E: Rayleigh Quotient and the Minimization Principle

We just consider here the Sturm-Liouville problem (11), page 5 in Section 18, with Dirichlet boundary conditions at both $x = a, b$ to give you a taste of the arguments needed for the minimization principle.

Referring back to the Rayleigh quotient on page 9 of Section 18, it is a *functional*, meaning it is a function that is defined on a domain of functions, and gives a real number. Thus, we need to define an admissible set of functions for its domain. Take $\mathcal{A}$ to mean the set of continuous functions $\psi = \psi(x)$ on $[a, b]$, ψ is not identically the zero function, such that $d\psi/dx$ is piecewise continuous on (a, b), and $\psi(a) = \psi(b) = 0$. Therefore, for any ψ in $\mathcal{A}$,

$$\mathcal{R}[\psi] = \frac{\int_a^b \{p(\frac{d\psi}{dx})^2 + q\psi^2\}dx}{\int_a^b \sigma\psi^2 dx}$$

is well-defined.

Theorem:

1. $\min_{\psi\in\mathcal{A}} \mathcal{R}[\psi]$ exists and is equal to the first eigenvalue λ_1 of the associated eigenvalue problem (12);

2. There exists a function $\phi \in \mathcal{A}$ such that $\mathcal{R}[\phi] = min_{\psi\in\mathcal{A}}\mathcal{R}[\psi]$. Up to an arbitrary multiplicative constant, ϕ is the eigenfunction associated with the eigenvalue λ_1.

This is a really neat result, but the proof is beyond the scope of these Notes. However, see the end of this appendix for a proof in a special case.

One can use this idea to estimate λ_1 in situations where variable coefficients in the equation prevent us from getting an explicit formula for λ_1. The idea is that for any ψ in $\mathcal{A}$, $\mathcal{R}[\psi] \geq \lambda_1$, so we would like to find a sequence of "trial" functions ψ_i from $\mathcal{A}$ such that $\mathcal{R}[\psi_{i+1}] \leq \mathcal{R}[\psi_i]$ and $\lim_{i\to\infty} \mathcal{R}[\psi_i] = \lambda_1$. Ideally, the $\psi_i's$ would be of one sign since, from the Sturm-Liouville theorem we know the function satisfying the minimization principle in part 1 of the Theorem is an eigenfunction of λ_1 and so has no zeros in (a, b).

Example:

$$\begin{array}{ll} \frac{d^2\phi}{dx^2} + \lambda\phi = 0 & 0 < x < \pi \\ \phi(0) = \phi(\pi) = 0 & \end{array}$$

So $p \equiv 1, q \equiv 0, \sigma \equiv 1$ and therefore $\mathcal{R}[\psi] = \int_0^\pi (\frac{d\psi}{dx})^2 dx / \int_0^\pi \psi^2 dx$. Of course, in this case, we know $\lambda_1 = 1$ and $\phi_1(x) = \sin(x)$. So,
$\mathcal{A} = \{\psi \in C[0, \pi], \psi'$ is piecewise continuous on $[0, \pi], \psi(0) = \psi(\pi) = 0\}$.

If, for example, $\psi_1(x) = x(\pi - x)$, which is in $\mathcal{A}$, then $\mathcal{R}[\psi_1] = \frac{\pi^3/3}{\pi^5/30} = \frac{10}{\pi^2} \simeq 1.0132$, which is a reasonable first estimate for λ_1. If we try $\psi_2(x) = rx$ for $0 \leq x \leq \pi/2$, and $\psi_2(x) = r(\pi - x)$ for $\pi/2 \leq x \leq \pi$, $r > 0$ fixed, the "roof" function, then $\mathcal{R}[\psi_2] = \frac{r^2\pi}{r^2\pi^3/12} = \frac{12}{\pi^2} \simeq 1.216$, which is not nearly as good. Part of the reason is that ψ_2 is "kinked"; it is not smooth enough to satisfy the equation in the whole interval, though $\mathcal{R}[\psi_2]$ is well-defined.

We are not going to pursue this line of thought further, but we will mention that the minimization principle can be extended to characterize the successive eigenvalues $\lambda_2, \lambda_3, \ldots$.

Outline of the Minimization Principle for the first eigenvalue for the simplest eigenvalue problem

Consider the eigenvalue problem

$$\begin{cases} \frac{d^2\phi}{dx^2} + \lambda\phi = 0 & 0 < x < 1 \\ \phi(0) = 0 = \phi(1) & \end{cases}$$

Then the Rayleigh quotient is $\mathcal{R}[\phi] = \int_0^1 (\phi')^2 dx / \int_0^1 \phi^2 dx$. Let $\mathcal{A}$:= all continuously differentiable functions defined on $[0, 1]$ which are zero at $x = 0, 1$, and let

$$m = \min_{\psi \in \mathcal{A}} \mathcal{R}[\psi] \quad . \tag{1}$$

The claim is that m equals the first (smallest) eigenvalue λ_1, and any solution $\phi(x)$ to (1) is its eigenfunction. By solution we mean that for all $\psi \in \mathcal{A}$, $\mathcal{R}[\phi] \leq \mathcal{R}[\psi]$, and $\phi \neq 0$. If we think of $\mathcal{R}[\cdot]$ as a form of energy functional, then we can interpret the minimization principle as stating a common physical principle, that is, the first eigenvalue is the minimum of the energy. Then the eigenfunction $\phi(x)$ is the physical system's "ground state." Our set of admissible functions, $\mathcal{A}$, is often called the set of *trial* functions.

