Jackson "formal" notes January 2020

1 Some formal theorems

A physics problem cannot be completely specified by a differential equation, but we also need an appropriate set of boundary conditions. Often we choose the electrostatic potential Φ to be zero at infinity. But sometimes we are concerned with a finite region of space with the potential or charge specified on the boundary walls. These boundary conditions result from the presence of charges *outside* the volume of interest, but we either do not know or do not care about these charges. For example, we may use a battery to set a conductor to a specified potential, and we do not care about the charge distribution in the battery.

To develop some useful theorems we start with some pure mathematics. Let ϕ and ψ be differentiable scalar functions of position defined in a volume V and on the bounding surface S. Then

$$\vec{\nabla} \cdot \left(\phi \vec{\nabla} \psi \right) = \phi \nabla^2 \psi + \vec{\nabla} \phi \cdot \vec{\nabla} \psi$$

Now integrate this expression over a volume V , and use the divergence theorem on the left side, to get

$$\begin{aligned} \int_V \vec{\nabla} \cdot \left(\phi \vec{\nabla} \psi \right) \, dV &= \int_V \left(\phi \nabla^2 \psi + \vec{\nabla} \phi \cdot \vec{\nabla} \psi \right) \, dV \\ \oint_S \left(\phi \vec{\nabla} \psi \right) \cdot \hat{n} \, dA &= \oint_S \phi \frac{\partial \psi}{\partial n} \, dA = \int_V \left(\phi \nabla^2 \psi + \vec{\nabla} \phi \cdot \vec{\nabla} \psi \right) \, dV \end{aligned} \qquad (1)$$

(Green's first identity) . As always when using the divergence theorem, $\hat{n}$ is the normal *outward* from the volume V. We have used the shorthand notation

$$\hat{n} \cdot \vec{\nabla} \equiv \frac{\partial}{\partial n}$$

Be careful with this: there is no variable "n" with respect to which we are diffferentiating. Next we interchange the functions ϕ and ψ and subtract the two relations to get

$$\begin{aligned} \int_V \left(\phi \nabla^2 \psi - \psi \nabla^2 \phi \right) \, dV &= \int_V \left[\vec{\nabla} \cdot \left(\phi \vec{\nabla} \psi \right) - \vec{\nabla} \cdot \left(\psi \vec{\nabla} \phi \right) \right] \, dV \\ &= \oint_S \left(\phi \vec{\nabla} \psi - \psi \vec{\nabla} \phi \right) \cdot \hat{n} \, dA \end{aligned} \qquad (2)$$

(Green's second identity.) This result is also sometimes called Green's theorem.

First we'll use these results to show that the solution to a well-defined potential problem is unique. We'll also learn what we need for the problem to be well-defined.

Suppose we have two solutions to a potential problem in a volume V, that is Φ_1 and Φ_2 both satisfy Poisson's equation in V with the same charge density $\rho(\vec{x})$:

$$\nabla^2 \Phi_i = -\frac{\rho}{\varepsilon_0}$$

and either Dirichlet boundary conditions (Φ specified on S) or Neumann boundary conditions ($\frac{\partial \Phi}{\partial n} \equiv \hat{n} \cdot \vec{\nabla} \Phi$ specified on S). The latter condition is equivalent to having a known charge density on S (Notes 1 eqn 11). Let the functions ϕ and ψ in Green's first identity (1) both equal χ, where $\chi \equiv \Phi_1 - \Phi_2$. Then :

$$\int_V \left(\chi \nabla^2 \chi + \vec{\nabla} \chi \cdot \vec{\nabla} \chi \right) \, dV = \oint_S \chi \frac{\partial \chi}{\partial n} \, dA$$

But $\nabla^2 \chi = 0$ in V and either $\chi = 0$ on S (Dirichlet conditions) or $\frac{\partial \chi}{\partial n} = 0$ on S (Neumann Conditions), so this equation reduces to

$$\int_V \left| \vec{\nabla} \chi \right|^2 \, dV = 0$$

Since the integrand is ≥ 0 everywhere in V, we conclude that

$$\vec{\nabla} \chi = 0 \quad \text{in } V$$

and thus the potentials can differ by at most a constant. That is, the solution is unique up to a constant. Notice that we needed to know either Φ on the surface or $\frac{\partial \Phi}{\partial n}$ on the surface, but not both. Thus the problem is well defined provided that we know (1) the charge density in the volume and (2) either Φ or $\frac{\partial \Phi}{\partial n}$ on the surface. In the event that Φ is specified on S, the constant must be zero and the potential is unique.

