SIMULATION OPTIMIZATION SYSTEMS
Research Laboratory

NOTES ON VECTORS, MATRICES AND SENSITIVITIES

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Matrix **A**

Let

$$\mathbf{A} \triangleq \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \cdot & \cdot & & \\ \cdot & \cdot & & \\ \cdot & \cdot & & \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$$

This mxn matrix has m rows and n columns.

Transpose of **A**

$$\mathbf{A}^T \triangleq \begin{bmatrix} a_{11} & a_{21} & \cdots & a_{m1} \\ a_{12} & a_{22} & \cdots & a_{m2} \\ \cdot & \cdot & & \\ \cdot & \cdot & & \\ \cdot & \cdot & & \\ a_{1n} & a_{2n} & \cdots & a_{mn} \end{bmatrix}$$

This nxm matrix has n rows and m columns.

Symmetric Matrix **A**

A square matrix **A** is said to be symmetric if

$$\mathbf{A}^T = \mathbf{A}$$

<u>Vector **a**</u>

Let

$$\mathbf{a} \triangleq \begin{bmatrix} a_1 \\ a_2 \\ \cdot \\ \cdot \\ \cdot \\ a_n \end{bmatrix}$$

This n-dimensional vector has n rows and 1 column.

<u>Transpose of **a**</u>

$$\mathbf{a}^T \triangleq [a_1 \quad a_2 \quad \ldots \quad a_n]$$

This n-dimensional vector has 1 row and n columns.

<u>Vector **a′**</u>

Let

$$\mathbf{a}' \triangleq \begin{bmatrix} a_1' \\ a_2' \\ \cdot \\ \cdot \\ \cdot \\ a_m' \end{bmatrix}$$

This m-dimensional vector has m rows and 1 column.

<u>Transpose of **a′**</u>

$$\mathbf{a}'^{T} \triangleq [a_1' \quad a_2' \quad \dots \quad a_m']$$

This m-dimensional vector has 1 row and m columns.

Forms of $\mathbf{A}$ and $\mathbf{A}^T$

Partitioned forms of $\mathbf{A}$ and $\mathbf{A}^T$ can be written as

$$\mathbf{A}^T = [\mathbf{a}_1 \quad \mathbf{a}_2 \quad \cdots \quad \mathbf{a}_m] = \begin{bmatrix} \mathbf{a}_1'^T \\ \mathbf{a}_2'^T \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{a}_n'^T \end{bmatrix} = \mathbf{A}'$$

and

$$\mathbf{A} = \begin{bmatrix} \mathbf{a}_1^T \\ \mathbf{a}_2^T \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{a}_m^T \end{bmatrix} = [\mathbf{a}_1' \quad \mathbf{a}_2' \quad \cdots \quad \mathbf{a}_n'] = \mathbf{A}'^T$$

Here, $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_m$ are n-dimensional, whereas $\mathbf{a}_1', \mathbf{a}_2', \ldots, \mathbf{a}_n'$ are m-dimensional.

<u>Rows of **A**</u>

$$\mathbf{A} = \begin{bmatrix} \mathbf{a}_1^T \\ \mathbf{a}_2^T \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{a}_m^T \end{bmatrix}$$

This mxn matrix has rows which are the transposes of the column vectors

$$\mathbf{a}_1 \triangleq \begin{bmatrix} a_{11} \\ a_{12} \\ \cdot \\ \cdot \\ \cdot \\ a_{1n} \end{bmatrix}, \quad \mathbf{a}_2 \triangleq \begin{bmatrix} a_{21} \\ a_{22} \\ \cdot \\ \cdot \\ \cdot \\ a_{2n} \end{bmatrix}, \quad \ldots, \quad \mathbf{a}_m \triangleq \begin{bmatrix} a_{m1} \\ a_{m2} \\ \cdot \\ \cdot \\ \cdot \\ a_{mn} \end{bmatrix}$$

Columns of **A**

$$\mathbf{A} = [\mathbf{a}_1' \quad \mathbf{a}_2' \quad \dots \quad \mathbf{a}_n']$$

