

Appendix - Gradient and Jacobian of multivariate functions

- We use thin/bold letters, $x, v/\mathbf{x}, \mathbf{v}$, for denoting scalar/vector inputs.
 - $\mathbf{x} \in \mathbb{R}^n \Rightarrow \mathbf{x} = (x_1, \dots, x_n)^T$, where $x_i \in \mathbb{R}, i \leq n$
- We use lower/upper case letters, $f, g, h/F, G, H$, for denoting scalar/vector functions.
 - $F \in \mathbb{R}^m \Rightarrow F = (f_1, \dots, f_m)^T$, where $f_i \in \mathbb{R}, i \leq m$

1 Definition of gradient and Jacobian

- Univariate functions

– Scalar function

- * (Function) $f(x) : \mathbb{R} \rightarrow \mathbb{R}$
- * (Gradient) $\nabla f(x) = df(x)/dx = \lim_{h \rightarrow 0} \{f(x+h) - f(x)\}/h : \mathbb{R} \rightarrow \mathbb{R}$
- * (Example)

$$f(x) = ax \Rightarrow \nabla f(x) = a$$

– (Column) Vector function

- * (Function) $F(x) = (f_1(x), \dots, f_m(x))^T : \mathbb{R} \rightarrow \mathbb{R}^m$ (a column vector)
- * (Jacobian) $\nabla F(x) = (df_1(x)/dx, \dots, df_m(x)/dx) : \mathbb{R} \rightarrow \mathbb{R}^{1 \times m}$ (a row vector)
- * (Example)

$$\begin{aligned} F(x) &= (3x+1, 2x^2-1, x^3-2x)^T \Rightarrow \nabla F(x) = (3, 4x, 3x^2-2) \rightarrow \text{변수는 } x \text{ 1개.} \\ F(x) &= \mathbf{x}\mathbf{a} = (a_1x, \dots, a_mx)^T \Rightarrow \nabla F(x) = \mathbf{a}^T \rightarrow \text{변수가 여러개.} \\ F(x) &= g(x)\mathbf{a} = (a_1g(x), \dots, a_mg(x))^T \Rightarrow \nabla F(x) = \nabla g(x)\mathbf{a}^T \end{aligned}$$

- Multivariate functions

– Scalar function

- * (Function) $f(\mathbf{x}) = f(x_1, \dots, x_n) : \mathbb{R}^n \rightarrow \mathbb{R}$
- * (Gradient) $\nabla f(\mathbf{x}) = (\partial f(\mathbf{x})/\partial x_1, \dots, \partial f(\mathbf{x})/\partial x_n)^T : \mathbb{R}^n \rightarrow \mathbb{R}^n$ (a column vector)
- * (Example)

$$\begin{aligned} f(\mathbf{x}) &= 3x_1^2 + 4x_2^2 + 5x_1x_2 \Rightarrow \nabla f(\mathbf{x}) = (6x_1 + 5x_2, 8x_2 + 5x_1)^T \\ f(\mathbf{x}) &= \mathbf{a}^T \mathbf{x} = \mathbf{x}^T \mathbf{a} = a_1x_1 + \dots + a_nx_n = \sum_{i=1}^n a_i x_i \Rightarrow \nabla f(\mathbf{x}) = \mathbf{a} \\ f(\mathbf{x}) &= \mathbf{a}^T G(\mathbf{x}) = G(\mathbf{x})^T \mathbf{a} = a_1g_1(\mathbf{x}) + \dots + a_mg_m(\mathbf{x}) = \sum_{j=1}^m a_j g_j(\mathbf{x}) \Rightarrow \nabla f(\mathbf{x}) = ??? \end{aligned}$$

