Linear Algebra – Lecture #12 Notes

In this class we'll apply the **Spectral Theorem** and the **Principal Axes Theorem** to understand **quadratic forms**. We'll also discuss the **Singular Value Decomposition** of any matrix.

Definition: A quadratic form is a homogeneous polynomial of degree 2, i.e. a polynomial function $q(\mathbf{x})$ such that $q(t\mathbf{x}) = t^2\mathbf{x}$, a pure quadratic expression in *n* variables. For example:

(a) $q(x,y) = 8x^2 - 4xy + 5y^2$ (b) $q(x_1,x_2,x_3) = x_1{}^2 - 2x_2{}^2 + 4x_3{}^2 + 2x_1x_2 - x_1x_3 + 4x_2x_3$

Observation: Any quadratic form can be expressed as $\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}$ where $\mathbf{x}$ is an $n\times 1$ (column) vector and **A** is a symmetric $n\times n$ matrix. For example:

(a) $q(x,y) = 8x^2 - 4xy + 5y^2 = \begin{bmatrix} x & y \end{bmatrix}\begin{bmatrix} 8 & -2 \\ -2 & 5 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}$

(b) $q(x_1,x_2,x_3) = x_1{}^2 - 2x_2{}^2 + 4x_3{}^2 + 2x_1x_2 - x_1x_3 + 4x_2x_3 = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}\begin{bmatrix} 1 & 1 & -\frac{1}{2} \\ 1 & -2 & 2 \\ -\frac{1}{2} & 2 & 4 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}$

Principal Axes Theorem: Any quadratic form $q(\mathbf{x}) = \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}$ may be expressed without cross terms in new coordinates via an orthonormal change of basis. That is, there exists an orthonormal basis $\mathcal{B} = \{\mathbf{u}_1,\cdots,\mathbf{u}_n\}$ and scalars $\{\lambda_1,\cdots,\lambda_n\}$ such that if $\{y_1,\cdots,y_n\}$ are the coordinates relative to the basis $\mathcal{B} = \{\mathbf{u}_1,\cdots,\mathbf{u}_n\}$, then $q(\mathbf{x}) = \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} = \mathbf{y}^{\mathrm{T}}\mathbf{D}\mathbf{y} = \lambda_1 y_1{}^2 + \cdots + \lambda_n y_n{}^2$.

Proof: By the Spectral Theorem, since **A** is symmetric it is orthogonally diagonalizable, i.e. it has real eigenvalues $\{\lambda_1,\cdots,\lambda_n\}$ and associated orthonormal eigenvectors $\mathcal{B} = \{\mathbf{u}_1,\cdots,\mathbf{u}_n\}$ for the matrix **A** such that if is the orthogonal change of basis matrix $\mathbf{S} = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{u}_1 & \cdots & \mathbf{u}_n \\ \downarrow & & \downarrow \end{bmatrix}$, then $[\mathbf{A}]_{\mathcal{B}} = \mathbf{S}^{-1}\mathbf{A}\mathbf{S} = \mathbf{S}^{\mathrm{T}}\mathbf{A}\mathbf{S} = \mathbf{D} = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}$, a diagonal matrix. We may therefore write $\mathbf{A} = \mathbf{S}\mathbf{D}\mathbf{S}^{\mathrm{T}}$, so $q(\mathbf{x}) = \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} = \mathbf{x}^{\mathrm{T}}\mathbf{S}\mathbf{D}\mathbf{S}^{\mathrm{T}}\mathbf{x} = (\mathbf{S}^{\mathrm{T}}\mathbf{x})^{\mathrm{T}}\mathbf{D}(\mathbf{S}^{\mathrm{T}}\mathbf{x}) = (\mathbf{S}^{-1}\mathbf{x})^{\mathrm{T}}\mathbf{D}(\mathbf{S}^{-1}\mathbf{x}) = \mathbf{y}^{\mathrm{T}}\mathbf{D}\mathbf{y} = \lambda_1 y_1{}^2 + \cdots + \lambda_n y_n{}^2$.