Now let ϕ be the electrostatic potential $\Phi(\vec{x}')$ in the volume V and let $\psi \equiv 1/R = 1/|\vec{x} - \vec{x}'|$. Then from Green's second identity (equation 2), with the primed variables as the integration variables, we have

$$\begin{aligned}
\int_V \left(\Phi(\vec{x}') \nabla'^2 \frac{1}{R} - \frac{1}{R} \nabla'^2 \Phi(\vec{x}') \right) \, dV' &= \oint_S \left(\Phi \vec{\nabla}' \frac{1}{R} - \frac{1}{R} \vec{\nabla}' \Phi \right) \cdot \hat{n}' \, dA' \\
\int_V \left\{ \Phi(\vec{x}') \left[-4\pi \delta(\vec{x} - \vec{x}') \right] - \frac{1}{R} \left(-\frac{\rho(\vec{x}')}{\varepsilon_0} \right) \right\} \, d^3\vec{x} &= \oint_S \left(\Phi \frac{\partial}{\partial n'} \frac{1}{R} - \frac{1}{R} \frac{\partial}{\partial n'} \Phi \right) \, dA'
\end{aligned}$$

We used Lea eqn 6.26 to evaluate $\nabla'^2 \frac{1}{R}$. Evaluating the first integral on the left with the sifting property, we have:

$$-4\pi \Phi(\vec{x}) = -\int_V \frac{1}{R} \frac{\rho(\vec{x}')}{\varepsilon_0} \, d^3\vec{x}' + \oint_S \left(\Phi \frac{\partial}{\partial n'} \frac{1}{R} - \frac{1}{R} \frac{\partial}{\partial n'} \Phi \right) \, dA'$$

or,

$$\Phi(\vec{x}) = \frac{1}{4\pi\varepsilon_0}\int_V \frac{\rho(\vec{x}')}{R}\, d^3\vec{x}' - \frac{1}{4\pi}\oint_S \left(\Phi(\vec{x}')\frac{\partial}{\partial n'}\frac{1}{R} - \frac{1}{R}\frac{\partial}{\partial n'}\Phi(\vec{x}')\right)\, dA'$$

This is, in principle, a solution for the potential in V. The first term is the same expression we derived for infinite space (Notes 1 eqn 29), now restricted to the volume V, and the second term, involving boundary conditions, is the effect of charges outside the volume. The problem is that we do not usually know both Φ and $\frac{\partial}{\partial n}\Phi$ on the boundary. In fact, if we did the problem would be overspecified and it is possible that no solution would exist (see Lea Appendix X.) To avoid this dilemma, we need to choose a better function ψ.

We want to retain the nice feature of $1/R$, that is $\nabla^2\psi = -4\pi\delta(\vec{x} - \vec{x}')$, because that is how we obtained $\Phi(\vec{x})$. But we need boundary conditions that eliminate one of the surface terms. Thus the *Green's function* is defined by the following mathematical problem:

$$\nabla'^2 G(\vec{x}, \vec{x}') = -4\pi\delta(\vec{x} - \vec{x}') \tag{3}$$

and either

$$G_D = 0 \qquad \text{on } S \qquad \text{(Dirichlet Green's function)} \tag{4}$$

or

$$\frac{\partial}{\partial n}G_N = \text{constant} \qquad \text{on } S \qquad \text{(Neumann Green's function)} \tag{5}$$

We cannot choose $\frac{\partial}{\partial n}G_N = 0$ on S in general, because

$$\int_V \nabla^2 G_N\, dV = \oint_S \frac{\partial G_D}{\partial n}\, dA$$

But the left hand side is not zero. From equation (3),

$$\int_V \nabla^2 G_N\, dV = \int_V -4\pi\delta(\vec{x} - \vec{x}')\, dV = -4\pi$$

Thus the best we can do is take $\frac{\partial G_D}{\partial n}$ to be constant, in which case

$$\frac{\partial G_D}{\partial n} = -\frac{4\pi}{A} \tag{6}$$

where A is the total area of the closed surface bounding the volume. If this area happens to be infinite, then (but only then) we may choose $\frac{\partial G_D}{\partial n} = 0$. With the Green's functions defined this way, we can find expressions for the potential as follows.

