Vv417 Lecture 26

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- We have only considered linear equations, and treated them in matrix form

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

Q: How to study a quadratic equation in two variables x and y in matrix form?

$$ax^2 + 2bxy + cy^2 + \alpha x + \beta y + \pi = 0$$

- We can write the above quadratic equation as

$$\underbrace{\begin{bmatrix} x & y \end{bmatrix}}_{\mathbf{x}^{\mathrm{T}}} \underbrace{\begin{bmatrix} a & b \\ b & c \end{bmatrix}}_{\mathbf{A}} \underbrace{\begin{bmatrix} x \\ y \end{bmatrix}}_{\mathbf{x}} + \underbrace{\begin{bmatrix} \alpha & \beta \end{bmatrix}}_{\mathbf{b}^{\mathrm{T}}} \underbrace{\begin{bmatrix} x \\ y \end{bmatrix}}_{\mathbf{x}} + \pi = 0$$

- The term in the quadratic equation

$$\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}$$

is called the quadratic form associated with the quadratic equation.

Definition

A quadratic form in n variables is a function $f\colon \mathbb{R}^n \to \mathbb{R}$ of the form

$$f(\mathbf{x}) = \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}$$

where $\mathbf{A}$ is a symmetric $n \times n$ matrix and $\mathbf{x} \in \mathbb{R}^n$.

- We refer to $\mathbf{A}$ as the matrix associated with f.

Exercise

Find the matrix associated with the quadratic form

$$f(x_1, x_2, x_3) = 2x_1^2 - x_2^2 + 5x_3^2 + 6x_1x_2 - 3x_1x_3$$

Solution

- In general,

$$\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} = \sum_i a_{ii}x_i^2 + \sum_{i<j} 2a_{ij}x_ix_j$$

Solution

- Since the squared terms are $2x_1^2 - x_2^2 + 5x_3^2$, thus the diagonals must be

$$\begin{bmatrix} 2 & & \\ & -1 & \\ & & 5 \end{bmatrix}$$

- Since cross-product terms are

$$6x_1x_2 - 3x_1x_3 + 0x_1x_2$$

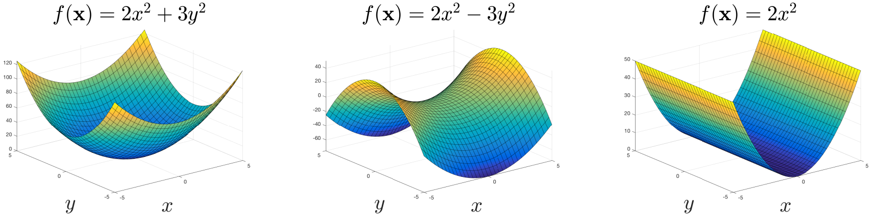
- The off-diagonals must be

$$\begin{bmatrix} & 3 & -1.5 \\ 3 & & 0 \\ -1.5 & 0 & \end{bmatrix} \Longrightarrow \mathbf{A} = \begin{bmatrix} 2 & 3 & -1.5 \\ 3 & -1 & 0 \\ -1.5 & 0 & 5 \end{bmatrix}$$

- For $\mathbf{x} \in \mathbb{R}^2$, when there is no cross-product term, the function

$$f(\mathbf{x}) = \mathbf{x}^{\mathrm{T}} \mathbf{A} \mathbf{x}$$

is relatively easy to study.



- Thus it is desirable to eliminate the cross-product terms before we study it

$$\mathbf{x}^{\mathrm{T}} \mathbf{A} \mathbf{x} = (\mathbf{Q}\mathbf{y})^{\mathrm{T}} \mathbf{A} (\mathbf{Q}\mathbf{y}) = \mathbf{y}^{\mathrm{T}} \mathbf{Q}^{\mathrm{T}} \mathbf{A} \mathbf{Q} \mathbf{y} = \mathbf{y}^{\mathrm{T}} \mathbf{D} \mathbf{y}$$

Q: Why can we always find a substitution $\mathbf{x} = \mathbf{Q}\mathbf{y}$ such that $\mathbf{D}$ is diagonal?