This mxn matrix has columns

$$\mathbf{a}_1' \triangleq \begin{bmatrix} a_{11} \\ a_{21} \\ \cdot \\ \cdot \\ \cdot \\ a_{m1} \end{bmatrix}, \quad \mathbf{a}_2' \triangleq \begin{bmatrix} a_{12} \\ a_{22} \\ \cdot \\ \cdot \\ \cdot \\ a_{m2} \end{bmatrix}, \quad \dots, \quad \mathbf{a}_n' \triangleq \begin{bmatrix} a_{1n} \\ a_{2n} \\ \cdot \\ \cdot \\ \cdot \\ a_{mn} \end{bmatrix}$$

Unit Vector $\mathbf{u}_i$

$$\mathbf{u}_i \triangleq \begin{bmatrix} 0 \\ \cdot \\ \cdot \\ \cdot \\ 1 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix} \begin{matrix} \\ \\ \\ \\ \leftarrow \text{ith row} \\ \\ \\ \\ \\ \end{matrix}$$

This vector is considered as having m elements, all of which are 0 except the ith, which is 1.

<u>Unit Vector $\mathbf{u}_j$</u>

$$\mathbf{u}_j \triangleq \begin{bmatrix} 0 \\ \cdot \\ \cdot \\ \cdot \\ 1 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix} \begin{matrix} \\ \\ \\ \\ \leftarrow \text{jth row} \\ \\ \\ \\ \\ \end{matrix}$$

This vector is considered as having n elements, all of which are 0 except the jth, which is 1.

The Identity Matrix

Let

$$\mathbf{u}_1 \triangleq \begin{bmatrix} 1 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix}, \quad \mathbf{u}_2 \triangleq \begin{bmatrix} 0 \\ 1 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix}, \ldots, \quad \mathbf{u}_n \triangleq \begin{bmatrix} 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 1 \end{bmatrix}.$$

Then

$$\mathbf{1} = [\mathbf{u}_1 \quad \mathbf{u}_2 \quad \cdots \quad \mathbf{u}_n]$$

is called the identity matrix.

Scalar Product

Let

$$\mathbf{a} \triangleq \begin{bmatrix} a_1 \\ a_2 \\ \cdot \\ \cdot \\ \cdot \\ a_n \end{bmatrix}, \quad \mathbf{b} \triangleq \begin{bmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ \cdot \\ b_n \end{bmatrix}.$$

Then

$$\mathbf{a}^T \mathbf{b} \triangleq a_1 b_1 + a_2 b_2 + \ldots + a_n b_n$$

The result is a scalar.

Element Selection from Vectors

$$\mathbf{u}_j^T \mathbf{a} \equiv \mathbf{a}^T \mathbf{u}_j = a_j$$

The result is the scalar element a_j.

$$\mathbf{u}_i^T \mathbf{a}' \equiv \mathbf{a}'^T \mathbf{u}_i = a_i'$$

The result is the scalar element a_i'.

Row Selection from Matrices

$$\mathbf{u}_i^T \mathbf{A} = \mathbf{u}_i^T \begin{bmatrix} \mathbf{a}_1^T \\ \mathbf{a}_2^T \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{a}_m^T \end{bmatrix} = \mathbf{a}_i^T$$

This result is the row vector corresponding to the ith row of $\mathbf{A}$. In transposed form, we have

$$\mathbf{A}^T \mathbf{u}_i = \mathbf{a}_i$$

Column Selection from Matrices

$$\mathbf{A}\,\mathbf{u}_j = [\mathbf{a}_1' \quad \mathbf{a}_2' \quad \ldots \quad \mathbf{a}_n']\ \mathbf{u}_j = \mathbf{a}_j'$$

This result is the column vector corresponding to the jth column of **A**. In transposed form, we have

$$\mathbf{u}_j^T \mathbf{A}^T = \mathbf{a}_j'^T$$

Element Selection from Matrices

$$\mathbf{u}_i^T \mathbf{A} \mathbf{u}_j = \begin{cases} \mathbf{u}_i^T (\mathbf{A} \mathbf{u}_j) = \mathbf{u}_i^T \mathbf{a}_j' = a_{ij} \\ (\mathbf{u}_i^T \mathbf{A}) \mathbf{u}_j = \mathbf{a}_i^T \mathbf{u}_j = a_{ij} \end{cases}$$

This result is the scalar element corresponding to the coefficient of A obtained from the intersection of row i and column j.