Definitions: A quadratic form $q(\mathbf{x}) = \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}$ with symmetric matrix **A** is called:

(a) **positive definite** if all of the eigenvalues $\{\lambda_1,\cdots,\lambda_n\}$ are strictly positive.
(b) **negative definite** if all of the eigenvalues $\{\lambda_1,\cdots,\lambda_n\}$ are strictly negative.
(c) **positive semi-definite** if all of the eigenvalues $\{\lambda_1,\cdots,\lambda_n\}$ are greater than or equal to 0.
(d) **negative semi-definite** if all of the eigenvalues $\{\lambda_1,\cdots,\lambda_n\}$ are less than or equal to 0.
(e) indefinite if some eigenvalues are positive and some or negative (and some may be equal to 0).

Some immediate applications are in **identifying the graphs of quadratic functions** $q(x,y)$ and **identifying level sets** of the form $q(x,y) = C$ (conic sections such as ellipses and hyperbolas) and $q(x,y,z) = C$ (quadric sections such as ellipsoids and hyperboloids of one or two sheets).

Example: The graph of the function $q(x,y) = 8x^2 - 4xy + 5y^2 = \begin{bmatrix} x & y \end{bmatrix}\begin{bmatrix} 8 & -2 \\ -2 & 5 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}$ can be easily identified by calculating the eigenvalues of **A** as $\lambda_1 = 9$ and $\lambda_2 = 4$ with orthonormal eigenbasis $\mathbf{u}_1 = \frac{1}{\sqrt{5}}\begin{bmatrix} 2 \\ -1 \end{bmatrix}$, $\mathbf{u}_2 = \frac{1}{\sqrt{5}}\begin{bmatrix} 1 \\ 2 \end{bmatrix}$. In (rotated) coordinates $\{u,v\}$ relative to this new basis, the graph $q = 9u^2 + 4v^2$ can be identified as an (upward, rotated) **paraboloid**. Similarly, the level set $q(x,y) = 8x^2 - 4xy + 5y^2 = 36$

may be re-expressed as $q = 9u^2 + 4v^2 = 36$ or $\left(\frac{u}{2}\right)^2 + \left(\frac{v}{3}\right)^2 = 1$, a (rotated) **ellipse** with semi-major axis 3 and semi-minor axis 2. Note that the longer axis corresponds to the *smaller* eigenvalue (slower growth) and the shorter axis corresponds to the *larger* eigenvalue (faster growth) to reach the given level set.

In the case of a level set of a **quadratic function in 3 variables**, if $q(x_1, x_2, x_3) = C > 0$.

If the signs of the eigenvalues are $\{+,+,+\}$, the level set will be a (rotated) **ellipsoid**.

If the signs of the eigenvalues are $\{+,+,-\}$, the level set will be a (rotated) **hyperboloid of one sheet**.

If the signs of the eigenvalues are $\{+,-,-\}$, the level set will be a (rotated) **hyperboloid of two sheets**.

Singular Values and the Singular Value Decomposition (SVD)

Given any $m \times n$ matrix **A**, it's possible to find an orthonormal basis $\mathcal{B} = \{\mathbf{u}_1, \cdots, \mathbf{u}_n\}$ for the domain ($\mathbf{R}^n$) as well as an orthonormal basis $\mathcal{C} = \{\mathbf{w}_1, \cdots, \mathbf{w}_m\}$ for the codomain ($\mathbf{R}^m$) such that the images $\{\mathbf{Au}_1, \cdots, \mathbf{Au}_n\}$ are orthogonal (some may be $\mathbf{0}$) and are scalar multiples, respectively, of the vectors $\{\mathbf{w}_1, \cdots, \mathbf{w}_m\}$ in the codomain. The scalars $\|\mathbf{Au}_i\| = \sigma_i$ are called the **singular values** of the matrix **A** (and the linear transformation that it represents).