The Principal Axes Theorem

Every quadratic form

$$f\left(\mathbf{x}\right)=\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}$$

can be diagonalised. Specifically, suppose $\mathbf{Q}$ is an orthogonal matrix such that

$$\mathbf{Q}^{\mathrm{T}}\mathbf{A}\mathbf{Q}=\mathbf{D}$$

is a diagonal matrix, then the substitution $\mathbf{x}=\mathbf{Q}\mathbf{y}$ transform the quadratic form

$$f\left(\mathbf{x}\right)=\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}$$

into the quadratic form

$$g\left(\mathbf{y}\right)=\mathbf{y}^{\mathrm{T}}\mathbf{D}\mathbf{y}$$

which has no cross-product term. If the eigenvalues of $\mathbf{A}$ are λ_1, λ_2, ..., λ_n, then

$$\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}=\mathbf{y}^{\mathrm{T}}\mathbf{D}\mathbf{y}=\lambda_1 y_1^2+\lambda_2 y_2^2+\cdots+\lambda_n y_n^2$$

Exercise

Find a substitution that transforms the quadratic form

$$f(x_1, x_2) = 5x_1^2 + 4x_1x_2 + 2x_2^2$$

into one without cross-product terms.

Solution

- The associated matrix is

$$\mathbf{A} = \begin{bmatrix} 5 & 2 \\ 2 & 2 \end{bmatrix}$$

- Solve the eigenvalue problem, we have

$$\left\{ \lambda_1 = 6, \quad \frac{1}{\sqrt{5}}\left(2\mathbf{e}_1 + \mathbf{e}_2\right) \right\} \quad \text{and} \quad \left\{ \lambda_2 = 1, \quad \frac{1}{\sqrt{5}}\left(\mathbf{e}_1 - 2\mathbf{e}_2\right) \right\}$$

- So the substitution is $x_1 = \dfrac{1}{\sqrt{5}}(2y_1 + y_2)$ and $x_2 = \dfrac{1}{\sqrt{5}}(y_1 - 2y_2)$.

Definition

A quadratic form $f(\mathbf{x}) = \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}$ is classified as one of the followings:

- Postive definite
$$f(\mathbf{x}) > 0 \qquad \text{for all} \quad \mathbf{x} \neq 0$$
- Negative definite
$$f(\mathbf{x}) < 0 \qquad \text{for all} \quad \mathbf{x} \neq 0$$
- Postive semidefinite
$$f(\mathbf{x}) \geq 0 \qquad \text{for all} \quad \mathbf{x}$$
- Negative semidefinite
$$f(\mathbf{x}) \leq 0 \qquad \text{for all} \quad \mathbf{x}$$
- Indefinite if $f(\mathbf{x})$ takes both positive and negatives values.

The associated the matrix $\mathbf{A}$ is classified according to the quadratic form $\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}$.

Q: How to determine whether a matrix is positive definite or not?

Q: What is the significance of having a positive definite $\mathbf{A}$?

Theorem

Let $\mathbf{A}$ be an $n \times n$ real symmetric matrix. The quadratic form $f(\mathbf{x}) = \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}$ is

- Positive definite if and only if all of the eigenvalues of $\mathbf{A}$ is positive.
- Negative definite if and only if all of the eigenvalues of $\mathbf{A}$ are negative.
- Positive semidefinite if and only if all of the eigenvalues of $\mathbf{A}$ are nonnegative
- Negative semidefinite if and only if all of the eigenvalues of $\mathbf{A}$ are nonpostive
- Indefinite if and only if $\mathbf{A}$ has both positive and negative eigenvalues.