Element Representation

$$\mathbf{A} = \begin{bmatrix} \mathbf{u}_1^T\mathbf{a}_1 & \mathbf{u}_2^T\mathbf{a}_1 & \cdots & \mathbf{u}_n^T\mathbf{a}_1 \\ \mathbf{u}_1^T\mathbf{a}_2 & \mathbf{u}_2^T\mathbf{a}_2 & \cdots & \mathbf{u}_n^T\mathbf{a}_2 \\ \vdots & \vdots & & \vdots \\ \mathbf{u}_1^T\mathbf{a}_m & \mathbf{u}_2^T\mathbf{a}_m & \cdots & \mathbf{u}_n^T\mathbf{a}_m \end{bmatrix} = \mathbf{A}'^T,$$

where $\mathbf{u}_j$, $j = 1, \ldots, n$ is n-dimensional.

$$\mathbf{A}'^T = \begin{bmatrix} \mathbf{u}_1^T\mathbf{a}_1' & \mathbf{u}_1^T\mathbf{a}_2' & \cdots & \mathbf{u}_1^T\mathbf{a}_n' \\ \mathbf{u}_2^T\mathbf{a}_1' & \mathbf{u}_2^T\mathbf{a}_2' & \cdots & \mathbf{u}_2^T\mathbf{a}_n' \\ \vdots & \vdots & & \vdots \\ \mathbf{u}_m^T\mathbf{a}_1' & \mathbf{u}_m^T\mathbf{a}_2' & \cdots & \mathbf{u}_m^T\mathbf{a}_n' \end{bmatrix} = \mathbf{A},$$

where $\mathbf{u}_i$, $i = 1, \ldots, m$ is m-dimensional.

<u>Assembly of an Element into a Column Vector</u>

To place the paramter ϕ into the ith row of a column vector we write

$$\mathbf{u}_i \phi = \begin{bmatrix} 0 \\ \cdot \\ \cdot \\ \cdot \\ \phi \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix} \leftarrow \text{ith row}$$

This results in a column vector containing zeros everywhere except in the ith row, which contains ϕ.

Assembly of an Element into a Row Vector

To place the parameter ϕ into the jth column of a row vector we write

$$\phi \mathbf{u}_j^T = [0 \quad \ldots \quad \phi \quad \ldots \quad 0]$$

$$\uparrow$$

jth col

This results in a row vector containing zeros everywhere except in the jth column, which contains ϕ.

Assembly of a Vector into a Row of a Matrix

To place the n-dimensional vector **a** into the ith row of a matrix we write

$$
\mathbf{u}_i\,\mathbf{a}^T = \begin{bmatrix} 0 & 0 & & 0 \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ 0 & 0 & & 0 \\ a_1 & a_2 & \cdots & a_n \\ 0 & 0 & & 0 \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ 0 & 0 & & 0 \end{bmatrix} \begin{matrix} \\ \\ \\ \\ \\ \leftarrow \text{ith row} \\ \\ \\ \\ \\ \\ \end{matrix}
$$

This results in a matrix containing zeros everywhere except in the ith row, which contains $\mathbf{a}^T$.

Assembly of a Vector into a Column of a Matrix

To place the m-dimensional vector **a′** into the jth column of a matrix we write

$$\mathbf{a}'\,\mathbf{u}_j^T = \begin{bmatrix} 0 & \cdots & 0 & a_1' & 0 & \cdots & 0 \\ 0 & \cdots & 0 & a_2' & 0 & \cdots & 0 \\ & & & \vdots & & & \\ 0 & \cdots & 0 & a_m' & 0 & \cdots & 0 \end{bmatrix}$$

$$\uparrow$$

jth col

This results in a matrix containing zeros everywhere except in the jth column, which contains **a′**.

