y_1''(z)\varepsilon + Y_2''(z)\varepsilon^2 + \cdots \\ & + Y_0'(z) + Y_1'(z)\varepsilon + Y_2'(z)\varepsilon^2 + \cdots \\ & + Y_0'(z)\varepsilon + Y_1'(z)\varepsilon^2 + Y_2'(z)\varepsilon^3 + \cdots \\ & + Y_0(z)\varepsilon + Y_1(z)\varepsilon^2 + Y_2(z)\varepsilon^3 + \cdots \end{aligned}$$

Equating like powers of ε we get the following recursive sequence of equations:

$$\begin{aligned} \varepsilon^0 : &\quad Y_0''(z) + Y_0'(z) = 0, \\ \varepsilon^1 : &\quad Y_1''(z) + Y_1'(z) = -(Y_0'(z) + Y_0(x)), \\ \varepsilon^2 : &\quad Y_2''(z) + Y_2'(z) = -(Y_1'(z) + Y_1(x)), \\ &\vdots \end{aligned}$$

Inner Solution: Leading-Order Approximation

Boundary conditions are found via

$$0 = Y_{\mathrm{in}}(0, \varepsilon) = Y_0(0) + Y_1(0)\varepsilon + Y_2(0)\varepsilon^2 + \cdots$$

which, upon equating powers, yields

$$\begin{aligned} \varepsilon^0 : &\quad Y_0(0) = 0, \\ \varepsilon^1 : &\quad Y_1(0) = 0, \\ \varepsilon^2 : &\quad Y_2(0) = 0, \\ &\vdots \end{aligned}$$

The general solution to the leading-order problem is

$$Y_0(z) = C_{0,1} e^{-z} + C_{0,2}.$$

Enforcing the boundary condition, we have

$$0 = Y_0(0) = C_{0,1} + C_{0,2} \quad \Longleftrightarrow \quad -C_{0,1} = A = C_{0,2}.$$

Thus,

$$Y_0(z) = A(1 - e^{-z}). \tag{16}$$

Simple Matching

Before we even consider trying to obtain Y_1, we want to determine the unknown coefficient A. This is done via what is called a **matching principle**. We will use the simplest such principle to start with. Later in the book we will invoke more complicated matching ideas.

Our simple rule is this:

$$\lim_{z \nearrow \infty} Y_0(z) = \lim_{z \searrow 0} y_0(x). \tag{17}$$

In other words, the leading-order inner and outer solutions should match as the stretched variable becomes large and as the original variable approaches the boundary layer. Applying this rule, we have

$$\lim_{z \nearrow \infty} A(1 - e^{-z}) = A = e^1 = \lim_{x \searrow 0} e^{1-x}. \tag{18}$$

Thus, $A = e^1$, and the leading-order inner solution is completely determined:

$$Y_0(z) = e^1 - e^{1-z}. \tag{19}$$

In principle, we can now find Y_1. We expect that it too will have one free parameter that can be determined via higher-order matching, and so on.

Composite Solution

For now, we content ourselves with constructing a composite solution that is valid over the whole of the domain, not just the inner region or the outer region. The general principle here is as follows. The leading-order **composite solution** or **uniform solution** is defined as

$$y_{\mathrm{c},0}(x) = Y_0\left(\frac{x}{\varepsilon}\right) + y_0(x) - \text{matching terms}. \tag{20}$$

In the present case, our composite leading-order solution is

$$y_{\mathrm{c},0}(x) = e^1 - e^{1-x/\varepsilon} + e^{1-x} - e^1, \tag{21}$$

or, equivalently,

$$y_{\mathrm{c},0}(x) = \frac{e^{-x} - e^{-x/\varepsilon}}{e^{-1}}, \tag{22}$$

which is remarkable like the true solution

$$y(x) = y(x,\varepsilon) := \frac{e^{-x} - e^{-x/\varepsilon}}{e^{-1} - e^{-1/\varepsilon}}. \tag{23}$$