Proof

- If $\mathbf{A}$ is positive definite and λ is an eigenvalue of

$$\mathbf{A}$$

and $\mathbf{x}$ is the corresponding eigenvector, then

$$\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} = \lambda\mathbf{x}^{\mathrm{T}}\mathbf{x} = \lambda \left\|\mathbf{x}\right\|^2$$

Proof

- Hence

$$\lambda = \frac{\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}}{\|\mathbf{x}\|^2} > 0$$

- Conversely, suppose that all eigenvalues of $\mathbf{A}$ are positive. Since $\mathbf{A}$ is real and symmetric, there always is an orthonormal set of n eigenvectors of $\mathbf{A}$.

$$\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$$

- Let $\mathbf{x}$ be any nonzero vector in $\mathbb{R}^n$, then

$$\mathbf{x} = \alpha_1\mathbf{x}_1 + \alpha_2\mathbf{x}_2 + \ldots + \alpha_n\mathbf{x}_n$$

where

$$\alpha_i = \mathbf{x}^{\mathrm{T}}\mathbf{x}_i \qquad \text{for} \quad i = 1, \ldots, n$$

Proof

- If follows that

$$\begin{aligned}\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} &= \mathbf{x}^{\mathrm{T}}\mathbf{A}\left(\alpha_1\mathbf{x}_1 + \alpha_2\mathbf{x}_2 + \ldots + \alpha_n\mathbf{x}_n\right) \\ &= \mathbf{x}^{\mathrm{T}}\left(\alpha_1\mathbf{A}\mathbf{x}_1 + \alpha_2\mathbf{A}\mathbf{x}_2 + \ldots + \alpha_n\mathbf{A}\mathbf{x}_n\right) \\ &= \mathbf{x}^{\mathrm{T}}\left(\alpha_1\lambda_1\mathbf{x}_1 + \alpha_2\lambda_2\mathbf{x}_2 + \ldots + \alpha_n\lambda_n\mathbf{x}_n\right) \\ &= \sum_{i=1}^{n}\alpha_i^2\lambda_i \\ &> 0\end{aligned}$$

  since all λ_i are positive and $\mathbf{x}$ is nonzero, which shows $\mathbf{A}$ is positive definite.
- Other statements can be proved in a similar fashion.

Q: What is the usefulness of a quadratic form?

Theorem

Let $f(\mathbf{x}) = \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}$ be a quadratic form with associated $n \times n$ matrix

$$\mathbf{A}$$

Let the eigenvalues of $\mathbf{A}$ be

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$$

Then the followings are true, subject to the constraint $\|\mathbf{x}\| = 1$:

1. $\lambda_n \leq f(\mathbf{x}) \leq \lambda_1$
2. The maximum value of $f(\mathbf{x})$ is
$$\lambda_1$$
and it is attained when $\mathbf{x}$ is a unit eigenvector corresponding to λ_1.
3. The minimum value of $f(\mathbf{x})$ is
$$\lambda_n$$
and it is attained when $\mathbf{x}$ is a unit eigenvector corresponding to λ_n.

Proof

- Consider an orthonormal eigenbasis corresponding to $\mathbf{A}$,

$$\mathcal{B} = \left\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\right\}$$

  then any vector in $\mathbb{R}^n$ can be expressed as

$$\mathbf{x} = \alpha_1\mathbf{x}_1 + \alpha_2\mathbf{x}_2 + \ldots + \alpha_n\mathbf{x}_n$$

  where

$$\alpha_{i} = \mathbf{x}^{\mathrm{T}}\mathbf{x}_{i} \qquad \text{for} \quad i = 1, \ldots, n$$

- If follows that

$$\begin{aligned} f(\mathbf{x}) = \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} &= \mathbf{x}^{\mathrm{T}}\mathbf{A}\left(\alpha_1\mathbf{x}_1 + \alpha_2\mathbf{x}_2 + \ldots + \alpha_n\mathbf{x}_n\right) \\ &= \mathbf{x}^{\mathrm{T}}\left(\alpha_1\lambda_1\mathbf{x}_1 + \alpha_2\lambda_2\mathbf{x}_2 + \ldots + \alpha_n\lambda_n\mathbf{x}_n\right) = \sum_{i=1}^{n}\alpha_i^2\lambda_i \end{aligned}$$