Assembly of an Element into a Matrix

To place the paramter ϕ into the intersection of row i and column j we write

$$\mathbf{u}_i \, \phi \, \mathbf{u}_j^T = \begin{bmatrix} & \cdot & \\ & \cdot & \\ & \cdot & \\ & \cdot & \\ \cdots\cdots & \phi & \cdots\cdots \\ & \cdot & \\ & \cdot & \\ & \cdot & \\ & \cdot & \end{bmatrix} \begin{matrix} \\ \\ \\ \\ \text{ith row} \\ \\ \\ \\ \\ \end{matrix}$$

$$\text{jth col}$$

This results in a matrix containing zeros everywhere except in the i,j location, which contains ϕ.

Two other forms are convenient to represent. The first one is

$$\mathbf{u}_i \, (\phi \, \mathbf{u}_j^T) = \begin{bmatrix} 0^T \\ 0^T \\ \cdot \\ \cdot \\ \cdot \\ \phi \, \mathbf{u}_j^T \\ \cdot \\ \cdot \\ 0^T \end{bmatrix} \begin{matrix} \\ \\ \\ \\ \\ \leftarrow \text{ith row} \\ \\ \\ \\ \end{matrix}$$

The other form is

$$(\mathbf{u}_i \, \phi) \, \mathbf{u}_j^T = [0 \quad 0 \quad \ldots \quad \underset{\substack{\uparrow \\ \text{jth col}}}{\mathbf{u}_i \, \phi} \quad \ldots \quad 0]$$

Assembly of a Matrix

To assemble **A** we may write

$$\mathbf{A} = \sum_{i=1}^{m} \sum_{j=1}^{n} \mathbf{u}_i \, a_{ij} \, \mathbf{u}_j^T$$

Assembly of the ith Row of a Matrix

To assemble the ith row of **A** we write

$$\mathbf{a}_i^T = \sum_{j=1}^{n} a_{ij} \mathbf{u}_j^T$$

Assembly of the jth Column of a Matrix

To assemble the jth column of **A** we write

$$\mathbf{a}_j' = \sum_{i=1}^{m} \mathbf{u}_i a_{ij}$$

Dyadic Product of **a** and **b**

Let

$$\mathbf{a} \triangleq \begin{bmatrix} a_1 \\ a_2 \\ \cdot \\ \cdot \\ \cdot \\ a_n \end{bmatrix}, \quad \mathbf{b} \triangleq \begin{bmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ \cdot \\ b_m \end{bmatrix}$$

Then

$$\mathbf{a}\ \mathbf{b}^T \triangleq \begin{bmatrix} a_1 b_1 & a_1 b_2 & \cdots & a_1 b_m \\ a_2 b_1 & a_2 b_2 & \cdots & a_2 b_m \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ a_n b_1 & a_n b_2 & \cdots & a_n b_m \end{bmatrix}$$

This result is the n by m matrix containing all possible products $a_i\ b_j$, $i = 1, 2, \ldots, n$; $j = 1, 2, \ldots, m$.

<u>Definitions of Derivative Operators</u>

$$\frac{\partial}{\partial \mathbf{a}} \triangleq \begin{bmatrix} \frac{\partial}{\partial a_1} \\ \frac{\partial}{\partial a_2} \\ \cdot \\ \cdot \\ \cdot \\ \frac{\partial}{\partial a_n} \end{bmatrix}$$

$$\frac{\partial}{\partial \mathbf{A}} \triangleq \begin{bmatrix} \frac{\partial}{\partial a_{11}} & \frac{\partial}{\partial a_{12}} & \cdots & \frac{\partial}{\partial a_{1n}} \\ \frac{\partial}{\partial a_{21}} & \frac{\partial}{\partial a_{22}} & \cdots & \frac{\partial}{\partial a_{2n}} \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ \frac{\partial}{\partial a_{m1}} & \frac{\partial}{\partial a_{m2}} & \cdots & \frac{\partial}{\partial a_{mn}} \end{bmatrix}$$