Composite Solution

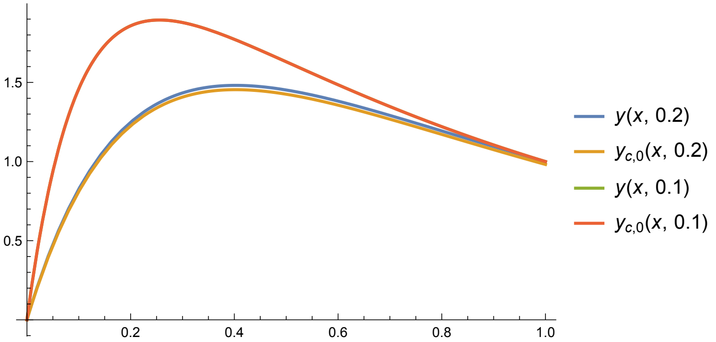

Figure: Plots of the solution $y(x, \varepsilon)$ and the leading-order composite solution $y_{c,0}(x, \varepsilon)$, for the values $\varepsilon = 0.2$ and $\varepsilon = 0.1$. Note that $y(x, 0.1)$ and $y_{c,0}(x, 0.1)$ are indistinguishable.

A Nonlinear Singular Perturbation Boundary Value Problem

The van der Waals-Cahn-Hilliard Phase Boundary

Next, consider the following two-point boundary value problem:

$$-\varepsilon^2 \frac{\mathrm{d}^2 u}{\mathrm{d}x^2} + u^3(x) - u(x) = 0, \quad u(-1) = -1, \quad u(1) = 1, \tag{24}$$

where $\varepsilon > 0$ is a small parameter. This equation models the transition of an order parameter from one pure phase, characterized by $u = -1$, to another, characterized by $u = +1$.

It comes up in thermodynamics and statistical physics when one wants to model an interface between two phases. The interfacial structure described by u, the solution of this problem, is called the van der Waals-Cahn-Hilliard phase boundary or van der Waals-Cahn-Hilliard diffuse interface.

The Limiting Structure is Singular

This is a singular perturbation problem, since when $\varepsilon = 0$, the differential equation is of reduced order. When $\varepsilon = 0$, we have a purely algebraic problem,

$$u^3(x) - u(x) = 0, \quad u(-1) = -1, \quad u(1) = 1$$

which has no solution, at least if we demand that u is continuous.

The Pure Phase or Homogeneous Free Energy

Let us make an attempt to solve the perturbed problem exactly. First, let us define the the **homogeneous free energy density**

$$W(u) := \frac{1}{4}u^4 - \frac{1}{2}u^2 + \frac{1}{4} = \frac{1}{4}\left(u^2 - 1\right)^2 .$$

Note that W is minimized by the states $u = \pm 1$, where $W(\pm 1) = 0$. See the figure on the next page. In any case,

$$W'(u) = u^3 - u,$$

and, therefore,

$$-\varepsilon^2 \frac{\mathrm{d}^2 u}{\mathrm{d}x^2} + W'(u(x)) = 0, \quad u(-1) = -1, \quad u(1) = 1. \tag{25}$$

Homogeneous Free Energy Density

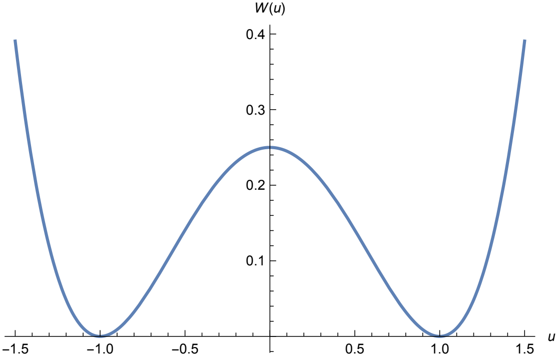

Figure: Plot of the homogeneous free energy density, $W(u)$.

Free Energy and States

Set $\Omega = (-1, 1)$. For each

$$u \in \mathcal{E} := \left\{ C^1(\Omega; \mathbb{R}) \cap C^0(\overline{\Omega}; \mathbb{R}) \;\middle|\; u(-1) = -1,\ u(1) = 1 \right\},$$

define the free energy functional

$$F(u) = \int_\Omega \left(\frac{1}{\varepsilon} W(u) + \frac{\varepsilon}{2} \left(\frac{\mathrm{d}u}{\mathrm{d}x} \right)^2 \right) \mathrm{d}x.$$

The set $\mathcal{E}$ is called the **energy set**. Members, u, of the set $\mathcal{E}$ are called **states**. So, for each state of the system, we can define an energy. Now, we want to figure out what state (or states) yields the lowest or smallest free energy.