Dirichlet problem:

Again we use eqn. (2), this time with ϕ equal to the electrostatic potential Φ in the volume V and ψ equal to the Green's function G_D.

$$\int_V \left(\Phi\nabla'^2 G_D - G_D\nabla'^2\Phi\right)\ dV' = \oint_S \left(\Phi\vec{\nabla}' G_D - G_D\vec{\nabla}'\Phi\right)\cdot\hat{n}'\ dA'$$

We use equations (3) and (4) for G and Poisson's equation for Φ to get:

$$\int_V \left\{\Phi\left[-4\pi\delta\left(\vec{x}-\vec{x}'\right)\right] - G_D\left(-\frac{\rho\left(\vec{x}'\right)}{\varepsilon_0}\right)\right\}\ d^3\vec{x}' = \oint_S \left(\Phi\frac{\partial G_D}{\partial n'} - 0\right)\ dA'$$

Thus

$$\Phi\left(\vec{x}\right) = \frac{1}{4\pi\varepsilon_0}\int_V G_D\left(\vec{x},\vec{x}'\right)\rho\left(\vec{x}'\right)\ d^3\vec{x}' - \frac{1}{4\pi}\oint_S \Phi\frac{\partial G_D}{\partial n'}\ dA' \tag{7}$$

which is Jackson's eqn. 1.44. We need to know Φ, but not $\partial\Phi/\partial n$, on S. The Dirichlet Green's function is symmetric in $\vec{x}$ and $\vec{x}'$ (see Lea §C.7.1 and Jackson problem 1.14.).

$$G_D\left(\vec{x},\vec{x}'\right) = G_D\left(\vec{x}',\vec{x}\right) \tag{8}$$

Neumann problem:

The analysis proceeds as before. Only the boundary conditions change. This time we use the condition (6).

$$\Phi\left(\vec{x}\right) = \frac{1}{4\pi\varepsilon_0}\int_V G_N\left(\vec{x},\vec{x}'\right)\rho\left(\vec{x}'\right)\ d^3\vec{x}' - \frac{1}{4\pi}\oint_S \left(\Phi\frac{\partial G_N}{\partial n'} - G_N\frac{\partial\Phi}{\partial n'}\right)\ dA'$$

$$\Phi\left(\vec{x}\right) = \frac{1}{4\pi\varepsilon_0}\int_V G_N\left(\vec{x},\vec{x}'\right)\rho\left(\vec{x}'\right)\ d^3\vec{x}' - \frac{1}{4\pi}\oint_S \Phi\left(-\frac{4\pi}{A}\right)dA' + \frac{1}{4\pi}\oint_S G_N\frac{\partial\Phi}{\partial n'}\ dA'$$

Then, writing $<\Phi>_S = \frac{1}{A}\oint_S \Phi\ dA$, the average value of the potential over the surface S, we obtain Φ in terms of ρ in V and $\partial\Phi/\partial n$ on S :

$$\Phi\left(\vec{x}\right) - \ <\Phi>_S = \frac{1}{4\pi\varepsilon_0}\int_V G_N\left(\vec{x},\vec{x}'\right)\rho\left(\vec{x}'\right)\ d^3\vec{x}' + \frac{1}{4\pi}\oint_S G_N\frac{\partial\Phi}{\partial n'}\ dA' \tag{9}$$

(Jackson 1.46) It is often possible to choose $<\Phi>_S$ to be zero.

The first step is, of course, to find the Green's function. This mathematical problem is easier than the original problem of finding Φ because (a) the differential equation is simpler since a delta function replaces the charge density function, and (b) the boundary conditions are also simpler, with zero replacing the potential function on S in the Dirichlet case, and a constant replacing the normal derivative in the Neumann case. As the semester progresses we will learn methods for finding G.

2 Numerical methods for finding potential

The big idea in all these methods is that energy is an extremum when a system is in equilibrium, and is a minimum when the equilibrium is stable. The electrostatic energy is proportional to

$$I(\Phi) = \int_V \left|\vec{E}\right|^2 \, dV = \int_V \left|\vec{\nabla}\Phi\right|^2 \, dV \tag{10}$$

(Notes 2 eqn 4). Thus we may guess the potential function Φ and refine the guess by making the energy-like functional $I(\Phi)$ (10) an extremum.

2.1 Relaxation methods

The relaxation method is a convenient method for solving 2-D boundary-value potential problems. You can even do this one on a spreadsheet!