– Vector function

- * (Function) $F(\mathbf{x}) = (f_1(\mathbf{x}), \dots, f_m(\mathbf{x}))^T : \mathbb{R}^n \rightarrow \mathbb{R}^m$
- * (Jacobian) $\nabla F(\mathbf{x}) = (\nabla f_1(\mathbf{x}), \dots, \nabla f_m(\mathbf{x})) : \mathbb{R}^n \rightarrow \mathbb{R}^{n \times m}$ (a matrix)
- * (Example)

$$\begin{aligned} F(\mathbf{x}) &= (2x_1x_2 + x_2^2, x_1^2 + 2x_1x_2)^T \Rightarrow \nabla F(\mathbf{x}) = \begin{pmatrix} 2x_2 & 2x_1 + 2x_2 \\ 2x_1 + 2x_2 & 2x_1 \end{pmatrix} \rightarrow \text{변수가 여러개.} \\ F(\mathbf{x}) &= \mathbf{A}\mathbf{x} = \begin{pmatrix} \mathbf{a}_1^T \\ \vdots \\ \mathbf{a}_m^T \end{pmatrix} \mathbf{x} = \begin{pmatrix} \mathbf{a}_1^T \mathbf{x} \\ \vdots \\ \mathbf{a}_m^T \mathbf{x} \end{pmatrix} \Rightarrow \nabla F(\mathbf{x}) = (\mathbf{a}_1, \dots, \mathbf{a}_m) = \mathbf{A}^T \end{aligned}$$

2 Gradient of products and ratios

• Univariate functions

- Product and ratio between two scalars - skipped
- Product of a vector and a scalar = vector

- ①
- * (Function) $F(x) = G(x)h(x) : \mathbb{R} \rightarrow \mathbb{R}^m$
 - * (Jacobian) $\nabla F(x) = \nabla G(x)h(x) + \nabla h(x)G(x)^T : \mathbb{R} \rightarrow \mathbb{R}^{1 \times m}$
 - * (Example)

$$F(x) = (\mathbf{a}x)h(x) \Rightarrow \nabla F(x) = \mathbf{a}^T h(x) + \nabla h(x)(\mathbf{a}x)^T$$

$$F(x) = \mathbf{a}\{xh(x)\} \Rightarrow \nabla F(x) = \{h(x) + \nabla h(x)x\}\mathbf{a}^T$$

- Ratio of a vector to a scalar = vector

- * (Function) $F(x) = G(x)/h(x) : \mathbb{R} \rightarrow \mathbb{R}^m$
- * (Jacobian) $\nabla F(x) = \{\nabla G(x)h(x) - \nabla h(x)G(x)^T\}/h(x)^2 : \mathbb{R} \rightarrow \mathbb{R}^{1 \times m}$
- * (Example)

$$F(x) = (\mathbf{a}x)/h(x) \Rightarrow \nabla F(x) = \{\mathbf{a}^T h(x) - \nabla h(x)(\mathbf{a}x)^T\}/h(x)^2$$

$$F(x) = \mathbf{a}\{x/h(x)\} \Rightarrow \nabla F(x) = [\{h(x) - x\nabla h(x)\}/h(x)^2]\mathbf{a}^T$$

• Multivariate functions

- Product of two scalars = scalar

- ~~이제~~ 벡터를 앞에.
- * (Function) $f(\mathbf{x}) = g(\mathbf{x})h(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}$
 - * (Gradient) $\nabla f(\mathbf{x}) = \nabla g(\mathbf{x})h(\mathbf{x}) + \nabla h(\mathbf{x})g(\mathbf{x})^T = \nabla g(\mathbf{x})h(\mathbf{x}) + \nabla h(\mathbf{x})g(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}^n$
 - * (Example)

$$f(\mathbf{x}) = (\mathbf{a}^T \mathbf{x})(\mathbf{c}^T \mathbf{x}) \Rightarrow \nabla f(\mathbf{x}) = \mathbf{a}(\mathbf{c}^T \mathbf{x}) + \mathbf{c}(\mathbf{a}^T \mathbf{x})$$