This observation follows by considering the symmetric $n \times n$ matrix $\mathbf{A}^\mathrm{T}\mathbf{A}$. By the Spectral Theorem, this matrix yields an orthonormal basis of eigenvectors $\mathcal{B} = \{\mathbf{u}_1, \cdots, \mathbf{u}_n\}$ with real eigenvalues $\{\lambda_1, \cdots, \lambda_n\}$. Furthermore, $(\mathbf{Au}_i)\cdot(\mathbf{Au}_j) = \langle \mathbf{Au}_i, \mathbf{Au}_j \rangle = (\mathbf{Au}_i)^\mathrm{T} \mathbf{Au}_j = \mathbf{u}_i^\mathrm{T}\mathbf{A}^\mathrm{T}\mathbf{Au}_j = \lambda_j \mathbf{u}_i^\mathrm{T}\mathbf{u}_j = \lambda_j \langle \mathbf{u}_i, \mathbf{u}_j \rangle$. In the case where $i \neq j$, this yields that $\langle \mathbf{Au}_i, \mathbf{Au}_j \rangle = 0$, i.e. that these images are orthogonal (or one or both could be $\mathbf{0}$). In the case where $i = j$, this yields that $\langle \mathbf{Au}_j, \mathbf{Au}_j \rangle = \|\mathbf{Au}_j\|^2 = \lambda_j$, so all of these eigenvalues must be greater than or equal to 0. Furthermore, $\|\mathbf{Au}_j\| = \sqrt{\lambda_j} = \sigma_j$ are the singular values. If we order the eigenvalues (and the singular values) in decreasing order, we can create the orthogonal $n \times n$ matrix $\mathbf{P} = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{u}_1 & \cdots & \mathbf{u}_n \\ \downarrow & & \downarrow \end{bmatrix}$ from the orthonormal basis for the domain. The vectors $\{\mathbf{Au}_1, \cdots, \mathbf{Au}_n\}$ will span the subspace $\mathrm{im}(\mathbf{A})$ of the codomain. If we arrange the orthonormal basis vectors $\{\mathbf{u}_1, \cdots, \mathbf{u}_n\}$ in such a way that any zero vectors in $\{\mathbf{Au}_1, \cdots, \mathbf{Au}_n\}$ appear at the end of the list, and if $\mathrm{rank}(\mathbf{A}) = \dim[\mathrm{im}(\mathbf{A})] = k$, then $\{\mathbf{Au}_1, \cdots, \mathbf{Au}_k\} = \{\sigma_1\mathbf{w}_1, \cdots, \sigma_k\mathbf{w}_k\}$ will be an orthogonal collection of vectors that span $\mathrm{im}(\mathbf{A})$. If we normalize these, we get an orthonormal basis $\{\mathbf{w}_1, \cdots, \mathbf{w}_k\}$ for $\mathrm{im}(\mathbf{A})$. [Note: For any $m \times n$ matrix **A,** $\mathrm{rank}(\mathbf{A}) = k = \dim[\mathrm{im}(\mathbf{A})] \leq \min(m, n)$.] Since $\mathrm{rank}(\mathbf{A}) = k < m$, we can find an orthonormal basis for $[\mathrm{im}(\mathbf{A})]^\perp$ to complete an orthonormal basis $\mathcal{C} = \{\mathbf{w}_1, \cdots, \mathbf{w}_m\}$ for the entire codomain $\mathbf{R}^m$. We define the orthogonal $m \times m$ matrix $\mathbf{Q} = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{w}_1 & \cdots & \mathbf{w}_m \\ \downarrow & & \downarrow \end{bmatrix}$ from this orthonormal basis for the codomain. Both **P** and **Q** represent rotations (with possible reflection) in the domain and codomain respectively. Using these matrices to change bases to the respective orthonormal bases, the following commuting diagram relates the matrix **A** (relative to the standard bases) to the matrix $\mathbf{\Sigma}$ (relative to these orthonormal bases):

$$\begin{array}{ccc} \{\mathbf{R}^n, \mathcal{E}_n\} & \xrightarrow{\mathbf{A}} & \{\mathbf{R}^m, \mathcal{E}_m\} \\ \mathbf{P}\uparrow & & \mathbf{Q}\uparrow \\ \{\mathbf{R}^n, \mathcal{B}\} & \xrightarrow{\Sigma} & \{\mathbf{R}^m, \mathcal{C}\} \end{array}$$