Proof

- Since the eigenvalues of $\mathbf{A}$ are given to be

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$$

  the quadratic form must be bounded

$$\sum_{i=1}^{n} \alpha_i^2 \lambda_n \leq f(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i^2 \lambda_i \leq \sum_{i=1}^{n} \alpha_i^2 \lambda_1$$

- By Parseval's formula, we have

$$\lambda_n \|\mathbf{x}\|^2 \leq f(\mathbf{x}) \leq \lambda_1 \|\mathbf{x}\|^2 \implies \lambda_n \leq f(\mathbf{x}) \leq \lambda_1$$

  when the constraint $\|\mathbf{x}\| = 1$ is invoked, which leads to the first statement.

- When $\mathbf{x}$ is the unit eigenvector corresponding to λ_1 or λ_n, only α_1 or α_n is nonzero and is equal to 1, respectively, only then the equality is achieved.

$\square$

Q: The last theorem is about the minimum and maximum of a quadratic form. How can we extend it to other functions of several variables,

$$f : \mathbb{R}^n \to \mathbb{R}$$

- To do that, we need two more pieces from Calculus, recall the followings:

Definition

If f is a function of n variables and if all second partial derivatives of f exist and are continuous over the domain of the function, then the Hessian matrix of f is

$$\mathbf{H} = \begin{bmatrix} f_{11} & f_{12} & f_{13} & \cdots & f_{1n} \\ f_{21} & f_{22} & f_{23} & \cdots & f_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ f_{n1} & f_{n2} & f_{n3} & \cdots & f_{nn} \end{bmatrix}$$

Taylor's Theorem

If $f\colon \mathbb{R} \to \mathbb{R}$ is three times differentiable at the point a, then

$$f(x) = f(a) + (x-a)f'(a) + \frac{1}{2}(x-a)^2 f''(a) + R(x)$$

where the remainder term $R(x)$ satisfies

$$\lim_{x\to a} \frac{R(x)}{\|x-a\|^2} = 0$$

- Similarly, if $f\colon \mathbb{R}^n \to \mathbb{R}$ is three times differentiable at $\mathbf{a} \in \mathbb{R}^n$, then

$$f(\mathbf{x}) = f(\mathbf{a}) + (\mathbf{x}-\mathbf{a})^{\mathrm{T}}\nabla f + \frac{1}{2}(\mathbf{x}-\mathbf{a})^{\mathrm{T}}\mathbf{H}(\mathbf{x}-\mathbf{a}) + R(\mathbf{x})$$

where the remainder term $R(x)$ satisfies

$$\lim_{\mathbf{x}\to \mathbf{a}} \frac{R(\mathbf{x})}{\|\mathbf{x}-\mathbf{a}\|^2} = 0$$

Theorem

Suppose $f\colon \mathbb{R}^n \to \mathbb{R}$ is three times differentiable, and f has a critical point at $\mathbf{a}$. If $\mathbf{H}$ is positive definite at $\mathbf{a}$, then $f(\mathbf{a})$ is a local minimum for f.

Proof

- Since $\mathbf{a}$ is a critical point for f, that is, the gradient at $\mathbf{a}$ is

$$\nabla f = \mathbf{0}$$

- According to Taylor, we have

$$\begin{aligned} f(\mathbf{x}) &= f(\mathbf{a}) + (\mathbf{x}-\mathbf{a})^{\mathrm{T}} \nabla f + \frac{1}{2}(\mathbf{x}-\mathbf{a})^{\mathrm{T}} \mathbf{H}(\mathbf{x}-\mathbf{a}) + R(\mathbf{x}) \\ &= f(\mathbf{a}) + \frac{1}{2}(\mathbf{x}-\mathbf{a})^{\mathrm{T}} \mathbf{H}(\mathbf{x}-\mathbf{a}) + R(\mathbf{x}) \end{aligned}$$