Suppose we want to find a solution to Laplace's equation in a volume V with a specifed potential function $V(\vec{x})$ on the boundary. We divide the volume up using a grid of rectangles and label the intersection points (the *grid points* or *lattice sites*) with indices i, j. For the example here I'll choose the grid to be made up of squares, h on a side. Then we can estimate the derivatives at a given grid point numerically using one of the following schemes:

centered difference:

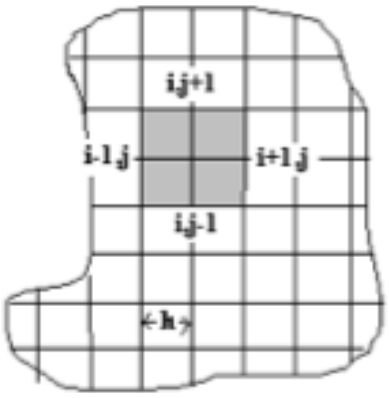
$$\left.\frac{\partial\psi}{\partial x}\right|_{i,j} = \frac{\psi_{i+1,j} - \psi_{i-1,j}}{2h}$$

forward difference

$$\left.\frac{\partial\psi}{\partial x}\right|_{i,j} = \frac{\psi_{i+1,j} - \psi_{i,j}}{h}$$

backward difference

$$\left.\frac{\partial\psi}{\partial x}\right|_{i,j} = \frac{\psi_{i,j} - \psi_{i-1,j}}{h}$$



Now we form the energy-like functional I over the top right corner of the shaded square using forward differences:

$$\begin{aligned} I &= \int \left(\vec{\nabla}\psi\right)^2 dV = \int \left\{ \left(\frac{\partial\psi}{\partial x}\right)^2 + \left(\frac{\partial\psi}{\partial y}\right)^2 \right\} dxdy \\ &= \left\{ \left[\frac{\psi_{i+1,j} - \psi_{i,j}}{h}\right]^2 + \left[\frac{\psi_{i,j+1} - \psi_{i,j}}{h}\right]^2 \right\} h^2 \end{aligned}$$

For the top left square we use backward differences. Then for the whole shaded square:

$$I = 2\left[\left(\psi_{i+1,j} - \psi_{i,j}\right)^2 + \left(\psi_{i,j+1} - \psi_{i,j}\right)^2 + \left(\psi_{i-1,j} - \psi_{i,j}\right)^2 + \left(\psi_{i,j-1} - \psi_{i,j}\right)^2\right]$$

and

$$\begin{aligned} \frac{\partial I}{\partial \psi_{i,j}} &= -4\left[\psi_{i+1,j} - \psi_{i,j} + \psi_{i,j+1} - \psi_{i,j} + \psi_{i-1,j} - \psi_{i,j} + \psi_{i,j-1} - \psi_{i,j}\right] \\ &= -4\left[\psi_{i+1,j} + \psi_{i,j+1} + \psi_{i-1,j} + \psi_{i,j-1} - 4\psi_{i,j}\right] \end{aligned}$$

Setting this equal to zero, we find the value of $\psi_{i,j}$ that makes I an extremum:

$$\begin{aligned} \psi_{i,j} &= \frac{1}{4}\left(\psi_{i+1,j} + \psi_{i,j+1} + \psi_{i-1,j} + \psi_{i,j-1}\right) \\ &= \text{ average of values at 4 surrounding sites} \end{aligned}$$

Thus the relaxation method amounts to filling the grid with values, any values, putting the exactly known boundary values at the lattice sites on the boundary, then re-computing the interior values by averaging, starting with the lattice sites next to the boundary. The process is iterated until it converges. Jackson (pg 48-49) discusses some ways to improve this scheme.

To iterate in EXCEL, you will need to set it up to do manual calculations. Under the tools tab, click "options" then "calculation" and check the manual box. (On a MAC the calculation options are under "formulas" .)

2.2 Variational methods

In this method we make a guess as to a function $\psi(x)$ that approximates the potential and form the energy-like functional

$$I(\psi) = \frac{1}{2}\int_V \vec{\nabla}\psi \cdot \vec{\nabla}\psi dV - \int_V g\frac{\psi}{\varepsilon_0} dV - \oint_S f\psi dA \tag{11}$$

Note that if the function ψ actually is the correct potential function, then the first volume integral gives the electrostatic energy in the volume V of interest, modulo a constant. We'll discuss the meaning of the other two terms below.