Derivatives of Scalar Products

$$\frac{\partial(\mathbf{a}^T\mathbf{b})}{\partial\mathbf{a}} = \left(\frac{\partial\mathbf{a}^T}{\partial\mathbf{a}}\right)\mathbf{b} = \mathbf{b}$$

Also,

$$\frac{\partial(\mathbf{b}^T\mathbf{a})}{\partial\mathbf{a}} = \frac{\partial(\mathbf{a}^T\mathbf{b})}{\partial\mathbf{a}} = \mathbf{b}$$

Jacobian Matrix [$\mathbf{b} \neq \mathbf{a}$]

Let

$$\mathbf{a} \triangleq \begin{bmatrix} a_1 \\ a_2 \\ \cdot \\ \cdot \\ \cdot \\ a_n \end{bmatrix}, \quad \mathbf{b} \triangleq \begin{bmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ \cdot \\ b_m \end{bmatrix}$$

Then

$$\frac{\partial \mathbf{b}^T}{\partial \mathbf{a}} \triangleq \left(\frac{\partial}{\partial \mathbf{a}} \right) \mathbf{b}^T = \begin{bmatrix} \frac{\partial b_1}{\partial a_1} & \frac{\partial b_1}{\partial a_2} & \cdots & \frac{\partial b_1}{\partial a_n} \\ \frac{\partial b_2}{\partial a_1} & \frac{\partial b_2}{\partial a_2} & \cdots & \frac{\partial b_2}{\partial a_n} \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ \frac{\partial b_m}{\partial a_1} & \frac{\partial b_m}{\partial a_2} & \cdots & \frac{\partial b_m}{\partial a_n} \end{bmatrix}^T$$

$$= \begin{bmatrix} \left(\frac{\partial b_1}{\partial \mathbf{a}} \right)^T \\ \left(\frac{\partial b_2}{\partial \mathbf{a}} \right)^T \\ \cdot \\ \cdot \\ \cdot \\ \left(\frac{\partial b_m}{\partial \mathbf{a}} \right)^T \end{bmatrix}^T = \begin{bmatrix} \frac{\partial b_1}{\partial \mathbf{a}} & \frac{\partial b_2}{\partial \mathbf{a}} & \cdots & \frac{\partial b_m}{\partial \mathbf{a}} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{\partial \mathbf{b}}{\partial a_1} & \frac{\partial \mathbf{b}}{\partial a_2} & \cdots & \frac{\partial \mathbf{b}}{\partial a_n} \end{bmatrix}^T$$

Jacobian Matrix [$\mathbf{b} \equiv \mathbf{a}$]

$$\frac{\partial \mathbf{a}^T}{\partial \mathbf{a}} = \left[\frac{\partial a_1}{\partial \mathbf{a}} \quad \frac{\partial a_2}{\partial \mathbf{a}} \quad \cdots \quad \frac{\partial a_n}{\partial \mathbf{a}} \right]$$

$$= [\mathbf{u}_1 \quad \mathbf{u}_2 \quad \cdots \quad \mathbf{u}_n] = \mathbf{1}$$

$$= \left[\frac{\partial \mathbf{a}}{\partial a_1} \quad \frac{\partial \mathbf{a}}{\partial a_2} \quad \cdots \quad \frac{\partial \mathbf{a}}{\partial a_n} \right]^T$$

$$= [\mathbf{u}_1 \quad \mathbf{u}_2 \quad \cdots \quad \mathbf{u}_n]^T = \mathbf{1}$$

where,

$$\mathbf{a} = \sum_{i=1}^{n} a_i \mathbf{u}_i$$

and

$$\frac{\partial}{\partial \mathbf{a}} = \sum_{i=1}^{n} \frac{\partial}{\partial a_i} \mathbf{u}_i$$

