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# Hermite radial basis function (HRBF). Gradient and matrix developments

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January 20, 2015

## 1 NOTATIONS

- $\mathbf{v}$ : vectors are in bold
- $\mathbf{M}$ : matrices are in bold capital.
- $\mathbf{v}_0 * \mathbf{v}_1$ : scalar product between  $\mathbf{v}_0$  and  $\mathbf{v}_1$ .
- $\mathbf{v}_0 \cdot \mathbf{v}_1$ : component wise product between  $\mathbf{v}_0$  and  $\mathbf{v}_1$ .
- $\mathbf{v}_0 \otimes \mathbf{v}_1$ : tensor product between  $\mathbf{v}_0$  and  $\mathbf{v}_1$  (outer product).
- $f_{x_0}(\mathbf{x}) = \frac{\partial f(\mathbf{x})}{\partial x_0}$  : is the partial derivative of the first variable  $x_0$  of  $f$ .

## 2 HRBF, GENERAL EXPRESSION

An HRBF is written:

$$f(\mathbf{x}) = \sum_i^N \alpha_i \phi(\|\mathbf{x} - \mathbf{p}_i\|) + \boldsymbol{\beta}_i * \nabla [\phi(\|\mathbf{x} - \mathbf{p}_i\|)] \quad (2.1)$$

With  $N$  the number of samples  $\mathbf{p}_i$ , then  $\alpha_i$  a scalar and  $\boldsymbol{\beta}_i$  a vector which are weights to be found to interpolate the data (pairs of points and normals). The expression  $\nabla[\phi(\|\mathbf{x} - \mathbf{p}_i\|)]$  can be developed by applying the formula :

$$\nabla [g(f(\mathbf{x}))] = g'(f(\mathbf{x})). \begin{pmatrix} \frac{\partial f(\mathbf{x})}{\partial x_0} \\ \vdots \\ \frac{\partial f(\mathbf{x})}{\partial x_n} \end{pmatrix} = g'(f(\mathbf{x})). \nabla f(\mathbf{x}) \quad (2.2)$$

with  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  and  $g : \mathbb{R} \rightarrow \mathbb{R}$ . If you're curious, you can find back this equality by using rules of *differentiabilities* for *multivariate* functions.<sup>1</sup>. These rules are rarely taught in secondary schools, I invite you to take a look at the multivariate chain rule. After this reading you should be able to understand why  $[g(f(\mathbf{x}))]_{x_0} = g'(x).f_{x_0}(\mathbf{x})$  and apply it to 2.2. So we have :

$$\nabla[\phi(\|\mathbf{x} - \mathbf{p}_i\|)] = \phi'(\|\mathbf{x} - \mathbf{p}_i\|). \nabla [\|\mathbf{x} - \mathbf{p}_i\|]$$

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<sup>1</sup>Function with multiple variables  $f(x_0, \dots, x_n)$  as opposed to univariate functions with a single variable  $f(x)$

$$\begin{aligned}
&= \phi'(\|\mathbf{x} - \mathbf{p}_i\|) \cdot \begin{pmatrix} \frac{(x_0 - p_{i,x_0})}{\|\mathbf{x} - \mathbf{p}_i\|} \\ \vdots \\ \frac{(x_n - p_{i,x_n})}{\|\mathbf{x} - \mathbf{p}_i\|} \end{pmatrix} \\
&= \phi'(\|\mathbf{x} - \mathbf{p}_i\|) \frac{\mathbf{x} - \mathbf{p}_i}{\|\mathbf{x} - \mathbf{p}_i\|}
\end{aligned}$$

Which enable us to write the equation 2.1 :

$$f(\mathbf{x}) = \sum_i^N \alpha_i \phi(\|\mathbf{x} - \mathbf{p}_i\|) + \phi'(\|\mathbf{x} - \mathbf{p}_i\|) \boldsymbol{\beta}_i * \frac{\mathbf{x} - \mathbf{p}_i}{\|\mathbf{x} - \mathbf{p}_i\|}$$

### 3 COMPUTING THE GRADIENT OF $f$

To Find the expression of the gradient  $\nabla f$  you'll need to know the arithmetic rules of the differential operator  $\nabla$ . Fortunately these are similar to the derivation rules of univariate functions:

$$\begin{aligned}
\nabla[f + g] &= \nabla f + \nabla g \\
\nabla[f \cdot g] &= \nabla f \cdot g + f \cdot \nabla g \\
\nabla\left[\frac{f}{g}\right] &= \frac{\nabla f \cdot g - f \cdot \nabla g}{g^2} \\
\nabla[\alpha \cdot f] &= \alpha \cdot \nabla f
\end{aligned}$$

