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 \( A \) to mean the set of continuous functions \( \psi(x) \) on \([a, b]\), \( \psi \) 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 \( \psi \) in \( A \),

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

is well-defined.

**Theorem:**

1. \( \min_{\psi \in A} R[\psi] \) exists and is equal to the first eigenvalue \( \lambda_1 \) of the associated eigenvalue problem (12);

2. There exists a function \( \phi \in A \) such that \( R[\phi] = \min_{\psi \in A} R[\psi] \). Up to an arbitrary multiplicative constant, \( \phi \) is the eigenfunction associated with the eigenvalue \( \lambda_1 \).

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 \( \lambda_1 \) in situations where variable coefficients in the equation prevent us from getting an explicit formula for \( \lambda_1 \). The idea is that for any \( \psi \) in \( A \), \( R[\psi] \geq \lambda_1 \), so we would like to find a sequence of “trial” functions \( \psi_i \) from \( A \) such that \( R[\psi_{i+1}] \leq R[\psi_i] \) and \( \lim_{i \to \infty} R[\psi_i] = \lambda_1 \). 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 \( \lambda_1 \) and so has no
zeros in \((a, b)\).

**Example:**

\[
\frac{d^2 \phi}{dx^2} + \lambda \phi = 0 \quad 0 < x < \pi \\
\phi(0) = \phi(\pi) = 0
\]

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

If, for example, \(\psi_1(x) = x(\pi - x)\), which is in \(A\), then \(R[\psi_1] = \frac{\pi^3/3}{\pi^3/30} = \frac{10}{\pi^2} \simeq 1.0132\), which is a reasonable first estimate for \(\lambda_1\). 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 \(R[\psi_2] = \frac{r^2 \pi}{r^2 \pi^2 / 12} = \frac{12}{\pi^2} \simeq 1.216\), which is not nearly as good. Part of the reason is that \(\psi_2\) is “kinked”; it is not smooth enough to satisfy the equation in the whole interval, though \(R[\psi_2]\) 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 \(R[\phi] = \int_0^1 (\phi')^2 dx / \int_0^1 \phi^2 dx\). Let \(\mathcal{A} := \text{all continuously differentiable functions defined on } [0, 1] \text{ which are zero at } x = 0, 1\), and let

\[
m = \min_{\psi \in \mathcal{A}} R[\psi].
\]

The claim is that \(m\) equals the first (smallest) eigenvalue \(\lambda_1\), and any solution \(\phi(\cdot)\) to (1) is its eigenfunction. By solution we mean that for all \(\psi \in \mathcal{A}\), \(R[\phi] \leq R[\psi], \) and \(\phi \neq 0\). If we think of \(R[\cdot]\) 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, \( A \), is often called the set of trial functions.

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

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

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

\[
f(\varepsilon) - f(0) = \frac{1}{\varepsilon} \left\{ \int_0^1 (\phi'^2 + 2\varepsilon \phi' v' + \varepsilon^2 v'^2) \, dx - \int_0^1 \phi'^2 \, dx \right\} = \frac{1}{\varepsilon} \left\{ \int_0^1 \phi'^2 \, dx \right\} \left( \int_0^1 \phi' v' \, dx \right) - \int_0^1 \phi'^2 \, dx \right) \]

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

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

\[
f'(0) = \lim_{\varepsilon \to 0} \frac{f(\varepsilon) - f(0)}{\varepsilon} = 2 \frac{\left( \int_0^1 \phi'^2 \, dx \right) \left( \int_0^1 \phi' v' \, dx \right) - \left( \int_0^1 \phi'^2 \, dx \right) \left( \int_0^1 \phi vdx \right)}{\left( \int_0^1 \phi'^2 \, dx \right)^2}
\]

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

\[
\left( \int_0^1 \phi'^2 \, dx \right) \left( \int_0^1 \phi' v' \, dx \right) = \left( \int_0^1 \phi'^2 \, dx \right) \left( \int_0^1 \phi vdx \right)
\]

that is,

\[
m = \mathsf{R}[\phi] = \int_0^1 \phi' v' \, dx \int_0^1 \phi vdx .
\]

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

\[
-\int_0^1 \phi'' vdx = m \int_0^1 \phi vdx , \text{ or } 0 = \int_0^1 v\{\phi'' + m\phi\} \, dx .
\]
Since this holds for all $v \in \mathcal{A}$, then $\phi'' + m\phi = 0$ in $(0, 1)$. Thus $m$ is an eigenvalue, with eigenfunction $\phi$. To show $m$ is the smallest eigenvalue of the problem, let $\lambda$ 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),

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

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

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

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