Concave/Convex functions and Maximum/Minimum Principles
Feb, 21st, 2019.

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

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

In Chinese, 
\[
\begin{array}{l}
- f''(x) > 0, \text{ then } f \text{ is called convex (or concave up).}
\end{array}
\]

\[f(x) = -x^2 + 1, \quad -f''(x) = 2 > 0 \text{ concave. (on any interval)} \]

\[f(x) = x^2, \quad -f''(x) = -2 < 0 \text{ convex.} \]

- 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
\[f(x) \geq 0 \text{ for all } x \in [a, b].\]

- This property is usually referred to as to be Minimum Principle, which
  can be defined in a very wide sense.
Def. For a function \( f \) defined on a compact domain \( D \subseteq \mathbb{R}^n \), if the minimum (maximum) cannot be obtained in the interior of the domain, then we say \( f \) 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 functions 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 \( D \subseteq \mathbb{R}^n \) 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., \( f|_{\partial D} = 0 \) for all \( \lambda \in \partial D \)).

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 functions: the second order differential operator \( H = -\frac{d^2}{dx^2} \) has Max-P on any closed interval \([a, b] \).
The Max-P can be extended to differential operators $H$ acting on (smooth) functions on $[a,b]$, given by

$$(Hf)(x) = ax^2 \frac{d^2 f}{dx^2} + bx \frac{d f}{dx} + v(x) f(x)$$

with appropriate assumptions on $a(x), b(x), v(x)$. 

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

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

eg. For $f(x,y)$ on $\mathbb{R}^2$, $\Delta f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}$

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

(Non-harmonic)

In particular, for smooth functions:

$f$ is called superharmonic if $-\Delta f \geq 0$

(f is 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 $\mathbb{R}^2$, $\Delta f = f'' + \Delta f \geq 0 \Rightarrow f(x) = ax + b$

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-P 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 \( \Delta \), (partial) second order derivative.

\textbf{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,
\[
f''(t) = -k f(t) \quad (\leftrightarrow -f''(t) = k f(t))
\]
The solution is
\[
f(t) = A \cos(wt + \phi), \text{ for arbitrary } A, \phi.
\]

\( w \) (frequency) is given explicitly by \( w = \sqrt{k} \).

Notice that the equation \(-f''(t) = k f(t)\) can be written as
\[
-1 f = k f \quad \text{by letting } H = -\frac{k}{\hbar^2}
\]
which is the (generalized) eigenvalue equation for \( H \).

The discrete version of \( \Delta \) and maximum principle \((m \mathbb{Z})\).

Recall the discrete version of the second order derivative \( \Delta x \) is the second order difference operator:

\[
(\Delta x)_n = x_{n+1} + x_{n-1} - 2x_n, \text{ for “function” } X : \mathbb{Z} \to \mathbb{R}.
\]

We are interested in eigenvalue problems and Max-P related to the discrete Laplacian. We also frequently drop the last term which simply shift the eigenvalue by \( 2 \).
If we consider a finite lattice \([1, 2, \ldots, n]\) and a vector \(x = (x_1, \ldots, x_n)\),

the operator
\[
(\Delta x)_n = x_{n+1} + x_n, \quad n = 1, \ldots, n
\]

is properly defined if we extend the lattice \([1, \ldots, n]\)
to \([0, 1, 2, \ldots, n, n+1]\) with the boundaries
\(j = 0\) and \(j = n+1\).

If we impose the zero boundary condition on the extended vector \(x = (x_0, x_1, \ldots, x_n, x_{n+1})\) such that
\(x_0 = x_{n+1} = 0\),
then \(\Delta\) will be consistent with the (free) Schrödinger
matrix \(H_0\) on \(\mathbb{R}^n\)
\[
H_0 = \begin{bmatrix}
0 & 1 & 0 \\
1 & \ddots & 1 \\
0 & \cdots & 0
\end{bmatrix}
\]

. The goal is to study the maximum principle for the
Schrödinger matrix \(H = -\Delta + V = -\begin{bmatrix}
0 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & 0
\end{bmatrix} + \begin{bmatrix}
v_1 & \cdots & v_n \\
\vdots & \ddots & \vdots \\
v_n & \cdots & v_1
\end{bmatrix}\)

Let \(y_j \geq 2, j = 1, \ldots, n\). For any vector \(y \in \mathbb{R}^n\),
(Max-P): if \(H y \geq 0\) (meaning all entries of \(H y \geq 0\)), then \(y_j > 0\) for all \(j\).

(Strong Max-P): if \(H y > 0\) (at least one entry of \(H y > 0\)), then \(y_j > 0\) for all \(j\).