Since $\mathbf{P}$ and $\mathbf{Q}$ are orthogonal matrices, $\mathbf{P}^{-1} = \mathbf{P}^{\mathrm{T}}$ and $\mathbf{Q}^{-1} = \mathbf{Q}^{\mathrm{T}}$, so we get $\mathbf{A} = \mathbf{Q}\boldsymbol{\Sigma}\mathbf{P}^{\mathrm{T}}$. This is known as the **Singular Value Decomposition** (SVD). If $m = n$, i.e. if $\mathbf{A}$ is a square matrix, then the matrix $\boldsymbol{\Sigma}$ will be diagonal with the singular values on the diagonal. However, the SVD also applies to any matrix – in which case the singular values will still appear along the "diagonal" starting at the upper-left position with 0's everywhere else.

Example: Consider the matrix $\mathbf{A} = \begin{bmatrix} 6 & 2 \\ -7 & 6 \end{bmatrix}$. We calculate $\mathbf{A}^{\mathrm{T}}\mathbf{A} = \begin{bmatrix} 6 & -7 \\ 2 & 6 \end{bmatrix}\begin{bmatrix} 6 & 2 \\ -7 & 6 \end{bmatrix} = \begin{bmatrix} 85 & -30 \\ -30 & 40 \end{bmatrix} = \mathbf{B}$. This yields the eigenvalues (in decreasing order) $\lambda_1 = 100$ and $\lambda_2 = 25$.
So the singular values are $\sigma_1 = 10$ and $\sigma_2 = 5$.

These eigenvalues yield, respectively, the orthonormal basis of eigenvectors $\mathbf{u}_1 = \frac{1}{\sqrt{5}}\begin{bmatrix} 2 \\ -1 \end{bmatrix}$, $\mathbf{u}_2 = \frac{1}{\sqrt{5}}\begin{bmatrix} 1 \\ 2 \end{bmatrix}$ for the domain. We then calculate $\mathbf{A}\mathbf{u}_1 = 10\left(\frac{1}{\sqrt{5}}\begin{bmatrix} 1 \\ -2 \end{bmatrix}\right) = 10\mathbf{w}_1$, $\mathbf{A}\mathbf{u}_2 = 5\left(\frac{1}{\sqrt{5}}\begin{bmatrix} 2 \\ 1 \end{bmatrix}\right) = 5\mathbf{w}_2$.

This yields the orthogonal matrices $\mathbf{P} = \frac{1}{\sqrt{5}}\begin{bmatrix} 2 & 1 \\ -1 & 2 \end{bmatrix}$ and $\mathbf{Q} = \frac{1}{\sqrt{5}}\begin{bmatrix} 1 & 2 \\ -2 & 1 \end{bmatrix}$ and $\boldsymbol{\Sigma} = \begin{bmatrix} 10 & 0 \\ 0 & 5 \end{bmatrix}$.

You can verify that $\mathbf{Q}\boldsymbol{\Sigma}\mathbf{P}^{\mathrm{T}} = \frac{1}{\sqrt{5}}\frac{1}{\sqrt{5}}\begin{bmatrix} 1 & 2 \\ -2 & 1 \end{bmatrix}\begin{bmatrix} 10 & 0 \\ 0 & 5 \end{bmatrix}\begin{bmatrix} 2 & -1 \\ 1 & 2 \end{bmatrix} = \frac{1}{5}\begin{bmatrix} 10 & 10 \\ -20 & 5 \end{bmatrix}\begin{bmatrix} 2 & -1 \\ 1 & 2 \end{bmatrix} = \frac{1}{5}\begin{bmatrix} 30 & 10 \\ -35 & 30 \end{bmatrix} = \begin{bmatrix} 6 & 2 \\ -7 & 6 \end{bmatrix} = \mathbf{A}$.