- Ratio of a scalar to a scalar = scalar

- * (Function) $f(\mathbf{x}) = g(\mathbf{x})/h(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}$
- * (Gradient) $\nabla f(\mathbf{x}) = \{\nabla g(\mathbf{x})h(\mathbf{x}) - \nabla h(\mathbf{x})g(\mathbf{x})^T\}/h(\mathbf{x})^2 = \{\nabla g(\mathbf{x})h(\mathbf{x}) - \nabla h(\mathbf{x})g(\mathbf{x})\}/h(\mathbf{x})^2 : \mathbb{R}^n \rightarrow \mathbb{R}^n$
- * (Example)

$$f(\mathbf{x}) = \mathbf{a}^T \mathbf{x} / \mathbf{c}^T \mathbf{x} \Rightarrow \nabla f(\mathbf{x}) = \{\mathbf{a}(\mathbf{c}^T \mathbf{x}) - \mathbf{c}(\mathbf{a}^T \mathbf{x})\}/(\mathbf{c}^T \mathbf{x})^2$$

$$f(\mathbf{x}) = 1/\mathbf{c}^T \mathbf{x} \Rightarrow \nabla f(\mathbf{x}) = \{\mathbf{0}(\mathbf{c}^T \mathbf{x}) - \mathbf{c}(1)\}/(\mathbf{c}^T \mathbf{x})^2 = -\mathbf{c}/(\mathbf{c}^T \mathbf{x})^2$$

②

- Product of a vector and a scalar = vector

- * (Function) $F(\mathbf{x}) = G(\mathbf{x})h(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}^m$
- * (Jacobian) $\nabla F(\mathbf{x}) = \nabla G(\mathbf{x})h(\mathbf{x}) + \nabla h(\mathbf{x})G(\mathbf{x})^T : \mathbb{R}^n \rightarrow \mathbb{R}^{n \times m}$
- * (Example)

$$F(\mathbf{x}) = \mathbf{A}\mathbf{x}(\mathbf{a}^T \mathbf{x}) \Rightarrow \nabla F(\mathbf{x}) = \mathbf{A}^T(\mathbf{a}^T \mathbf{x}) + \mathbf{a}(\mathbf{A}\mathbf{x})^T$$

$$F(\mathbf{x}) = \mathbf{c}(\mathbf{a}^T \mathbf{x}) \Rightarrow \nabla F(\mathbf{x}) = \mathbf{0}(\mathbf{a}^T \mathbf{x}) + \mathbf{a}\mathbf{c}^T$$

$$F(\mathbf{x}) = (\mathbf{c}\mathbf{a}^T)\mathbf{x} \Rightarrow \nabla F(\mathbf{x}) = (\mathbf{c}\mathbf{a}^T)^T$$

- Ratio of a vector to a scalar = vector

- * (Function) $F(\mathbf{x}) = G(\mathbf{x})/h(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}^m$

* (Jacobian) $\mathbb{R}^n \rightarrow \mathbb{R}^{n \times m} : \nabla F(\mathbf{x}) = \{\nabla G(\mathbf{x})h(\mathbf{x}) - \nabla h(\mathbf{x})G(\mathbf{x})^T\}/h(\mathbf{x})^2$

* (Example)

$$F(\mathbf{x}) = \mathbf{Ax}/\mathbf{a}^T \mathbf{x} \Rightarrow \nabla F(\mathbf{x}) = \{\mathbf{A}^T(\mathbf{a}^T \mathbf{x}) - \mathbf{a}(\mathbf{Ax})^T\}/(\mathbf{a}^T \mathbf{x})^2$$

$$F(\mathbf{x}) = \mathbf{c}/\mathbf{a}^T \mathbf{x} \Rightarrow \nabla f(\mathbf{x}) = \{\mathbf{0}(\mathbf{a}^T \mathbf{x}) - \mathbf{ac}^T\}/(\mathbf{a}^T \mathbf{x})^2$$

★ Inner product of two vectors = scalar

* (Function) $f(\mathbf{x}) = G(\mathbf{x})^T H(\mathbf{x}) = \sum_{j=1}^m g_j(\mathbf{x})h_j(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}$

* (Gradient) $\nabla f(\mathbf{x}) = \nabla G(\mathbf{x})H(\mathbf{x}) + \nabla H(\mathbf{x})G(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}$