Note that the free energy is always non-negative.

Energy Variation

We want to take a derivative of the free energy functional. How can we do this? First, define

$$\mathcal{T} := \left\{ C^1(\Omega; \mathbb{R}) \cap C^0(\overline{\Omega}; \mathbb{R}) \;\middle|\; w(-1) = 0,\ w(1) = 0 \right\},$$

which is called the **test space**. Then, for each $s \in \mathbb{R}$ and $w \in \mathcal{T}$, $u + sw \in \mathcal{E}$, and

$$F(u + sw) = \int_\Omega \left(\frac{1}{\varepsilon} W(u + sw) + \frac{\varepsilon}{2} \left(\frac{\mathrm{d}u}{\mathrm{d}x} + s \frac{\mathrm{d}w}{\mathrm{d}x} \right)^2 \right) \mathrm{d}x.$$

This computation measures the change in the energy given a change in the state of the system.

An element w from the test space $\mathcal{T}$ is called a **test function**.

Directional Derivatives

Let us compute the analog of a directional derivative. To this end, observe that, for arbitrary $w \in \mathcal{T}$.

$$\frac{\mathrm{d}}{\mathrm{d}s} F(u + sw) = \int_\Omega \left(\frac{1}{\varepsilon} W'(u + sw) w + \varepsilon \left(\frac{\mathrm{d}u}{\mathrm{d}x} + s \frac{\mathrm{d}w}{\mathrm{d}x} \right) \frac{\mathrm{d}w}{\mathrm{d}x} \right) \mathrm{d}x,$$

which leads to

$$\left. \frac{\mathrm{d}}{\mathrm{d}s} F(u + sw) \right|_{s=0} = \int_\Omega \left(\frac{1}{\varepsilon} W'(u) w + \varepsilon \frac{\mathrm{d}u}{\mathrm{d}x} \frac{\mathrm{d}w}{\mathrm{d}x} \right) \mathrm{d}x.$$

Using integration-by-parts, we have

$$\begin{aligned} \left. \frac{\mathrm{d}}{\mathrm{d}s} F(u + sw) \right|_{s=0} &= \int_\Omega \left(\frac{1}{\varepsilon} W'(u) - \varepsilon \frac{\mathrm{d}^2 u}{\mathrm{d}x^2} \right) w \, \mathrm{d}x + \varepsilon \left. \frac{\mathrm{d}u}{\mathrm{d}x} w \right|_{x=-1}^{x=1} \\ &= \int_\Omega \left(\frac{1}{\varepsilon} W'(u) - \varepsilon \frac{\mathrm{d}^2 u}{\mathrm{d}x^2} \right) w \, \mathrm{d}x, \end{aligned}$$

where we used $w(\pm 1) = 0$.

The Variational Derivative

The object

$$\delta_u F := \frac{1}{\varepsilon} W'(u) - \varepsilon \frac{\mathrm{d}^2 u}{\mathrm{d}x^2} \tag{26}$$

is called the **variational derivative** of F, and it satisfies the important relation

$$\left. \frac{\mathrm{d}}{\mathrm{d}s} F(u + sw) \right|_{s=0} = \int_\Omega \delta_u F \, w \, \mathrm{d}x, \quad \forall \, w \in \mathcal{T}. \tag{27}$$

Observe that it is essentially the representation of the directional derivative of the functional F.

Think about the standard directional derivative of a function $f \in C^1(\mathbb{R}^d; \mathbb{R})$, which satisfies

$$\left. \frac{\mathrm{d}}{\mathrm{d}s} f(\mathbf{x} + s\mathbf{y}) \right|_{s=0} = \nabla f(\mathbf{x}) \cdot \mathbf{y}, \quad \forall \, \mathbf{y} \in \mathbb{R}^d.$$

Here it is obvious that the vector $\nabla f(\mathbf{x})$, which is, of course, the gradient, is the representation of the directional derivative.