Example: Consider the matrix $\mathbf{A} = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 1 & 0 \end{bmatrix}$. We calculate $\mathbf{A}^{\mathrm{T}}\mathbf{A} = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & 1 & 1 \\ 1 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 1 \end{bmatrix} = \mathbf{B}$. The characteristic polynomial of $\mathbf{B}$ is $p_{\mathbf{B}}(\lambda) = \lambda^3 - 4\lambda^2 + 3\lambda = \lambda(\lambda - 3)(\lambda - 1)$. This yields the eigenvalues (in decreasing order) $\lambda_1 = 3$, $\lambda_2 = 1$, and $\lambda_3 = 0$. The singular values will therefore be $\sigma_1 = \sqrt{3}$, $\sigma_2 = 1$, and $\sigma_3 = 0$ ($\sigma_3 = 0$ will not figure into the singular value decomposition). The eigenvalues yield, respectively, the orthonormal basis vectors $\mathbf{u}_1 = \frac{1}{\sqrt{6}}\begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix}$, $\mathbf{u}_2 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$, and $\mathbf{u}_3 = \frac{1}{\sqrt{3}}\begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix}$. We then calculate

$\mathbf{A}\mathbf{u}_1 = \sqrt{3}\left(\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}\right) = \sqrt{3}\mathbf{w}_1$, $\mathbf{A}\mathbf{u}_2 = 1\left(\frac{1}{\sqrt{2}}\begin{bmatrix} -1 \\ 1 \end{bmatrix}\right) = 1\mathbf{w}_2$, and $\mathbf{A}\mathbf{u}_3 = \mathbf{0}$.

This yields the orthogonal matrices $\mathbf{P} = \begin{bmatrix} 1/\sqrt{6} & 1/\sqrt{2} & 1/\sqrt{3} \\ 2/\sqrt{6} & 0 & -1/\sqrt{3} \\ 1/\sqrt{6} & -1/\sqrt{2} & 1/\sqrt{3} \end{bmatrix}$ for the domain and $\mathbf{Q} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$ for the codomain, and $\boldsymbol{\Sigma} = \begin{bmatrix} \sqrt{3} & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \end{bmatrix}$.

So $\mathbf{A} = \mathbf{Q}\boldsymbol{\Sigma}\mathbf{P}^{\mathrm{T}} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} \sqrt{3} & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}\begin{bmatrix} 1/\sqrt{6} & 2/\sqrt{6} & 1/\sqrt{6} \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 1/\sqrt{3} & -1/\sqrt{3} & 1/\sqrt{3} \end{bmatrix}$ is the corresponding singular value decomposition.

Application of Principal Axes Theorem to critical points analysis and the 2nd derivative test

A typical question from Multivariable Calculus is:

Find all critical points of the function $f(x,y)=\frac{1}{3}x^3-3x^2+\frac{1}{4}y^2+xy+13x-y+2$. Determine which give relative maxima, relative minima, or saddle points.

As you recall, we first find the critical points for this function. This gives us:

$$f_x(x,y)=x^2-6x+y+13=0$$
$$f_y(x,y)=\tfrac{1}{2}y+x-1 \quad \Rightarrow \quad y=2-2x$$

So, we must have $x^2-6x+(2-x)+13=x^2-8x+15=(x-3)(x-5)=0$.
These yield the two critical points $(3,-4)$ and $(5,-8)$. The next question is then:

Do these critical points give maxima, minima, saddle points, or what?

To answer this question, we generally appeal to the **2nd Derivative Test**, which can be formulated as follows:

Let $f(x,y)$ be a function which is continuous, with continuous first and second partial derivatives. Define the Hessian matrix to be the (symmetric) matrix consisting of the 2nd partial derivatives, i.e. $H_f=\begin{bmatrix} f_{xx} & f_{xy} \\ f_{yx} & f_{yy}\end{bmatrix}$. Let (x_0,y_0) be a critical point for this function.

If $\det[H_f(x_0,y_0)]>0$, then (x_0, y_0) will give a relative maximum or minimum for this function.

If either $f_{xx}(x_0,y_0)>0$ or $f_{yy}(x_0,y_0)>0$, then there is a relative minimum at (x_0,y_0).

If either $f_{xx}(x_0,y_0)<0$ or $f_{yy}(x_0,y_0)<0$, then there is a relative maximum at (x_0,y_0).

If $\det[H_f(x_0,y_0)]<0$, then (x_0,y_0) will give a saddle point for this function.