* (Example)

$$f(\mathbf{x}) = (\mathbf{Ax})^T (\mathbf{Bx}) \Rightarrow \nabla f(\mathbf{x}) = \mathbf{A}^T (\mathbf{Bx}) + \mathbf{B}^T (\mathbf{Ax}) = (\mathbf{A}^T \mathbf{B} + \mathbf{B}^T \mathbf{A})\mathbf{x}$$

$$f(\mathbf{x}) = \mathbf{x}^T \mathbf{Cx} = (\mathbf{C}^T \mathbf{x})^T (\mathbf{Ix}) \Rightarrow \nabla f(\mathbf{x}) = \mathbf{C}(\mathbf{Ix}) + \mathbf{I}(\mathbf{C}^T \mathbf{x}) = (\mathbf{C} + \mathbf{C}^T)\mathbf{x}$$

3 Chain rules

• Outer univariate scalar

– Inner univariate scalar - skipped

– Inner multivariate scalar

* (Function) $f(\mathbf{x}) = g(h(\mathbf{x})) \Leftrightarrow f = g(t), t = h(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R} \rightarrow \mathbb{R}$

* (Gradient) $\nabla f(\mathbf{x}) = \nabla h(\mathbf{x}) \nabla g(h(\mathbf{x})) : \mathbb{R}^n \rightarrow \mathbb{R}$

* (Example)

$$f(\mathbf{x}) = (\mathbf{a}^T \mathbf{x})^2 \Rightarrow \nabla f(\mathbf{x}) = \mathbf{a}2(\mathbf{a}^T \mathbf{x})$$

$$f(\mathbf{x}) = (\mathbf{a}^T \mathbf{x})(\mathbf{a}^T \mathbf{x}) \Rightarrow \nabla f(\mathbf{x}) = \mathbf{a}(\mathbf{a}^T \mathbf{x}) + \mathbf{a}(\mathbf{a}^T \mathbf{x})$$

$$f(\mathbf{x}) = g(\mathbf{a}^T \mathbf{x}) \Rightarrow \nabla f(\mathbf{x}) = \mathbf{a} \nabla g(\mathbf{a}^T \mathbf{x})$$

• Outer univariate vector

– Inner univariate scalar

* (Function) $F(x) = G(h(x)) \Leftrightarrow F = G(v), v = h(x) : \mathbb{R} \rightarrow \mathbb{R} \rightarrow \mathbb{R}^m$

* (Jacobian) $\nabla F(x) = \nabla h(x) \nabla G(h(x)) : \mathbb{R} \rightarrow \mathbb{R}^{1 \times m}$

* (Example)

$$F(x) = \mathbf{a}(x^2 + x) \Rightarrow \nabla F(x) = (2x + 1)\mathbf{a}^T$$

$$F(x) = \mathbf{a}h(x) \Rightarrow \nabla F(x) = \nabla h(x)\mathbf{a}^T$$

– Inner multivariate scalar

* (Function) $F(\mathbf{x}) = G(h(\mathbf{x})) \Leftrightarrow F = G(v), v = h(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R} \rightarrow \mathbb{R}^m$

* (Gradient) $\nabla F(\mathbf{x}) = \nabla h(\mathbf{x}) \nabla G(h(\mathbf{x})) : \mathbb{R}^n \rightarrow \mathbb{R}^{n \times m}$

* (Example)

$$F(\mathbf{x}) = \mathbf{a}(\mathbf{c}^T \mathbf{x}) \Rightarrow \nabla F(\mathbf{x}) = \mathbf{ca}^T$$

$$F(\mathbf{x}) = (\mathbf{ac}^T)\mathbf{x} \Rightarrow \nabla F(\mathbf{x}) = \mathbf{ca}^T$$

$$F(\mathbf{x}) = \mathbf{a}(\mathbf{c}^T \mathbf{x}) \Rightarrow \nabla F(\mathbf{x}) = \mathbf{0}(\mathbf{c}^T \mathbf{x}) + \mathbf{ca}^T$$