Energy Minimization and Equilibrium

Observe that, if we set $\delta_u F = 0$ in $\Omega = (-1, 1)$, and mind the boundary conditions, this is equivalent to the problem that we stated earlier:

$$-\varepsilon \frac{\mathrm{d}^2 u}{\mathrm{d}x^2} + \frac{1}{\varepsilon} W'(u(x)) = 0, \quad u(-1) = -1, \quad u(1) = 1. \tag{28}$$

In other words, solving this problem is related to finding the minimum free energy state, just as setting $\nabla f(\mathbf{x}) = \mathbf{0}$ is related to finding a (local or global) minimizer of f.

We can prove, though it requires some significant machinery to do so, that if $u \in \mathcal{E}$ solves the problem (28), then it is the minimum free energy state, also called the **equilibrium state**.

An Analytic Representation of the Equilibrium Problem

Remarkably, for this nonlinear problem, we can find and analytic representation of the solution, sort of. Multiplying the ODE by u' and integrating, we get

$$\frac{\varepsilon^2}{2}\left|u'(x)\right|^2 = \zeta + W(u(x)), \quad x \in (-1,1), \tag{29}$$

where ζ is an integration constant. Let us assume that $\zeta > 0$, and define

$$\chi_{\varepsilon,\zeta}(u) := \int_0^u \frac{\varepsilon\, ds}{\sqrt{2\zeta + 2W(s)}}\ , \quad u \in [-1,1]\,.$$

Clearly $\chi_{\varepsilon,\zeta}(0) = 0$ and, by symmetry of W, $\chi_{\varepsilon,\zeta}$ is an odd function, with

$$-\chi_{\varepsilon,\zeta}(-1) = \chi_{\varepsilon,\zeta}(1) =: x_\varepsilon(\zeta).$$

Since $\chi_{\varepsilon,\zeta}$ is smooth, odd, and monotonically increasing on $[-1,1]$, $\chi_{\varepsilon,\zeta}$ has a smooth, odd, and monotonically increasing inverse

$$u = \chi_{\varepsilon,\zeta}^{-1} : [-x_\varepsilon(\zeta), x_\varepsilon(\zeta)] \to [-1,1].$$

An Analytic Representation of the Equilibrium Solution

Further, observe that

$$\frac{\mathrm{d}\chi_{\varepsilon,\zeta}^{-1}}{\mathrm{d}x}(x) = \frac{1}{\chi_{\varepsilon,\zeta}'\left(\chi_{\varepsilon,\zeta}^{-1}(x)\right)} = \frac{\sqrt{2\zeta + 2W\left(\chi_{\varepsilon,\zeta}^{-1}(x)\right)}}{\varepsilon}, \quad \forall\, x \in [-x_\varepsilon(\zeta), x_\varepsilon(\zeta)],$$

which shows that $u = \chi_{\varepsilon,\zeta}^{-1}$ satisfies (29), at least on the interval $[-x_\varepsilon(\zeta), x_\varepsilon(\zeta)]$, where it is defined and smooth.

The idea is this: we wish to pick the value of the integration constant $\zeta > 0$, if possible, so that $x_\varepsilon(\zeta) = 1$. Fix $\varepsilon > 0$, and recall that

$$x_\varepsilon(\zeta) := \varepsilon \int_0^1 \frac{\mathrm{d}s}{\sqrt{2\zeta + 2W(s)}}.$$

It is not hard to see that $x_\varepsilon(\zeta)$ is a monotonically decreasing, continuous function of ζ on $(0, \infty)$. A little more effort shows that

$$x_\varepsilon(\zeta) \nearrow +\infty, \quad \text{as} \quad \zeta \searrow 0 \quad \text{and} \quad x_\varepsilon(\zeta) \searrow 0, \quad \text{as} \quad \zeta \nearrow +\infty.$$

An Analytic Representation of the Equilibrium Solution

We conclude from all this that here is a unique value $\zeta = \zeta_o \in (0, \infty)$ such that $x_\varepsilon(\zeta_o) = 1$. The solution that we seek is, precisely,

$$u = \chi_{\varepsilon,\zeta_o}^{-1} : [-x_\varepsilon(\zeta_o) = -1, x_\varepsilon(\zeta_o) = 1] \to [-1, 1],$$

with

$$u(\pm 1) = \chi_{\varepsilon,\zeta_o}^{-1}(\pm 1) = \pm 1 \quad \text{and} \quad u(0) = \chi_{\varepsilon,\zeta_o}^{-1}(0) = 0.$$

Constructed Solutions for Various $\zeta > 0$.

