

Concave/Convex functions and Maximum/Minimum Principles

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- We will mainly focus on smooth function $f(x)$ on a closed interval $[a, b]$

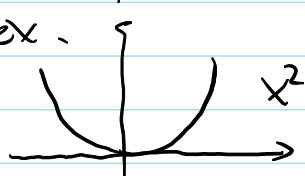
Def. If $-f''(x) \geq 0$, then f is called concave (or concave down)

If $-f''(x) \leq 0$, then f is called convex (or concave up)

eg $f(x) = -x^2 + 1$. $-f''(x) = 2 > 0$ concave. (on any interval)



eg. $f(x) = x^2$, $-f''(x) = -2 < 0$ convex.



- We will mainly focus on concave (down) functions since if $f(x)$ is convex, then $-f(x)$ is concave.

- One property of concave function is that we can predict where its minimum value will be obtained.

Prop. If $f(x)$ is concave on $[a, b]$, then the minimum of $f(x)$ cannot be obtained in the interior of the domain, (a, b) .

Cor. If $f(x)$ is concave on $[a, b]$ and $f(a) = f(b) = 0$, then $f(x) \geq 0$ for all $x \in [a, b]$.

- This property is usually referred as to be Minimum Principle, which can be defined in a very wide sense.

Def. For a function $f(x)$ defined on a compact domain $D \subset \mathbb{R}^n$, if the minimum (maximum) cannot be obtained in the interior of the domain, then we say $f(x)$ satisfies the Minimum Principle (Maximum Principle).

Remark. People sometimes abuse the terminologies and refer both Min/Max Principle to Maximum Principle for simplicity. We will also call both Maximum Principle (Max-P) from now on.

The previous discussion on concave function shows that concave function (on a closed interval) satisfies Max-P.

We also see that this is actually a property associated to the second order derivative (negative), which is a differential operator.

We are particularly interested in operators acting on functions on a compact domain $D \subset \mathbb{R}^n$ with zero boundary conditions.

Def. We say an operator H has maximum principle (in domain D) if $Hf \geq 0$ in D implies $f \geq 0$ in D for all f with zero boundary condition (i.e., $f(x) = 0$ for all $x \in \partial D = \text{boundary of } D$)

Remark. This is a non-rigorous definition. The domain of the function space and the domain of the operator (to which functions can this operator be applied) have to be more precise in different context.

- Using this definition, we may express the Max-P of concave function as: the second order differential operator $H = -\frac{d^2}{dx^2}$ has Max-P on any closed interval $[a, b]$.

- The Max-Principle for $-\frac{d^2}{dx^2}$ can be extended to differential operator H acting on (smooth) functions on $[a, b]$, given by

$$(Hf)(x) = a(x) \cdot \frac{d^2}{dx^2} f(x) + b(x) \cdot \frac{d}{dx} f(x) + v(x) \cdot f(x)$$
 with appropriate assumptions on $a(x)$, $b(x)$, $v(x)$.

- The generalization of $\frac{d^2}{dx^2}$ on \mathbb{R}^n ($n \geq 2$) is called Laplacian operator, given by the sum of all second order partial derivatives:

$$\Delta = \frac{\partial^2}{\partial x_1^2} + \dots + \frac{\partial^2}{\partial x_n^2}$$

e.g. For $f(x_1, x_2)$ on \mathbb{R}^2 , $\Delta f = \frac{\partial^2}{\partial x_1^2} f + \frac{\partial^2}{\partial x_2^2} f$

- The concept of concave function on \mathbb{R} is generalized to be the so-called superharmonic function on \mathbb{R}^n .
 (convex)
 (subharmonic)

- In particular, for smooth functions, f is called superharmonic if $-\Delta f \geq 0$
 subharmonic if $-\Delta f \leq 0$

f is called harmonic if f is both superharmonic and subharmonic (i.e. $\Delta f = 0$).

Notice that on \mathbb{R}^1 , $\Delta f = f''(x) \geq 0 \Rightarrow f(x) = ax + b$

The only non-trivial harmonic function is linear function.