Now perform a variation on the function ψ by letting $\psi \rightarrow \psi + \delta\psi$. We obtain a corresponding variation in I :

$$\delta I = \int_V \vec{\nabla}\psi \cdot \vec{\nabla}\delta\psi \; dV - \frac{1}{\varepsilon_0}\int_V g\delta\psi \; dV - \oint_S f\delta\psi \; dA$$

Next use the relation (1)

$$\int \left(\phi\nabla^2\psi + \vec{\nabla}\phi \cdot \vec{\nabla}\psi\right) \; dV = \oint_S \phi\frac{\partial\psi}{\partial n} \; dA$$

with $\phi = \delta\psi$:

$$\int \left(\delta\psi\nabla^2\psi + \vec{\nabla}\delta\psi \cdot \vec{\nabla}\psi\right) \; dV = \oint_S \delta\psi\frac{\partial\psi}{\partial n} \; dA$$

and substitute into the first term of δI

$$\begin{aligned} \delta I &= \oint_S \delta\psi\frac{\partial\psi}{\partial n} \; dA - \int_V \delta\psi\nabla^2\psi \; dV - \frac{1}{\varepsilon_0}\int_V g\delta\psi \; dV - \oint_S f \; \delta\psi \; dA \\ &= -\int_V \delta\psi\left(\nabla^2\psi + \frac{g}{\varepsilon_0}\right) \; dV + \oint_S \delta\psi\left(\frac{\partial\psi}{\partial n} - f\right) \; dA \end{aligned}$$

To have an extremum, we need $\delta I = 0$ for any variation $\delta\psi$, which we can achieve if

$$\nabla^2\psi = -\frac{g}{\varepsilon_0} = -\frac{\rho}{\varepsilon_0}$$

(Poisson's equation for the potential in V) and

$$\frac{\partial\psi}{\partial n} = f \text{ on S} \;\; \text{(Neumann conditions)}$$

or

$$\delta\psi = 0 \text{ on S (Dirichlet conditions)}$$

(f may be taken to be identically zero for a Dirichlet problem.)

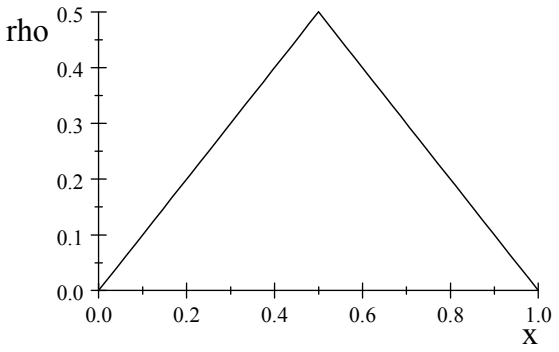
Thus we can solve for the potential using the following method:

- Pick a trial function $\psi(\vec{x})$ that fits the boundary conditions on the bounding surface S. The function $\psi(\vec{x})$ must contain one or more adjustable parameters α_i.
- Form the energy-like functional $I(\psi(\alpha_i))$ (11).
- Make I an extremum by setting the derivatives $\frac{\partial I}{\partial \alpha_i} = 0$. This determines the α_i.

Example: The volume of interest is the infinite slab occupying the volume $0 < x < 1$. Within the volume there is a charge density

$$\frac{\rho(x)}{\varepsilon_0} = \begin{cases} kx & \text{if} \quad x < 1/2 \\ k(1-x) & \text{if} \quad x > 1/2 \end{cases}$$

where k is a constant.



$\rho(x)$

and the boundary conditions are $\Phi = 0$ at $x = 0$ and at $x = 1$. We choose the trial function:

$$\text{Trial} : \psi = Ax(1-x)$$

that satisfies the boundary conditions. It has only one parameter: A. Its derivative is:

$$\frac{d\psi}{dx} = A(1-2x)$$

The function g is the function $\rho(x)$ given above, and since we have a Dirichlet problem, we take $f \equiv 0$. Then our energy-like functional (11) is:

$$\begin{aligned} I &= I(\psi) = \frac{1}{2}\int_V \vec{\nabla}\psi \cdot \vec{\nabla}\psi dV - \int_V g\frac{\psi}{\varepsilon_0}dV \\ &= \frac{1}{2}\int_0^1 A^2(1-2x)^2\,dx - \int_0^{1/2} Akx^2(1-x)\,dx - \int_{1/2}^1 Akx(1-x)^2\,dx \\ &= \frac{1}{6}A^2 - \frac{5}{96}Ak \end{aligned}$$