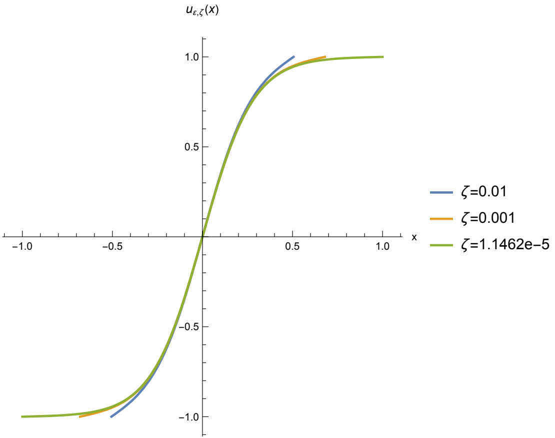

Figure: Plot plot of the constructed solution $u_{\varepsilon,\zeta}$ with the domain $[-x_\varepsilon(\zeta), x_\varepsilon(\zeta)]$, for $\varepsilon = 0.2$ and three decreasing values of ζ: $\zeta = 0.01$, $\zeta = 0.001$, and $\zeta = 1.1462 \times 10^{-05}$. Note that $x_\varepsilon(1.1462 \times 10^{-05}) \approx 1$, when $\varepsilon = 0.2$.

The quantity $x_\varepsilon(\zeta)/\varepsilon$ as $\zeta \searrow 0$, with $\varepsilon = 0.1$.

ζ	$x_\varepsilon(\zeta)/\varepsilon$
0.1	1.56094
0.01	2.52835
0.001	3.39852
0.0001	4.22931
0.00001	5.04843
0.000001	5.86407
0.0000001	6.67864
0.00000001	7.49288
0.000000001	8.30702
0.0000000001	9.12112
0.00000000001	9.93521
0.000000000001	10.7493

Table: The quantity $x_\varepsilon(\zeta)/\varepsilon$, as $\zeta \searrow 0$, is growing logarithmically slowly. But, one can prove that $x_\varepsilon(\zeta) \nearrow +\infty$ as $\zeta \searrow 0$. The values of $x_\varepsilon(\zeta)/\varepsilon$ are computed via numerical integration in Mathematica.

The Special Case of $\Omega = (-\infty, \infty)$

Finally, we point out that $\zeta = 0$ is special:

$$\chi_{\varepsilon,0}(u) = \int_0^u \frac{\varepsilon \, ds}{\sqrt{2W(s)}} = \sqrt{2}\varepsilon \operatorname{arctanh}(u), \quad -1 < u < 1.$$

Thus,

$$u_{\varepsilon,0}(x) = \tanh\left(\frac{x}{\sqrt{2}\varepsilon}\right), \quad -\infty < x < \infty,$$

$$\lim_{x \searrow -\infty} u_{\varepsilon,0}(x) = -1 \quad u_{\varepsilon,0}(0) = 0, \quad \lim_{x \nearrow +\infty} u_{\varepsilon,0}(x) = +1,$$

and

$$-\varepsilon^2 u_{\varepsilon,0}''(x) + W'(u_{\varepsilon,0}(x)) = 0, \quad -\infty < x < \infty.$$

See the next two figures.