Hence,

$$\frac{\partial \mathbf{a}}{\partial a_i} \equiv \frac{\partial a_i}{\partial \mathbf{a}} \equiv \mathbf{u}_i$$

Jacobian Matrix [$\mathbf{b} = \mathbf{A}\,\mathbf{a}$]

$$\frac{\partial \mathbf{b}^T}{\partial \mathbf{a}} = \frac{\partial(\mathbf{a}^T \mathbf{A}^T)}{\partial \mathbf{a}} = \mathbf{A}^T$$

Jacobian Matrix [$\mathbf{b} = \mathbf{A}^T \mathbf{a}$]

$$\frac{\partial \mathbf{b}^T}{\partial \mathbf{a}} = \frac{\partial(\mathbf{a}^T \mathbf{A})}{\partial \mathbf{a}} = \mathbf{A}$$

Jacobian Matrix [$b = \mathbf{c}^T \mathbf{A}\,\mathbf{a}$]

$$\frac{\partial b}{\partial \mathbf{a}} = \mathbf{A}^T \mathbf{c}$$

Jacobian Matrix [$b = \mathbf{a}^T \mathbf{A}\,\mathbf{c}$]

$$\frac{\partial b}{\partial \mathbf{a}} = \mathbf{A}\,\mathbf{c}$$

Jacobian Matrix [$b = \mathbf{a}^T \mathbf{A}\,\mathbf{a}$]

$$\frac{\partial b}{\partial \mathbf{a}} = \mathbf{A}\,\mathbf{a} + \mathbf{A}^T \mathbf{a} = (\mathbf{A} + \mathbf{A}^T)\,\mathbf{a}$$

<u>Derivative of an Element of a Matrix w.r.t. **A**</u>

$$\frac{\partial a_{ij}}{\partial \mathbf{A}} = \begin{bmatrix} & \vdots & \\ & \vdots & \\ \cdots\cdots & 1 & \cdots\cdots \\ & \vdots & \\ & \vdots & \end{bmatrix} \quad \text{ith row}$$

$$\text{jth col}$$

$$= \mathbf{u}_i \mathbf{u}_j^T$$

The result is a matrix with zeros everywhere except at the intersection of row i and column j, which has a 1.

Derivative of **A** w.r.t. a_{ij}

$$\frac{\partial \mathbf{A}}{\partial a_{ij}} = \mathbf{u}_i \mathbf{u}_j^T \equiv \frac{\partial a_{ij}}{\partial \mathbf{A}}$$

Derivative of $\mathbf{A}^{-1}$ where m = n

We have, by definition

$$\mathbf{A}^{-1}\mathbf{A} = \mathbf{1}$$

from which

$$\frac{\partial \mathbf{A}^{-1}}{\partial \phi} = -\mathbf{A}^{-1}\frac{\partial \mathbf{A}}{\partial \phi}\mathbf{A}^{-1}$$

Derivative of $\mathbf{A}^{-1}$ w.r.t. a_{ij}

$$\frac{\partial \mathbf{A}^{-1}}{\partial a_{ij}} = -\mathbf{A}^{-1}\mathbf{u}_i\mathbf{u}_j^T\mathbf{A}^{-1}$$

$$= -\mathbf{p}_i\mathbf{q}_j^T$$

where $\mathbf{p}_i$ and $\mathbf{q}_j$ are solutions to

$$\mathbf{A}\mathbf{p}_i = \mathbf{u}_i$$

$$\mathbf{A}^T\mathbf{q}_j = \mathbf{u}_j$$

Derivatives of the Solution of $\mathbf{Ax} = \mathbf{b}$

Let $\mathbf{A}$ be n x n, $\mathbf{x}$ and $\mathbf{b}$ be n-dimensional. Then,

$$\frac{\partial \mathbf{x}}{\partial a_{ij}} = \frac{\partial(\mathbf{A}^{-1}\mathbf{b})}{\partial a_{ij}}$$

$$= -\mathbf{A}^{-1}\mathbf{u}_i\mathbf{u}_j^T\mathbf{A}^{-1}\mathbf{b} = -\mathbf{p}_i x_j$$