So

$$\frac{dI}{dA} = \frac{1}{3}A - \frac{5}{96}k = 0 \Rightarrow A = \frac{5}{32}k$$

and the variational solution is:

$$\psi = \frac{5k}{32} x\left(1-x\right)$$

Let's compare with the exact solution. We start with the differential equation:

$$\frac{d^2\psi}{dx^2} = \begin{array}{ll} -kx & \text{if} \quad x < 1/2 \\ k\left(x-1\right) & \text{if} \quad x > 1/2 \end{array}$$

Integrating once, we get

$$\frac{1}{k}\frac{d\psi}{dx} = \left\{ \begin{array}{ll} -\frac{x^2}{2} + A & \text{if} \quad x < 1/2 \\ \frac{x^2}{2} - x + B & \text{if} \quad x > 1/2 \end{array} \right.$$

$d\psi/dx$ is continuous for $0 < x < 1$, so matching at $x = 1/2$, we find

$$\begin{aligned} -\frac{1}{2}\left(\frac{1}{2}\right)^2 + A &= \frac{1}{2}\left(\frac{1}{2}\right)^2 - \frac{1}{2} + B \\ A &= \frac{1}{4} - \frac{1}{2} + B = B - \frac{1}{4} \end{aligned}$$

Integrating again, and applying the boundary condition at $x = 0$, we get:

$$\frac{\psi}{k} = \left\{ \begin{array}{ll} \left(B - \frac{1}{4}\right) x - \frac{x^3}{6} & \text{if} \quad x < 1/2 \\ \frac{x^3}{6} - \frac{x^2}{2} + Bx + C & \text{if} \quad x > 1/2 \end{array} \right.$$

At $x = 1$ the boundary condition is:

$$0 = \frac{1}{6} - \frac{1}{2} + B + C = -\frac{1}{3} + B + C \Rightarrow C = \frac{1}{3} - B$$

and matching at $x = 1/2$, we have

$$\begin{aligned} \left(B - \frac{1}{4}\right)\frac{1}{2} - \frac{\left(1/2\right)^3}{6} &= \frac{\left(1/2\right)^3}{6} - \frac{1}{2}\left(\frac{1}{2}\right)^2 + \frac{B}{2} + \frac{1}{3} - B \\ \frac{1}{2}B - \frac{7}{48} &= \frac{11}{48} - \frac{1}{2}B \\ B &= \frac{11}{48} + \frac{7}{48} = \frac{3}{8} \end{aligned}$$

Then

$$C = \frac{1}{3} - B = \frac{1}{3} - \frac{3}{8} = -\frac{1}{24}$$

and

$$A = B - \frac{1}{4} = \frac{3}{8} - \frac{1}{4} = \frac{1}{8}$$

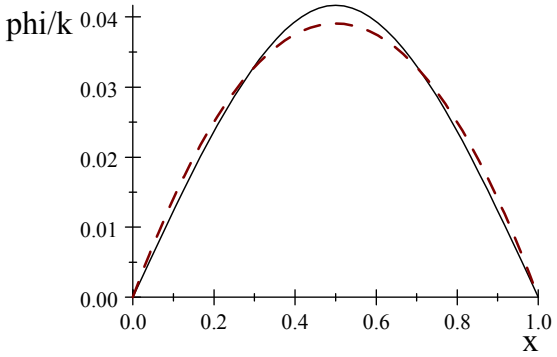
So the exact solution is:

$$\psi\left(x\right) = k\left\{ \begin{array}{ll} \frac{x}{8} - \frac{x^3}{6} & \text{if} \quad 0 < x < 1/2 \\ -\frac{1}{24} + \frac{3x}{8} - \frac{x^2}{2} + \frac{x^3}{6} & \text{if} \quad 1 > x > 1/2 \end{array} \right.$$

The two solutions are compared in the graph below. The variational solution is a very good approximation to the exact solution, even though we chose a very simple trial function. At $x = 0.5$,

$$\frac{\text{true-approx}}{\text{true}} = \frac{4.166\,7 \times 10^{-2} - \frac{5}{32}\frac{1}{4}}{4.166\,7 \times 10^{-2}} = 6.25 \times 10^{-2}$$

The approximate solution is good to about 6%. We could achieve better agreement near the peak by adding an additional parameter to the trial solution.



Black: exact dashed: variational