• Outer multivariate scalar

- Inner univariate vector

- * (Function) $f(x) = g(H(x)) \Leftrightarrow f = g(\mathbf{v}), \mathbf{v} = H(x) : \mathbb{R} \rightarrow \mathbb{R}^m \rightarrow \mathbb{R}$
- * (Gradient) $\nabla f(x) = \nabla H(x) \nabla g(H(x)) : \mathbb{R} \rightarrow \mathbb{R}$
- * (Example)

$$\begin{aligned} f(x) &= \mathbf{a}^T(\mathbf{c}x) \Rightarrow \nabla f(x) = \mathbf{c}^T \mathbf{a} \\ f(x) &= (\mathbf{a}^T \mathbf{c})x \Rightarrow \nabla f(x) = (\mathbf{a}^T \mathbf{c})^T \end{aligned}$$

- Inner multivariate vector

- * (Function) $f(\mathbf{x}) = g(H(\mathbf{x})) \Leftrightarrow f = g(\mathbf{v}), \mathbf{v} = H(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}^m \rightarrow \mathbb{R}$
- * (Gradient) $\nabla f(\mathbf{x}) = \nabla H(\mathbf{x}) \nabla g(H(\mathbf{x})) : \mathbb{R}^n \rightarrow \mathbb{R}^n$
- * (Example)

$$\begin{aligned} f(\mathbf{x}) &= \mathbf{a}^T(\mathbf{C}\mathbf{x}) \Rightarrow \nabla f(\mathbf{x}) = \mathbf{C}^T \mathbf{a} \\ f(\mathbf{x}) &= (\mathbf{a}^T \mathbf{C})\mathbf{x} \Rightarrow \nabla f(\mathbf{x}) = (\mathbf{a}^T \mathbf{C})^T \end{aligned}$$

• Outer multivariate vector

- Inner univariate vector

- * (Function) $F(x) = G(H(x)) \Leftrightarrow F = G(\mathbf{v}), \mathbf{v} = H(x) : \mathbb{R} \rightarrow \mathbb{R}^m \rightarrow \mathbb{R}^\ell$
- * (Jacobian) $\nabla F(x) = \nabla H(x) \nabla G(H(x)) : \mathbb{R} \rightarrow \mathbb{R}^{1 \times \ell}$
- * (Example)

$$\begin{aligned} F(x) &= \mathbf{C}(\mathbf{a}x) \Rightarrow \nabla F(x) = \mathbf{a}^T \mathbf{C}^T \\ F(x) &= (\mathbf{C}\mathbf{a})x \Rightarrow \nabla F(x) = (\mathbf{C}\mathbf{a})^T \end{aligned}$$

- Inner multivariate vector

- * (Function) $F(\mathbf{x}) = G(H(\mathbf{x})) \Leftrightarrow F = G(\mathbf{v}), \mathbf{v} = H(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}^m \rightarrow \mathbb{R}^l$
- * (Jacobian) $\nabla F(\mathbf{x}) = \nabla H(\mathbf{x}) \nabla G(H(\mathbf{x})) : \mathbb{R}^n \rightarrow \mathbb{R}^l$
- * (Example)

$$\begin{aligned} F(\mathbf{x}) &= \mathbf{A}(\mathbf{C}\mathbf{x}) \Rightarrow \nabla F(\mathbf{x}) = \mathbf{C}^T \mathbf{A}^T \\ F(\mathbf{x}) &= (\mathbf{A}\mathbf{C})\mathbf{x} \Rightarrow \nabla F(\mathbf{x}) = (\mathbf{A}\mathbf{C})^T \end{aligned}$$

