OPTIMUM DESIGN

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Lecture 6

Fall 2017

Taylor Series Expansion

Assume *f*(x) is:

1. Continuous function of a single variable x
2. Differentiable n times
3. x ∈ *S*, where *S* is non-empty, closed, and bounded
4. therefore x* is a possible optima

$$f(x) = f(x^*) + \frac{df(x^*)}{dx}(x - x^*) + \frac{1}{2}\frac{d^2 f(x^*)}{dx^2}(x - x^*)^2 + \frac{1}{3!}\frac{d^3 f(x^*)}{dx^3}(x - x^*)^3 + h.o.t.$$

Taylor Series Approximations

let $x - x^* = d$, a small change or vicinity of x^*...then

$$f(x) = f(x^* + d)$$

$$f(x) = f(x^*) + \frac{df(x^*)}{dx} d + \frac{1}{2} \frac{d^2 f(x^*)}{dx^2} d^2 + \frac{1}{3!} \frac{d^3 f(x^*)}{dx^3} d^3 + h.o.t.$$

$$f(x) \approx f(x^*) + \frac{df(x^*)}{dx} d \qquad \text{First Order Approximation}$$

$$f(x) \approx f(x^*) + \frac{df(x^*)}{dx} d + \frac{1}{2} \frac{d^2 f(x^*)}{dx^2} d^2 \qquad \text{Second Order Approximation}$$

Taylor Series – Mult. Variables

Estimate $f(\mathbf{x})$ using Taylor Series

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

Let $\mathbf{d} = (\mathbf{x} - \mathbf{x}^*)$, therefore $\mathbf{x} = \mathbf{x}^* + \mathbf{d}$

$$f(\mathbf{x}) = f(\mathbf{x}^* + \mathbf{d}) = f(\mathbf{x}^*) + \nabla f^T(\mathbf{x}^*)\mathbf{d} + \frac{1}{2}\mathbf{d}^T \mathbf{H}\,\mathbf{d} + R$$

Change in function

Let's define a change in the function with the symbol Δ

$$\Delta f = f(\mathbf{x}) - f(\mathbf{x}^*)$$

$$\Delta f = \nabla f^T \mathbf{d} + \frac{1}{2}\mathbf{d}^T \mathbf{H}\,\mathbf{d} + R$$

Δ-Delta ∇-Del

Let's define a first order change in the function

$$\delta f = \nabla f^T \delta\mathbf{x} = \nabla f \bullet \delta\mathbf{x}$$

EXAMPLE 4.8 TAYLOR'S EXPANSION OF A FUNCTION OF TWO VARIABLES

Obtain a second-order Taylor's expansion for the function $f(\mathbf{x}) = 3x_1^3 x_2$ at the point $\mathbf{x}^* = (1, 1)$.

Solution

The gradient and Hessian of the function $f(\mathbf{x})$ at the point $\mathbf{x}^* = (1,1)$ using Eqs. (4.5) and (4.8) are

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \dfrac{\partial f}{\partial x_1} \\ \dfrac{\partial f}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 9x_1^2 x_2 \\ 3x_1^3 \end{bmatrix} = \begin{bmatrix} 9 \\ 3 \end{bmatrix}; \quad \mathbf{H} = \begin{bmatrix} 18x_1 x_2 & 9x_1^2 \\ 9x_1^2 & 0 \end{bmatrix} = \begin{bmatrix} 18 & 9 \\ 9 & 0 \end{bmatrix} \tag{a}$$

Substituting these in the matrix form of Taylor's expression given in Eq. (4.12), and using $\mathbf{d} = \mathbf{x} - \mathbf{x}^*$, we obtain an approximation $\bar{f}(\mathbf{x})$ for $f(\mathbf{x})$ as

$$\bar{f}(\mathbf{x}) = 3 + \begin{bmatrix} 9 \\ 3 \end{bmatrix}^T \begin{bmatrix} (x_1 - 1) \\ (x_2 - 1) \end{bmatrix} + \frac{1}{2} \begin{bmatrix} (x_1 - 1) \\ (x_2 - 1) \end{bmatrix}^T \begin{bmatrix} 18 & 9 \\ 9 & 0 \end{bmatrix} \begin{bmatrix} (x_1 - 1) \\ (x_2 - 1) \end{bmatrix} \tag{b}$$

where $f(\mathbf{x}^*) = 3$ has been used. Simplifying the expression by expanding vector and matrix products, we obtain Taylor's expansion for $f(\mathbf{x})$ about the point (1, 1) as

$$\bar{f}(\mathbf{x}) = 9x_1^2 + 9x_1 x_2 - 18x_1 - 6x_2 + 9 \tag{c}$$

EXAMPLE 4.9 LINEAR TAYLOR'S EXPANSION OF A FUNCTION

Obtain a linear Taylor's expansion for the function

$$f(\mathbf{x}) = x_1^2 + x_2^2 - 4x_1 - 2x_2 + 4 \tag{a}$$

at the point $\mathbf{x}^* = (1, 2)$. Compare the approximate function with the original function in a neighborhood of the point (1, 2).