Derivative of an Element of the Solution of $\mathbf{A}\,\mathbf{x} = \mathbf{b}$

Let

$$\frac{\partial x_k}{\partial a_{ij}} = \mathbf{u}_k^T \frac{\partial \mathbf{x}}{\partial a_{ij}} = -\mathbf{u}_k^T\mathbf{A}^{-1}\mathbf{u}_i\mathbf{u}_j^T\mathbf{A}^{-1}\mathbf{b}$$

$$= -\hat{\mathbf{x}}_k^T\mathbf{u}_i\mathbf{u}_j^T\mathbf{x}$$

$$= -\hat{x}_{ki}\,x_j$$

Hence,

$$\frac{\partial x_k}{\partial \mathbf{A}} = -\hat{\mathbf{x}}_k\mathbf{x}^T$$

where $\hat{\mathbf{x}}_k$ is the solution of

$$\mathbf{A}^T\hat{\mathbf{x}}_k = \mathbf{u}_k$$

Derivative of a Linear Combination of the Elements of the Solution of $\mathbf{A}\,\mathbf{x} = \mathbf{b}$

Let $\bar{x} = \mathbf{u}^T \mathbf{x}$

Then

$$\frac{\partial \bar{x}}{\partial a_{ij}} = \frac{\partial(\mathbf{u}^T \mathbf{x})}{\partial a_{ij}} = -\,\mathbf{u}^T \mathbf{p}_i\, \mathbf{q}_j^T\, \mathbf{b}$$

$$= -\,(\mathbf{u}^T \mathbf{p}_i)\,(\mathbf{b}^T \mathbf{q}_j)$$

The result comes from the appropriate linear combinations of $\mathbf{p}_i$ and $\mathbf{q}_j$.

Alternatively,

$$\frac{\partial \bar{x}}{\partial a_{ij}} = -\,\mathbf{q}^T \mathbf{u}_i\, \mathbf{u}_j^T\, \mathbf{x}$$

$$= -\,q_i\, x_j$$

where $\mathbf{q}$ is the solution of

$$\mathbf{A}^T \mathbf{q} = \mathbf{u}$$

Hence

$$\frac{\partial \bar{x}}{\partial \mathbf{A}} = -\mathbf{q}\,\mathbf{x}^T$$

Also,

$$\frac{\partial \bar{x}}{\partial a_{ij}} = \mathbf{u}_i^T\, \frac{\partial \bar{x}}{\partial \mathbf{A}}\, \mathbf{u}_j$$

Hence

$$\frac{\partial \bar{\mathbf{x}}}{\partial \phi} = \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial \bar{\mathbf{x}}}{\partial a_{ij}} \frac{\partial a_{ij}}{\partial \phi} = \sum_{i=1}^{n} \sum_{j=1}^{n} \mathbf{u}_i^T \frac{\partial \bar{\mathbf{x}}}{\partial \mathbf{A}} \mathbf{u}_j \frac{\partial a_{ij}}{\partial \phi}$$

Special Case 1

Let

$$\frac{\partial \mathbf{A}}{\partial \phi} \equiv \mathbf{u}\,\mathbf{u}_i^T - \mathbf{u}\,\mathbf{u}_j^T$$

Then

$$\frac{\partial \bar{x}}{\partial \phi} = -\mathbf{u}^T \frac{\partial \mathbf{x}}{\partial \phi} = -\mathbf{u}^T \mathbf{A}^{-1} \frac{\partial \mathbf{A}}{\partial \phi} \mathbf{A}^{-1} \mathbf{b}$$

$$= -\mathbf{u}^T \mathbf{A}^{-1} \mathbf{u}\,(\mathbf{u}_i - \mathbf{u}_j)^T \mathbf{A}^{-1} \mathbf{b}$$