If $\det[H_f(x_0,y_0)]=0$, then there is insufficient information provided by the 2nd derivatives to distinguish between a possible relative maximum, relative minimum, or saddle point at (x_0,y_0) for this function. That is, the 2nd derivative test is inconclusive.

The 2nd Derivative Test is derived from the idea of **quadratic approximation**. It is easily shown that the quadratic function that best approximates a given (sufficiently differentiable) function $f(x,y)$ in the vicinity of a point (x_0,y_0) is given by:

$$\begin{aligned} f(x,y)\cong Q(x,y)&=f(x_0,y_0)+f_x(x_0,y_0)(x-x_0)+f_y(x_0,y_0)(y-y_0)\\ &\quad+\tfrac{1}{2}f_{xx}(x_0,y_0)(x-x_0)^2+f_{xy}(x_0,y_0)(x-x_0)(y-y_0)+\tfrac{1}{2}f_{yy}(x_0,y_0)(y-y_0)^2\end{aligned}$$

If we denote by $\overrightarrow{\nabla f}$ the (gradient) row vector $\overrightarrow{\nabla f}=\begin{bmatrix} f_x & f_y\end{bmatrix}$, and let $\mathbf{h}=[\mathbf{x}-\mathbf{x}_0]=\begin{bmatrix} x-x_0 \\ y-y_0\end{bmatrix}$, and if we further write $\mathbf{x}=(x,y)$ and $\mathbf{x}_0=(x_0,y_0)$, then the above expression becomes:

$$f(\mathbf{x})\cong f(\mathbf{x}_0)+\overrightarrow{\nabla f}(\mathbf{x}_0)\cdot[\mathbf{x}-\mathbf{x}_0]+\tfrac{1}{2}[\mathbf{x}-\mathbf{x}_0]^{\mathrm{T}}[H_f(\mathbf{x}_0)][\mathbf{x}-\mathbf{x}_0]=f(\mathbf{x}_0)+\overrightarrow{\nabla f}(\mathbf{x}_0)\cdot\mathbf{h}+\tfrac{1}{2}\mathbf{h}^{\mathrm{T}}[H_f(\mathbf{x}_0)]\mathbf{h}$$

At a critical point $\mathbf{x}_0=(x_0,y_0)$ the situation is much simpler, since $\overrightarrow{\nabla f}(\mathbf{x}_0)=\mathbf{0}$ (the zero vector). In this case, the quadratic approximation is simply:

$$f(\mathbf{x})=f(\mathbf{x}_0+\mathbf{h})\cong f(\mathbf{x}_0)+\tfrac{1}{2}\mathbf{h}^{\mathrm{T}}[H_f(\mathbf{x}_0)]\mathbf{h}$$ where **h** is small

Thus, the question of whether there is a maximum, minimum, saddle point, or whatever at $\mathbf{x}_0 = (x_0, y_0)$ boils down to our being able to understand the **quadratic form** $\mathbf{h}^{\mathrm{T}}[H_f(\mathbf{x}_0)]\mathbf{h}$, and, in particular, what its sign is for any $\mathbf{h}$. Note that in the context of quadratic approximation we are only interested in the case where the components of $\mathbf{h}$ are all relatively small.

Definition: A quadratic form in $\mathbf{R}^n$ is a function $q(\mathbf{h})$ of the form $q(\mathbf{h}) = \mathbf{h}^{\mathrm{T}}\mathbf{A}\mathbf{h}$ for some symmetric matrix $\mathbf{A}$. In other words, a quadratic form is just a 2nd degree expression involving the coordinates $(h_1, h_2, \cdots, h_n)$.

We can apply the **Principal Axes Theorem** to $q(\mathbf{h}) = \mathbf{h}^{\mathrm{T}}[H_f(\mathbf{x}_0)]\mathbf{h}$ because the Hessian matrix $\mathbf{A} = H_f(\mathbf{x}_0)$ is symmetric (Clairaut's Theorem, or equality of mixed partial derivatives). There is a orthonormal basis $\mathcal{B} = \{\mathbf{u}_1, \cdots, \mathbf{u}_n\}$ of eigenvectors of $\mathbf{A} = H_f(\mathbf{x}_0)$, an orthogonal matrix $\mathbf{S}$ whose columns are the vectors of $\mathcal{B}$, and $\mathbf{S}^{-1}\mathbf{A}\mathbf{S} = \mathbf{S}^{\mathrm{T}}\mathbf{A}\mathbf{S} = \mathbf{D}$, a diagonal matrix whose diagonal entries are the (real) eigenvalues of $\mathbf{A} = H_f(\mathbf{x}_0)$.