Solution

The gradient of the function at the point (1, 2) is given as

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \dfrac{\partial f}{\partial x_1} \\ \dfrac{\partial f}{\partial x_2} \end{bmatrix} = \begin{bmatrix} (2x_1 - 4) \\ (2x_2 - 2) \end{bmatrix} = \begin{bmatrix} -2 \\ 2 \end{bmatrix} \tag{b}$$

Since $f(1, 2) = 1$, Eq. (4.13) gives a linear Taylor's approximation for $f(\mathbf{x})$ as

$$\bar{f}(\mathbf{x}) = 1 + [-2 \;\; 2] \begin{bmatrix} (x_1 - 1) \\ (x_2 - 2) \end{bmatrix} = -2x_1 + 2x_2 - 1 \tag{c}$$

To see how accurately $\bar{f}(x)$ approximates the original $f(x)$ in the neighborhood of (1, 2), we calculate the functions at the point (1.1, 2.2), a 10% change in the point as $\bar{f}(x) = 1.20$ and $f(x) = 1.25$. We see that the approximate function underestimates the real function by 4%. An error of this magnitude is quite acceptable in many applications. However, note that the errors will be different for different functions and can be larger for highly nonlinear functions.

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$$f(x) = f(x^*) + \frac{df(x^*)}{dx}(x - x^*) + \frac{1}{2}\frac{d^2 f(x^*)}{dx^2}(x - x^*)^2 + \ldots$$
$$\frac{1}{3!}\frac{d^3 f(x^*)}{dx^3}(x - x^*)^3 + \frac{1}{4!}\frac{d^4 f(x^*)}{dx^4}(x - x^*)^4 + h.o.t.$$

Taylor Series Approximations

let $x - x^* = d$, a small change or vicinity of x^*...then

$$f(x) = f(x^* + d)$$

$$f(x) = f(x^*) + \frac{df(x^*)}{dx} d + \frac{1}{2} \frac{d^2 f(x^*)}{dx^2} d^2 + \frac{1}{3!} \frac{d^3 f(x^*)}{dx^3} d^3 + h.o.t.$$

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Single variable minimization

Given that x* is the minimum of *f*(x), then any movement away from x* is “uphill”, therefore to guarantee that a move goes uphill

$$\Delta f(x) \geq 0$$

$$\Delta f(x) = f(x) - f(x^*) = f'(x^*)d + \frac{1}{2} f''(x^*)d^2 + \ldots$$

$$\frac{1}{3!} f'''(x^*)d^3 + \frac{1}{4!} f^{iv}(x^*)d^4 + h.o.t.$$

First-order necessary condition

$$f'(x^*) = 0$$

Stationary point=max,min,neither

Any points satisfying $f'(x^*) = 0$

Are called “stationary” points.

Those points are a:

1. Min pt, or
2. Max pt, or
3. Neither (i.e. an inflection pt)

We need another test!

Second-order sufficient condition

Look at second order term

$$\Delta f(x) = f(x) - f(x^*) = f'(x^*)d + \frac{1}{2} f''(x^*)d^2 + \ldots$$

$$\frac{1}{3!} f'''(x^*)d^3 + \frac{1}{4!} f^{iv}(x^*)d^4 + h.o.t.$$

Second-order sufficient condition for a minimum

$$f''(x^*) > 0$$

Second-order condition?

What if $f''(x^*) < 0$

Then *f*(x*) is not a minimum of *f*(x*).

It is a maximum of *f*(x*).

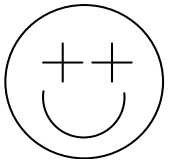
Single variable optimization

First-order necessary condition

$$f'(x^*) = 0$$

$$f''(x^*) > 0$$

Second-order sufficient condition for a minimum



$$f''(x^*) < 0$$

Second-order sufficient condition for a maximum

Higher—order tests?

What if $f''(x^*) = 0$

Then the second order test fails. We need higher order derivatives…

Min $f^{even}(x^*) > 0$

Max $f^{even}(x^*) < 0$

Second-order necessary conditions

Note the "= 0" possibility

$f''(x^*) \geq 0$

A pt not satisfying this test is not a min!

$f''(x^*) \leq 0$

A pt not satisfying this test is not a max!