$$= -\mathbf{u}^T \mathbf{p}\,(x_i - x_j)$$

Let

$$\mathbf{u} = \mathbf{u}_i - \mathbf{u}_j$$

Then

$$\frac{\partial \bar{x}}{\partial \phi} = -(p_i - p_j)(x_i - x_j)$$

and

$$\frac{\partial \mathbf{A}}{\partial \phi} = (\mathbf{u}_i - \mathbf{u}_j)(\mathbf{u}_i - \mathbf{u}_j)^T$$

$$= \begin{bmatrix} & \vdots & & \vdots & \\ \cdots & 1 & \cdots & -1 & \cdots \\ & \vdots & & \vdots & \\ \cdots & -1 & \cdots & 1 & \cdots \\ & \vdots & & \vdots & \end{bmatrix} \begin{matrix} \\ \leftarrow \text{ith row} \\ \\ \leftarrow \text{jth row} \\ \\ \end{matrix}$$

$$\begin{matrix} \uparrow & \qquad & \uparrow \\ \text{ith col} & & \text{jth col} \end{matrix}$$

Special Case 2

Let

$$\frac{\partial \mathbf{A}}{\partial \phi} \equiv (\mathbf{u}_k - \mathbf{u}_\ell)(\mathbf{u}_k - \mathbf{u}_\ell)^T$$

Then

$$\frac{\partial \bar{x}}{\partial \phi} = -\mathbf{u}^T \mathbf{A}^{-1} (\mathbf{u}_k - \mathbf{u}_\ell)(\mathbf{u}_k - \mathbf{u}_\ell)^T \mathbf{A}^{-1} \mathbf{b}$$

$$= -(q_k - q_\ell)(x_k - x_\ell)$$

where $\mathbf{q}$ is the solution to

$$\mathbf{A}^T \mathbf{q} = \mathbf{u}$$

and $\mathbf{u}$ is the vector leading to $\bar{x} = \mathbf{u}^T \mathbf{x}$.

Placing Elements Arbitrarily

Let

$$\mathbf{u}_0 \triangleq \begin{bmatrix} 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix}$$

$$\mathbf{u}_1 \triangleq \begin{bmatrix} 1 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix}$$

$$\mathbf{u}_2 \triangleq \begin{bmatrix} 0 \\ 1 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix}$$

$$\mathbf{u}_n \triangleq \begin{bmatrix} 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 1 \end{bmatrix}$$

and denote

$$\mathbf{u}_{i,j} \triangleq \mathbf{u}_i - \mathbf{u}_j$$

$$\mathbf{u}_{rs,k\ell} \triangleq \mathbf{u}_r + \mathbf{u}_s - \mathbf{u}_k - \mathbf{u}_\ell$$

hence

$$\mathbf{u}_{i_1 i_2 \ldots i_p, j_1 j_2 \ldots j_q} \triangleq \sum_{k=1}^{p} \mathbf{u}_{i_k} - \sum_{\ell=1}^{q} \mathbf{u}_{j_\ell}$$

For example,

$$\mathbf{u}_{345,16} = \begin{bmatrix} -1 \\ 0 \\ 1 \\ 1 \\ 1 \\ -1 \end{bmatrix}$$

Then if

$$\mathbf{u} \equiv \mathbf{u}_{345,16}$$

we have

$$\mathbf{u}^T \mathbf{u} = \text{card}\,\{3, 4, 5, 1, 6\} = 5$$

and

$$\mathbf{u}\,\mathbf{u}^T = \begin{bmatrix} 1 & 0 & -1 & -1 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 1 & 1 & -1 \\ -1 & 0 & 1 & 1 & 1 & -1 \\ -1 & 0 & 1 & 1 & 1 & -1 \\ 1 & 0 & -1 & -1 & -1 & 1 \end{bmatrix} \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{matrix}$$

$$\begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 \end{matrix}$$

$$= (\mathbf{u}_3 + \mathbf{u}_4 + \mathbf{u}_5 - \mathbf{u}_1 - \mathbf{u}_6)(\mathbf{u}_3 + \mathbf{u}_4 + \mathbf{u}_5 - \mathbf{u}_1 - \mathbf{u}_6)^T$$