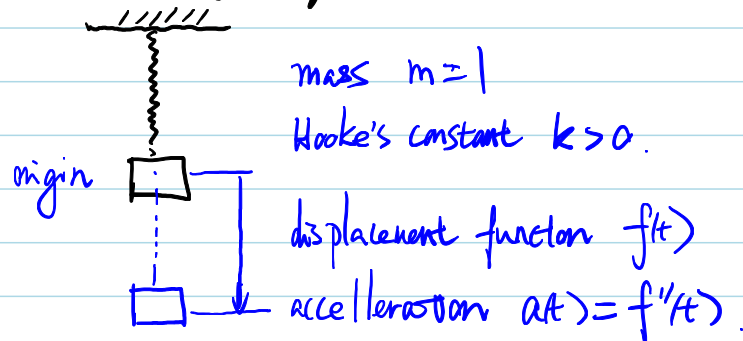
- On \mathbb{R}^n ($n \geq 2$), the harmonic functions are more complicated (and interesting)
- The Max-Principle is still true for $-\Delta$ on compact domain. But the proof is highly non-trivial on \mathbb{R}^n , $n \geq 2$.

- The phrase "harmonic" (in math) is frequently used in problems related to Δ , (partial) second order derivative.

e.g. Harmonic Oscillator (of a Mass-spring system).

Newton's Second Law:
 $F = ma = f''(t)$

Hooke's Law:
 $F = -kf$



Putting two laws together,

$$f''(t) = -k \cdot f(t) \quad (\Leftrightarrow -f''(t) = k \cdot f(t))$$

The solution is

$$f(t) = A \cos(\omega t + \varphi), \text{ for arbitrary } A, \varphi.$$

ω (frequency) is given explicitly by $\omega = \sqrt{k}$

Notice that the equation $-f''(t) = k \cdot f(t)$ can be written as

$$Hf = k \cdot f \quad \text{by letting } H = -\frac{d^2}{dt^2},$$

which is the (generalized) eigenvalue equation for H .

- The discrete version of Δ and maximum principle. ($n \in \mathbb{Z}$)

Recall the discrete version of the second order derivative $\frac{d^2}{dt^2}$ is the second order difference operator:

$$(\Delta X)_n = X_{n+1} + X_{n-1} - 2X_n, \text{ for "function" } X: \mathbb{Z} \rightarrow \mathbb{R}.$$

- We are interested in eigenvalue problems and Max-P related to this discrete Laplacian. We also frequently drop the last term which simply shifts the eigenvalue by 2.

If we consider a finite lattice $[1, 2, \dots, n]$ and a vector $x = (x_1, \dots, x_n)$,

the operator

$$(\Delta x)_n = x_{n+1} + x_{n-1}, \quad n=1, \dots, n$$

is properly defined if we extend the lattice $[1, \dots, n]$

to $[0, 1, 2, \dots, n, n+1]$ with the boundaries $j=0$ and $j=n+1$.

If we impose the zero boundary condition on the extended vector $\overset{m}{x} = (x_0, x_1, \dots, x_n, x_{n+1})$ such that

$$x_0 = x_{n+1} = 0,$$

then Δ will be consistent with the (free) Schrödinger matrix H_0 on \mathbb{R}^n

$$H_0 = \begin{bmatrix} 0 & 1 & & 0 \\ 1 & & & \\ & & \ddots & \\ 0 & & & 1 \\ & & & & 0 \end{bmatrix}$$

- The goal is to study the maximum principle for the Schrödinger matrix $H = -\Delta + V := -\begin{bmatrix} 0 & 1 & & 0 \\ 1 & & & \\ & & \ddots & \\ 0 & & & 1 \\ & & & & 0 \end{bmatrix} + \begin{bmatrix} v_1 & & 0 \\ & \ddots & \\ 0 & & v_n \end{bmatrix}$

lem. Assume that $v_j \geq 2, j=1, \dots, n$. For any vector $\vec{u} \in \mathbb{R}^n$,

(Max-P): if $H\vec{u} \geq 0$ (meaning all entries of $H\vec{u} \geq 0$), then $u_j \geq 0$ for all j .

(Strong Max-P): if $H\vec{u} > 0$ (at least one entry of $H\vec{u} > 0$), then $u_j > 0$ for all j .