Multiple variable optimization

If x* is the minimum of $f(\mathbf{x})$, then any movement away from $\mathbf{x}^*$ is "uphill".

$$\Delta f = f(\mathbf{x}) - f(\mathbf{x}^*) > 0$$

$$\Delta f = f(\mathbf{x}^* + \mathbf{d}) - f(\mathbf{x}^*) = \nabla f^T(\mathbf{x}^*)\mathbf{d} + \frac{1}{2}\mathbf{d}^T\mathbf{H}\,\mathbf{d} + R$$

$$\Delta f = \nabla f^T(\mathbf{x}^*)\mathbf{d} + \frac{1}{2}\mathbf{d}^T\mathbf{H}\,\mathbf{d} \quad \text{(second order)}$$

dot product → scalar

triple product → scalar

$$\Delta f = scalar$$

How can we guarantee that for a move in any **d,** we make away from $\mathbf{x}^*$, we go "uphill"?

First-order necessary Condition

For **x*** to be a local minimum: $\Delta f = f(\mathbf{x}) - f(\mathbf{x}^*) > 0$

$$\Delta f = \nabla f^T(\mathbf{x}^*)\mathbf{d} + \frac{1}{2}\mathbf{d}^T\mathbf{H}\,\mathbf{d}$$

1rst order term

$$\nabla f^T(\mathbf{x}^*) = \mathbf{0} \qquad \nabla f(\mathbf{x}^*) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix}_{\mathbf{x}^*} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \\ 0 \end{bmatrix} = \mathbf{0}$$

Second-order sufficient condition

For **x*** to be local minimum:

$$\mathbf{d}^T \mathbf{H}\, \mathbf{d} > 0$$

That is **H(x***) must be positive definite

Remember that $\mathbf{d}^T \mathbf{H}\, \mathbf{d}$

has “quadratic form”

Quadratic form of a matrix

Given $F(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathbf{A}\,\mathbf{x}$ where $\mathbf{A}$ is symmetric, for example :

$$\mathbf{x}^T = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \qquad \mathbf{A} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$\mathbf{x}^T\mathbf{A}\,\mathbf{x} = \mathbf{x}^T \bullet (\mathbf{A}\mathbf{x}) \qquad \mathbf{A}\mathbf{x} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$\mathbf{x}^T\mathbf{A}\,\mathbf{x} = \mathbf{x}^T \bullet (\mathbf{A}\mathbf{x}) = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}^T \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = x_1^2 + x_2^2 + x_3^2$$

$$F(\mathbf{x}) = \frac{1}{2}\left(x_1^2 + x_2^2 + x_3^2\right)$$

EXAMPLE 4.10 MATRIX OF THE QUADRATIC FORM

Identify a matrix associated with the quadratic form:

$$F(x_1, x_2, x_3) = 2x_1^2 + 2x_1x_2 + 4x_1x_3 - 6x_2^2 - 4x_2x_3 + 5x_3^2 \tag{a}$$

Solution

Writing F in the matrix form ($F(\mathbf{x}) = \mathbf{x}^T\mathbf{P}\mathbf{x}$), we obtain

$$F(\mathbf{x}) = [x_1 \; x_2 \; x_3]\begin{bmatrix} 2 & 2 & 4 \\ 0 & -6 & -4 \\ 0 & 0 & 5 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \tag{b}$$

For example, the following matrices are also associated with the same quadratic form:

$$\mathbf{P} = \begin{bmatrix} 2 & 0.5 & 1 \\ 1.5 & -6 & -6 \\ 3 & 2 & 5 \end{bmatrix}; \quad \mathbf{P} = \begin{bmatrix} 2 & 4 & 5 \\ -2 & -6 & 4 \\ -1 & -8 & 5 \end{bmatrix} \tag{c}$$

EXAMPLE 4.10 MATRIX OF THE QUADRATIC FORM

Identify a matrix associated with the quadratic form:

$$F(x_1, x_2, x_3) = 2x_1^2 + 2x_1x_2 + 4x_1x_3 - 6x_2^2 - 4x_2x_3 + 5x_3^2 \qquad \text{(a)}$$

Dividing the coefficients equally between the off-diagonal terms, we obtain the symmetric matrix associated with the quadratic form in E q. (a) as

$$\mathbf{A} = \begin{bmatrix} 2 & 1 & 2 \\ 1 & -6 & -2 \\ 2 & -2 & 5 \end{bmatrix} \qquad \text{(d)}$$

The diagonal elements of the symmetric matrix **A** are obtained from the coefficient of x_i^2 as before. The off-diagonal elements are obtained by dividing the coefficient of the term x_ix_j equally between a_{ij} and a_{ji}. Any of the matrices in Eqs. (b)–(d) gives a matrix associated with the quadratic form.