2.15: Appendix II- Legendre Transformations

A *convex function* of a single variable $f(x)$ is one for which $f''(x)>0$ everywhere. The *Legendre transform* of a convex function $f(x)$ is a function $g(p)$ defined as follows. Let p be a real number, and consider the line $y=px$, as shown in Figure 2.15.1. We define the point $x(p)$ as the value of x for which the difference $F(x,p)=px-f(x)$ is greatest. Then define $g(p)=F\big(x(p),p\big)$.[26] The value $x(p)$ is unique if $f(x)$ is convex, since $x(p)$ is determined by the equation

$$f'\big(x(p)\big)=p\ . \tag{2.15.1}$$

Note that from $p=f'\big(x(p)\big)$ we have, according to the chain rule,

$$\frac{d}{dp}\,f'\big(x(p)\big)=f''\big(x(p)\big)\,x'(p) \qquad\Longrightarrow\qquad x'(p)=\Big[f''\big(x(p)\big)\Big]^{-1}\ . \tag{2.15.2}$$

From this, we can prove that $g(p)$ is itself convex:

$$\begin{aligned} g'(p)&=\frac{d}{dp}\Big[p\,x(p)-f\big(x(p)\big)\Big]\\ &=p\,x'(p)+x(p)-f'\big(x(p)\big)\,x'(p)=x(p)\ , \end{aligned}$$

hence

$$g''(p)=x'(p)=\Big[f''\big(x(p)\big)\Big]^{-1}>0\ . \tag{2.15.3}$$

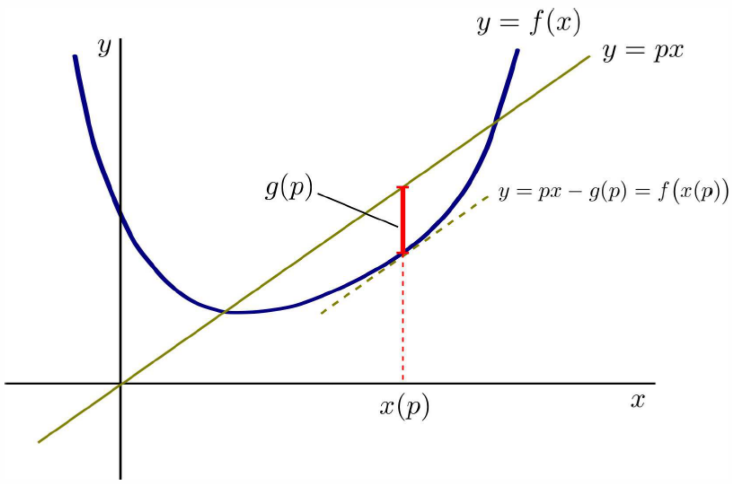

Figure 2.15.1: Construction for the Legendre transformation of a function $f(x)$.

In higher dimensions, the generalization of the definition $f''(x)>0$ is that a function $F(x_1,\ldots,x_n)$ is convex if the matrix of second derivatives, called the *Hessian*,

$$H_{ij}(\mathbf{x})=\frac{\partial^2 F}{\partial x_i\,\partial x_j} \tag{2.15.4}$$

is positive definite. That is, all the eigenvalues of $H_{ij}(\mathbf{x})$ must be positive for every $\mathbf{x}$. We then define the Legendre transform $\mathbf{G}(\mathbf{p})$ as

$$\mathbf{G}(\mathbf{p})=\mathbf{p}\cdot\mathbf{x}-F(\mathbf{x}) \tag{2.15.5}$$

where

$$\mathbf{p}=\boldsymbol{\nabla}F\ . \tag{2.15.6}$$

Note that

$$dG=\mathbf{x}\cdot d\mathbf{p}+\mathbf{p}\cdot d\mathbf{x}-\boldsymbol{\nabla}F\cdot d\mathbf{x}=\mathbf{x}\cdot d\mathbf{p}\ , \tag{2.15.7}$$

which establishes that G is a function of $\mathbf{p}$ and that

$$\frac{\partial G}{\partial p_j} = x_j \,. \tag{2.15.8}$$

Note also that the Legendre transformation is *self dual*, which is to say that the Legendre transform of $G(\mathbf{p})$ is $F(\mathbf{x})$: $F \to G \to F$ under successive Legendre transformations.

We can also define a *partial Legendre transformation* as follows. Consider a function of q variables $F(\mathbf{x}, \mathbf{y})$, where $\mathbf{x} = \{x_1, \ldots, x_m\}$ and $\mathbf{y} = \{y_1, \ldots, y_n\}$, with $q = m + n$. Define $\mathbf{p} = \{p_1, \ldots, p_m\}$, and

$$G(\mathbf{p}, \mathbf{y}) = \mathbf{p} \cdot \mathbf{x} - F(\mathbf{x}, \mathbf{y}) \,, \tag{2.15.9}$$

where

$$p_a = \frac{\partial F}{\partial x_a} \qquad (a = 1, \ldots, m) \,. \tag{2.15.10}$$

These equations are then to be inverted to yield

$$x_a = x_a(\mathbf{p}, \mathbf{y}) = \frac{\partial G}{\partial p_a} \,. \tag{2.15.11}$$

Note that

$$p_a = \frac{\partial F}{\partial x_a} \big(\mathbf{x}(\mathbf{p}, \mathbf{y}), \mathbf{y}\big) \,. \tag{2.15.12}$$

Thus, from the chain rule,

$$\delta_{ab} = \frac{\partial p_a}{\partial p_b} = \frac{\partial^2 F}{\partial x_a \, \partial x_c} \, \frac{\partial x_c}{\partial p_b} = \frac{\partial^2 F}{\partial x_a \, \partial x_c} \, \frac{\partial^2 G}{\partial p_c \, \partial p_b} \,, \tag{2.15.13}$$

which says

$$\frac{\partial^2 G}{\partial p_a \, \partial p_b} = \frac{\partial x_a}{\partial p_b} = \mathsf{K}^{-1}_{ab} \,, \tag{2.15.14}$$

where the $m \times m$ partial Hessian is

$$\frac{\partial^2 F}{\partial x_a \, \partial x_b} = \frac{\partial p_a}{\partial x_b} = \mathsf{K}_{ab} \,. \tag{2.15.15}$$

Note that $\mathsf{K}_{ab} = \mathsf{K}_{ba}$ is symmetric. And with respect to the $\mathbf{y}$ coordinates,

$$\frac{\partial^2 G}{\partial y_\mu \, \partial y_\nu} = -\frac{\partial^2 F}{\partial y_\mu \, \partial y_\nu} = -\mathsf{L}_{\mu\nu} \,, \tag{2.15.16}$$

where

$$\mathsf{L}_{\mu\nu} = \frac{\partial^2 F}{\partial y_\mu \, \partial y_\nu} \tag{2.15.17}$$

is the partial Hessian in the $\mathbf{y}$ coordinates. Now it is easy to see that if the full $q \times q$ Hessian matrix H_{ij} is positive definite, then any submatrix such as K_{ab} or $\mathsf{L}_{\mu\nu}$ must also be positive definite. In this case, the partial Legendre transform is convex in $\{p_1, \ldots, p_m\}$ and concave in $\{y_1, \ldots, y_n\}$.