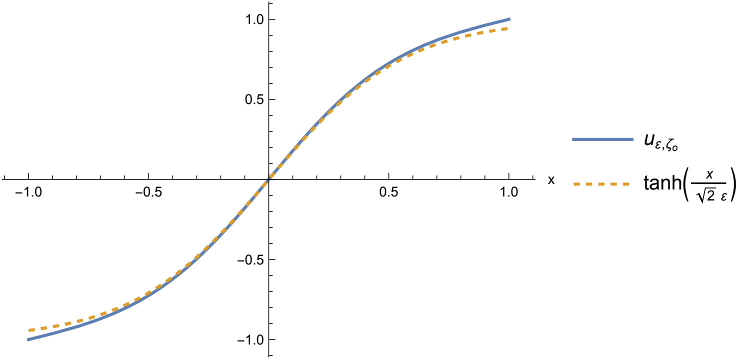

Figure: Plot of the constructed solution u_{ε,ζ_o}, with the values $\varepsilon = 0.4$ and $\zeta_o = 1.0743 \times 10^{-02}$, in comparison with the function $u_{\varepsilon,0}(x) = \tanh\left(\frac{x}{\sqrt{2}\varepsilon}\right)$, with $\varepsilon = 0.4$. Note that, for this value of ε, the hyperbolic tangent approximates the shape of the interface well, but gets the boundary values incorrect.

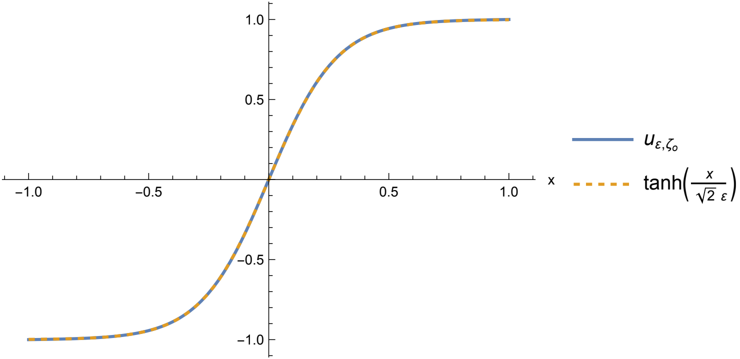

Figure: Plot of the constructed solution u_{ε,ζ_o}, with the values $\varepsilon = 0.2$ and $\zeta_o = 1.1462 \times 10^{-05}$, in comparison with the function $u_{\varepsilon,0}(x) = \tanh\left(\frac{x}{\sqrt{2}\varepsilon}\right)$, with $\varepsilon = 0.2$. These functions are indistinguishable.

Outer Solution

Now that we have gotten the “exact” solutions out of the way, next, let us attempt to approximate the solution using asymptotic methods. Of course, we expect difficulty since this is a singular perturbation problem, as we pointed out above.

First, let us assume that

$$u(x) = u_0(x) + \varepsilon u_1(x) + \varepsilon^2 u_2(x) + \cdots ,$$

and plug this expansion into (24). We get the following leading-order and correction problems:

$$\begin{aligned} \varepsilon^0 : &\quad u_0^3(x) - u_0(x) = 0, \quad u_0(\pm 1) = \pm 1, \\ \varepsilon^1 : &\quad 3u_0(x)u_1(x) - u_1(x) = 0, \quad u_1(\pm 1) = 0. \end{aligned}$$

Outer Solution

We know from the exact solutions, that there is a rapid transition, that is, a boundary layer, in an ε-neighborhood of $x = 0$. The outer solutions will hold outside of that region. Thus,

$$u_0(x) = \begin{cases} -1, & -1 \leq x < -O(\varepsilon), \\ +1, & O(\varepsilon) < x \leq +1, \end{cases}$$

The correction satisfies

$$u_1(x) = \begin{cases} 0, & -1 \leq x < -O(\varepsilon), \\ 0, & O(\varepsilon) < x \leq +1, \end{cases}$$

Inner Solution: Dominant Balance

Next we want to find an expansion for a solution inside the boundary layer. As with the singularly perturbed algebraic problems, we use a change of variables and the method of dominant balance to make progress. Suppose that $z = \varepsilon^{\alpha} x$. Set $U(z) := u(\varepsilon^{-\alpha} z) = u(x)$. Then,

$$\frac{\mathrm{d}u}{\mathrm{d}x}(x) = \frac{\mathrm{d}z}{\mathrm{d}x}\frac{\mathrm{d}U}{\mathrm{d}z}(z) = \varepsilon^{\alpha}\frac{\mathrm{d}U}{\mathrm{d}z}(z).$$

and

$$\frac{\mathrm{d}^2 u}{\mathrm{d}x^2}(x) = \varepsilon^{2\alpha}\frac{\mathrm{d}^2 U}{\mathrm{d}z^2}(z).$$