- Since $\mathbf{H}$ is positive definite at $\mathbf{a}$, if λ is the smallest eigenvalue of $\mathbf{H}$ at $\mathbf{a}$,

$$(\mathbf{x}-\mathbf{a})^{\mathrm{T}} \mathbf{H}(\mathbf{x}-\mathbf{a}) \geq \lambda \left\|\mathbf{x}-\mathbf{a}\right\|^2$$

Proof

- If follows that

$$f(\mathbf{x}) \geq f(\mathbf{a}) + \frac{\lambda}{2} \|\mathbf{x} - \mathbf{a}\|^2 + R(\mathbf{x})$$
$$f(\mathbf{x}) - f(\mathbf{a}) \geq \frac{\lambda}{2} \|\mathbf{x} - \mathbf{a}\|^2 + R(\mathbf{x})$$

- From Taylor's, we have

$$\lim_{\mathbf{x} \to \mathbf{a}} \frac{R(\mathbf{x})}{\|\mathbf{x} - \mathbf{a}\|^2} = 0$$

which means there exists $\delta > 0$, for $\epsilon = \frac{\lambda}{2}$, such that any $\mathbf{x}$ satisfies

$$\|\mathbf{x} - \mathbf{a}\| < \delta \implies \left| \frac{R(\mathbf{x})}{\|\mathbf{x} - \mathbf{a}\|^2} - 0 \right| < \frac{\lambda}{2} \implies |R(\mathbf{x})| < \frac{\lambda}{2} \|\mathbf{x} - \mathbf{a}\|^2$$

Proof

- Since $\mathbf{H}$ is positive definite at $\mathbf{a}$, all eigenvalues of it must be positive,

$$|R(\mathbf{x})| < \frac{\lambda}{2}\|\mathbf{x}-\mathbf{a}\|^2 \implies -\frac{\lambda}{2}\|\mathbf{x}-\mathbf{a}\|^2 < R(\mathbf{x}) < \frac{\lambda}{2}\|\mathbf{x}-\mathbf{a}\|^2$$

- It follows that

$$f(\mathbf{x}) - f(\mathbf{a}) \geq \frac{\lambda}{2}\|\mathbf{x}-\mathbf{a}\|^2 + R(\mathbf{x})$$

$$f(\mathbf{x}) - f(\mathbf{a}) > \frac{\lambda}{2}\|\mathbf{x}-\mathbf{a}\|^2 - \frac{\lambda}{2}\|\mathbf{x}-\mathbf{a}\|^2$$

$$f(\mathbf{x}) - f(\mathbf{a}) > 0$$

  for any $\mathbf{x}$ that satisfies $\|\mathbf{x}-\mathbf{a}\| < \delta$.

- Therefore, $f(\mathbf{a})$ is a local minimum of f.

Exercise

Find the local extreme values and determine their nature for,

$$f(x, y, z) = x^2 + y^2 + 7z^2 - xy - 3yz$$

```
>> syms x y z real
>> f = symfun(x^2 + y^2 + 7*z^2 - x*y - 3*y*z,[x,y,z]);
>> gradf=jacobian(f,[x,y,z]); % Finds the gradient
>> sol = solve(gradf == 0); % Sets the gradient to zero
>> sol.x
ans =    0
>> sol.y
ans =    0
>> sol.z
ans =    0
>> subs(f,x,y,z, [sol.x],[sol.y],[sol.z])
ans(x, y, z) = 0
>> hessianf = hessian(f, [x,y,z]); % Finds the hessian matrix
[  2, -1,  0]
[ -1,  2, -3]
[  0, -3, 14]

>> lambda = eig(vpa(hessianf));
>> eval(lambda)
ans =
   14.7124
    2.6786
    0.6090
```