Thus $\mathbf{A} = \mathbf{S}\mathbf{D}\mathbf{S}^{\mathrm{T}}$ and, if we define $\mathbf{y} = [\mathbf{h}]_{\mathcal{B}} = \mathbf{S}^{-1}\mathbf{h} = \mathbf{S}^{\mathrm{T}}\mathbf{h} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$ we have:

$$\boxed{q(\mathbf{h}) = \mathbf{h}^{\mathrm{T}}\mathbf{A}\mathbf{h} = \mathbf{h}^{\mathrm{T}}\mathbf{S}\mathbf{D}\mathbf{S}^{\mathrm{T}}\mathbf{h} = (\mathbf{S}^{\mathrm{T}}\mathbf{h})^{\mathrm{T}}\mathbf{D}\mathbf{S}^{\mathrm{T}}\mathbf{h} = \mathbf{y}^{\mathrm{T}}\mathbf{D}\mathbf{y} = \lambda_1 {y_1}^2 + \cdots + \lambda_n {y_n}^2}$$

In this form, it is easy to see that:

A quadratic form $q(\mathbf{h})$ is positive definite if all eigenvalues of $\mathbf{A}$ are strictly positive.
A quadratic form $q(\mathbf{h})$ is negative definite if all eigenvalues of $\mathbf{A}$ are strictly negative.
A quadratic form $q(\mathbf{h})$ is positive semi-definite if all eigenvalues of $\mathbf{A}$ are either positive or zero.
A quadratic form $q(\mathbf{h})$ is negative semi-definite if all eigenvalues of $\mathbf{A}$ are either negative or zero.
A quadratic form $q(\mathbf{h})$ is indefinite if some of the eigenvalues of $\mathbf{A}$ are positive and some are negative.

From this, we conclude:

2nd Derivative Test (second form): A critical point for a function $f(\mathbf{x})$ will give:
(1) a relative minimum if all eigenvalues of the Hessian matrix $H_f(\mathbf{x}_0)$ are strictly positive.
(2) a relative maximum if all eigenvalues of the Hessian matrix $H_f(\mathbf{x}_0)$ are strictly negative.
(3) neither a relative maximum nor a relative minimum if some of the eigenvalues of $H_f(\mathbf{x}_0)$ are positive and some are negative.
(4) Further analysis is necessary in the case where the Hessian matrix $H_f(\mathbf{x}_0)$ is positive semi-definite (a relative minimum or neither) or negative semi-definite (a relative maximum or neither).

The reasoning behind (4) is simply that the second derivative test is based on a quadratic *approximation* and in the borderline case where an eigenvalue is zero, we cannot rely on this approximation to make any valid conclusions.