It follows that

$$-\varepsilon^{2+2\alpha}\frac{\mathrm{d}^2 U}{\mathrm{d}z^2}(z) + W'(U(z)) = 0.$$

In this case, there is no third term, and we can balance the first and second, to get $\alpha = -1$. So $z = \frac{x}{\varepsilon}$ and

$$-\frac{\mathrm{d}^2 U}{\mathrm{d}z^2}(z) + W'(U(z)) = 0. \tag{30}$$

Inner Solution: Leading Order Approximation

Assume that

$$U(z) = U_0(z) + \varepsilon U_1(z) + \varepsilon^2 U_2(z) + \cdots .$$

Inserting the expansion into (30) we obtain the following leading-order problems:

$$\begin{aligned} \varepsilon^0 : &\quad -U_0''(z) + U_0^3(z) - U_0(z) = 0, \\ \varepsilon^1 : &\quad -U_1''(z) + 3U_0(z)U_1(z) - U_1(z) = 0. \end{aligned}$$

We immediately see two possible leading-order solutions

$$U_0(z) = \tanh\left(\frac{z}{\sqrt{2}}\right)$$

or

$$U_0(z) = \tanh\left(\frac{-z}{\sqrt{2}}\right).$$

A solution to the linear first-order correction problem could be determined once the leading-order solution, U_0 is known.

Matching: Connecting the Inner and Outer Solutions

In order to determine the expansion for the inner solution, we need to determine boundary conditions for the U_i. The simplest way to do this for the leading order approximation, U_0, is via the conditions

$$\lim_{z \to -\infty} U_0(z) = \lim_{x \nearrow 0} u_0(x) \quad \text{and} \quad \lim_{z \to +\infty} U_0(z) = \lim_{x \searrow 0} u_0(x).$$

This works out to be

$$\lim_{z \to -\infty} U_0(z) = -1 \quad \text{and} \quad \lim_{z \to +\infty} U_0(z) = +1,$$

and implies that the leading-order solution is

$$U_0(z) = \tanh\left(\frac{z}{\sqrt{2}}\right).$$

Leading-Order Composite Approximation

To sum up, we can approximate the solution to the boundary value problem via

$$u(x) \approx u_{\mathrm{c},0}(x, \varepsilon) = \tanh\left(\frac{x}{\sqrt{2}\varepsilon}\right).$$

We point out that the leading-order term in our approximation satisfies the original differential equation exactly. The boundary conditions do not hold exactly. However, the approximations of the boundary conditions are quite remarkable. See the table on the next page.

The Composite Approximation Evaluated at the End Points

ε	$1.0 - \tanh\left(\frac{1}{\sqrt{2\varepsilon}}\right)$
0.10	1.44271×10^{-06}
0.09	2.99744×10^{-07}
0.08	4.20451×10^{-08}
0.07	3.36478×10^{-09}
0.06	1.16041×10^{-10}
0.05	1.04072×10^{-12}
0.04	8.88178×10^{-16}

Table: The difference between the exact boundary value, 1, and the value given by the approximation, $\tanh\left(\frac{x}{\sqrt{2\varepsilon}}\right)$, for decreasing values of ε.

Hyperbolic Tangent Solutions/Approximations

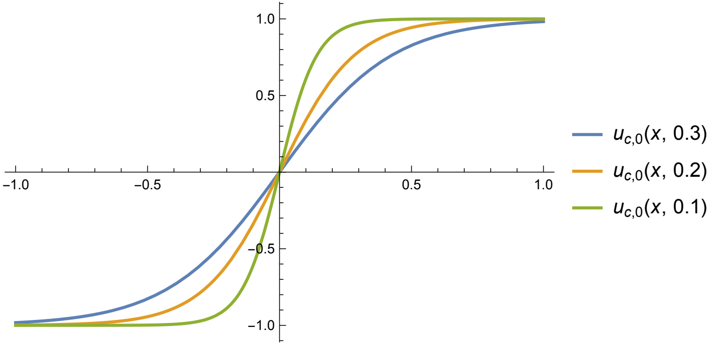

Figure: Plots of the hyperbolic tangent interface for the values $\varepsilon = 0.3$, $\varepsilon = 0.2$, and $\varepsilon = 0.1$.