Suppose ϕ is a solution to (1), and let ε be any constant, and v be any admissible (trial) function. Then

$$\mathcal{R}[\phi] \leq \mathcal{R}[\phi + \varepsilon v] := f(\varepsilon)$$

By ordinary calculus, $f'(0) = 0$ (since f has a critical point at $\varepsilon = 0$). Now

$$\frac{f(\varepsilon) - f(0)}{\varepsilon} =$$

$$\frac{1}{\varepsilon}\left\{ \frac{\int_0^1 (\phi'^2 + 2\varepsilon\phi' v' + \varepsilon^2 v'^2) dx}{\int_0^1 (\phi^2 + 2\varepsilon\phi v + \varepsilon^2 v^2) dx} - \frac{\int_0^1 \phi'^2 dx}{\int_0^1 \phi^2 dx} \right\} =$$

$$\frac{1}{\varepsilon}\left\{ \frac{(\int_0^1 \phi^2 dx)[\int_0^1 \phi'^2 dx + 2\varepsilon \int_0^1 \phi' v' dx + O(\varepsilon^2)] - (\int_0^1 \phi'^2 dx)[\int_0^1 \phi^2 dx + 2\varepsilon \int_0^1 \phi v dx + O(\varepsilon^2)]}{(\int_0^1 \phi^2 dx)(\int_0^1 (\phi^2 + 2\varepsilon\phi v + \varepsilon^2 v^2) dx)} \right\} =$$

$$2\left\{ \frac{(\int_0^1 \phi^2 dx)[\int_0^1 \phi' v' dx + O(\varepsilon)] - (\int_0^1 \phi'^2 dx)[\int_0^1 \phi v dx + O(\varepsilon)]}{(\int_0^1 \phi^2 dx)^2 + O(\varepsilon)} \right\}$$

where $O(\varepsilon)$ means terms of the order ε. Thus

$$f'(0) = \lim_{\varepsilon \to 0} \frac{f(\varepsilon) - f(0)}{\varepsilon} = 2\frac{(\int_0^1 \phi^2 dx)(\int_0^1 \phi' v' dx) - (\int_0^1 \phi'^2 dx)(\int_0^1 \phi v dx)}{(\int_0^1 \phi^2 dx)^2}$$

Therefore, $f'(0) = 0$ if, and only if

$$(\int_0^1 \phi^2 dx)(\int_0^1 \phi' v' dx) = (\int_0^1 (\phi')^2 dx)(\int_0^1 \phi v dx) \ ,$$

that is,

$$m = \mathcal{R}[\phi] = \frac{\int_0^1 \phi' v' dx}{\int_0^1 \phi v dx} \ .$$

Since $\int_0^1 \phi' v' dx = -\int_0^1 \phi'' v dx$ (integration-by-parts)
we have

$$-\int_0^1 \phi'' v dx = m \int_0^1 \phi v dx \ , \ \text{or} \ \ 0 = \int_0^1 v\{\phi'' + m\phi\} dx \ .$$

Since this holds for all $v \in \mathcal{A}$, then $\phi'' + m\phi = 0$ in $(0,1)$. Thus m is an eigenvalue, with eigenfunction ϕ. To show m is the *smallest* eigenvalue of the problem, let λ be any other eigenvalue, with eigenfunction w; i.e. $w'' + \lambda w = 0$ in $(0,1)$, with $w(0) = w(1) = 0$, $w \neq 0$. By the definition of m in (1),

$$m \leq \mathcal{R}[w] = \frac{\int_0^1 w'^2 dx}{\int_0^1 w^2 dx} = \frac{-\int_0^1 ww'' dx}{\int_0^1 w^2 dx} = \frac{\lambda \int_0^1 w^2 dx}{\int_0^1 w^2 dx} = \lambda\ .$$

So, m is smaller than any other eigenvalue.

Remark: This whole argument generalizes to higher dimensions, that is, to $\nabla^2 \phi + \lambda\phi = 0$ in bounded domain $\Omega \subset \mathbb{R}^n$, $\phi_{|\partial\Omega} = 0$, where now the claim would be

$$\lambda_1 = m = \min\{\int_\Omega |\nabla\psi|^2 dx / \int_\Omega |\psi|^2 dx\}$$

Green's first identity is used to get to the result rather than using the 1D integration-by-parts formula.