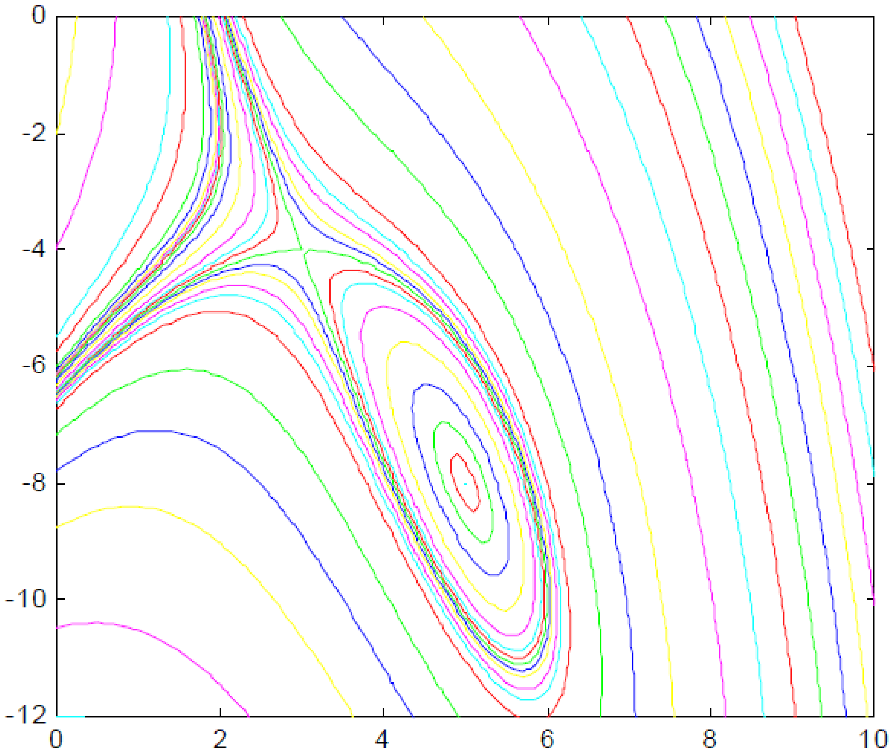
Notice that for a function of two variables, in cases (1) and (2) the determinant of the Hessian matrix will be the product of the two eigenvalues and will be positive. In the case where both eigenvalues are positive, the trace of the Hessian matrix (the sum of its diagonal terms = the sum of its eigenvalues) will be positive and hence either $f_{xx}(x_0, y_0)$ or $f_{yy}(x_0, y_0)$ must be positive. In the case where both eigenvalues are negative, the trace of the Hessian will be negative and hence either $f_{xx}(x_0, y_0)$ or $f_{yy}(x_0, y_0)$ must be negative. In case (3) for a function of two variables, the determinant will thus be negative. In case (4), the determinant will be zero. These observations yield our earlier version of the 2nd derivative test.

This second version of the second derivative test actually tells us quite a bit more. It tells us that there is a new coordinate system defined in the vicinity of a given critical point, based on the principal axes, in which:

$$\boxed{f(\mathbf{x}) \cong f(\mathbf{x}_0) + \tfrac{1}{2}\mathbf{h}^{\mathrm{T}}[H_f(\mathbf{x}_0)]\mathbf{h} = f(\mathbf{x}_0) + \tfrac{1}{2}\mathbf{y}^{\mathrm{T}}\mathbf{D}\mathbf{y} = f(\mathbf{x}_0) + \tfrac{1}{2}(\lambda_1 y_1{}^2 + \cdots + \lambda_n y_n{}^2)}$$

This tells us, in particular, that, in the vicinity of this critical point, changes in the function will be most sensitive to changes in the direction of the eigenvector associated with the eigenvalue of largest magnitude.

Here's a contour diagram for the function $f(x,y) = \frac{1}{3}x^3 - 3x^2 + \frac{1}{4}y^2 + xy + 13x - y + 2$ with its two critical points – a saddle point at $(3,-4)$ with $f(3,-4) = 19$ and a relative minimum at $(5,-8)$ with $f(5,-8) = 17\frac{2}{3}$.



In this example, the Hessian matrix is $H_f = \begin{bmatrix} 2x-6 & 1 \\ 1 & \frac{1}{2} \end{bmatrix}$.

At the critical point $(3,-4)$, we have $H_f(3,-4) = \begin{bmatrix} 0 & 1 \\ 1 & \frac{1}{2} \end{bmatrix}$ with eigenvalues $\lambda = \dfrac{1 \pm \sqrt{17}}{4}$ (one positive, one negative) indicating a saddle point.

At the critical point $(5,-8)$, we have $H_f(5,-8) = \begin{bmatrix} 4 & 1 \\ 1 & \frac{1}{2} \end{bmatrix}$ with eigenvalues $\lambda = \dfrac{9 \pm \sqrt{65}}{4}$ (both positive) indicating a relative minimum.

You may want to carry out the calculations to find the associated principal axes at each of these critical points and relate them to the shape of the contours. In particular, note the approximately elliptical contours in the vicinity of the relative minimum at $(5,-8)$, and which directions yield most rapid growth.

Notes by Robert Winters