4 Statistical Example: Multivariate analysis

• Linear regression

- (Function) $L(\beta) = \sum_{i=1}^n (y_i - \mathbf{x}_i^T \beta)^2 \Leftrightarrow (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta) : \mathbb{R}^p \rightarrow \mathbb{R}$
- (Gradient) $\nabla L(\beta) = \sum_{i=1}^n \{-2\mathbf{x}_i(y_i - \mathbf{x}_i^T \beta)\} \Leftrightarrow -2\mathbf{X}^T (\mathbf{y} - \mathbf{X}\beta) : \mathbb{R}^p \rightarrow \mathbb{R}^p$
- (Hessian: Jacobian of gradient): $\nabla^2 L(\beta) = \sum_{i=1}^n 2\mathbf{x}_i \mathbf{x}_i^T \Leftrightarrow 2\mathbf{X}^T \mathbf{X} : \mathbb{R}^p \rightarrow \mathbb{R}^{p \times p}$

• Logistic regression

- (Function) $L(\beta) = \sum_{i=1}^n \{-y_i \mathbf{x}_i^T \beta + \log(1 + \exp(\mathbf{x}_i^T \beta))\} : \mathbb{R}^p \rightarrow \mathbb{R}$
- (Gradient) $\mathbb{R}^p \rightarrow \mathbb{R}^p$

$$\begin{aligned} \nabla L(\beta) &= \sum_{i=1}^n \{-(y_i \mathbf{x}_i^T)^T + \mathbf{x}_i \exp(\mathbf{x}_i^T \beta) / (1 + \exp(\mathbf{x}_i^T \beta))\} \\ &= \sum_{i=1}^n \left[-y_i + \frac{\exp(\mathbf{x}_i^T \beta)}{1 + \exp(\mathbf{x}_i^T \beta)} \right] \mathbf{x}_i \end{aligned}$$

$$\frac{e^{x_i^T \beta}}{(1 + e^{x_i^T \beta})^2} \cdot x_i \quad \left(\frac{x_i \exp(x_i^T \beta) \cdot (1 + \exp(x_i^T \beta)) - x_i \exp(x_i^T \beta) \exp(x_i^T \beta)}{(1 + \exp(x_i^T \beta))^2} \right) x_i$$

★ (Hessian) $\nabla^2 L(\beta) = \sum_{i=1}^n \exp(\mathbf{x}_i^T \beta) / \{1 + \exp(\mathbf{x}_i^T \beta)\}^2 \mathbf{x}_i \mathbf{x}_i^T : \mathbb{R}^p \rightarrow \mathbb{R}^{p \times p}$

• General scheme

- (Function) $L(\beta) = \sum_{i=1}^n \ell_i(\mathbf{x}_i^T \beta) : \mathbb{R}^p \rightarrow \mathbb{R}$
- (Gradient) $\nabla L(\beta) = \sum_{i=1}^n \mathbf{x}_i \nabla \ell_i(\mathbf{x}_i^T \beta) : \mathbb{R}^p \rightarrow \mathbb{R}^p$
- (Hessian) $\nabla^2 L(\beta) = \sum_{i=1}^n \mathbf{x}_i \nabla^2 \ell_i(\mathbf{x}_i^T \beta) \mathbf{x}_i^T : \mathbb{R}^p \rightarrow \mathbb{R}^{p \times p}$

? ~~Gradient~~

$$\nabla^2 L(\beta) = \nabla \sum_{i=1}^n \left(\frac{e^{x_i \beta}}{1 + e^{x_i \beta}} \right) x_i \rightarrow x_i \text{ 는 헤지라 } \cancel{\phi}$$

$$= \nabla \sum_{i=1}^n x_i \left(\frac{e^{x_i \beta}}{1 + e^{x_i \beta}} \right)$$

헤지라 는 헤지라 인데
A.
 $\nabla G.H + \nabla H.G.T.$

$$= \sum_{i=1}^n \nabla x_i \left(\frac{e^{x_i \beta}}{1 + e^{x_i \beta}} \right) + \nabla \left(\frac{e^{x_i \beta}}{1 + e^{x_i \beta}} \right) x_i^T$$

$$= \sum_{i=1}^n \frac{x_i \cdot \exp(x_i^T \beta)}{\{1 + \exp(x_i^T \beta)\}^2} \cdot x_i^T$$

$$\frac{e^{x_i \beta}}{1 + e^{x_i \beta}} \cdot \frac{1}{1 + e^{x_i \beta}}$$