Unless needed we won't developed the expression of the gradient of the norml:

$$\nabla[\|\mathbf{x} - \mathbf{p}_i\|] = \frac{\mathbf{x} - \mathbf{p}_i}{\|\mathbf{x} - \mathbf{p}_i\|}$$

We are finally ready to compute the gradient of  $f$ . Don't be afraid of the length of the development, because each line represents only a single simplification. The changes only happen in the blue expressions:

$$\begin{aligned}
\nabla f(\mathbf{x}) &= \nabla \left[ \sum_i^N \alpha_i \phi(\|\mathbf{x} - \mathbf{p}_i\|) + \phi'(\|\mathbf{x} - \mathbf{p}_i\|) \boldsymbol{\beta}_i * \nabla[\|\mathbf{x} - \mathbf{p}_i\|] \right] \\
&= \sum_i^N \nabla[\alpha_i \phi(\|\mathbf{x} - \mathbf{p}_i\|)] + \nabla[\phi'(\|\mathbf{x} - \mathbf{p}_i\|) \boldsymbol{\beta}_i * \nabla[\|\mathbf{x} - \mathbf{p}_i\|]] \\
&= \sum_i^N \alpha_i \nabla[\phi(\|\mathbf{x} - \mathbf{p}_i\|)] + \nabla[\phi'(\|\mathbf{x} - \mathbf{p}_i\|) \boldsymbol{\beta}_i * \nabla[\|\mathbf{x} - \mathbf{p}_i\|]] \\
&= \sum_i^N \alpha_i \underbrace{\phi'(\|\mathbf{x} - \mathbf{p}_i\|) \nabla[\|\mathbf{x} - \mathbf{p}_i\|]}_{\mathbf{a}_i(\mathbf{x})} + \nabla[\phi'(\|\mathbf{x} - \mathbf{p}_i\|) \boldsymbol{\beta}_i * \nabla[\|\mathbf{x} - \mathbf{p}_i\|]] \\
&= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + \nabla[\phi'(\|\mathbf{x} - \mathbf{p}_i\|) (\boldsymbol{\beta}_i * \nabla[\|\mathbf{x} - \mathbf{p}_i\|])] \\
&= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + (\nabla[\phi'(\|\mathbf{x} - \mathbf{p}_i\|)] \cdot (\boldsymbol{\beta}_i * \nabla[\|\mathbf{x} - \mathbf{p}_i\|]) + \phi'(\|\mathbf{x} - \mathbf{p}_i\|) \nabla[\boldsymbol{\beta}_i * \nabla[\|\mathbf{x} - \mathbf{p}_i\|]]) \\
&= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + \underbrace{\phi''(\|\mathbf{x} - \mathbf{p}_i\|) \nabla[\|\mathbf{x} - \mathbf{p}_i\|] \cdot (\boldsymbol{\beta}_i * \nabla[\|\mathbf{x} - \mathbf{p}_i\|])}_{\mathbf{z}_i(\mathbf{x})} + \phi'(\|\mathbf{x} - \mathbf{p}_i\|) \nabla[\boldsymbol{\beta}_i * \nabla[\|\mathbf{x} - \mathbf{p}_i\|]] \\
&= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + \mathbf{z}_i(\mathbf{x}) + \phi'(\|\mathbf{x} - \mathbf{p}_i\|) \nabla[\boldsymbol{\beta}_i * \nabla[\|\mathbf{x} - \mathbf{p}_i\|]] \\
&= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + \mathbf{z}_i(\mathbf{x}) + \phi'(\|\mathbf{x} - \mathbf{p}_i\|) \nabla\left[\frac{\boldsymbol{\beta}_i * (\mathbf{x} - \mathbf{p}_i)}{\|\mathbf{x} - \mathbf{p}_i\|}\right] \\
&= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + \mathbf{z}_i(\mathbf{x}) + \phi'(\|\mathbf{x} - \mathbf{p}_i\|) \left( \frac{\nabla[\boldsymbol{\beta}_i * (\mathbf{x} - \mathbf{p}_i)] \|\mathbf{x} - \mathbf{p}_i\| - \boldsymbol{\beta}_i * (\mathbf{x} - \mathbf{p}_i) \cdot \nabla[\|\mathbf{x} - \mathbf{p}_i\|]}{\|\mathbf{x} - \mathbf{p}_i\|^2} \right) \\
&= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + \mathbf{z}_i(\mathbf{x}) + \phi'(\|\mathbf{x} - \mathbf{p}_i\|) \left( \nabla[\boldsymbol{\beta}_i * (\mathbf{x} - \mathbf{p}_i)] \frac{\|\mathbf{x} - \mathbf{p}_i\|}{\|\mathbf{x} - \mathbf{p}_i\|^2} - \frac{\boldsymbol{\beta}_i * (\mathbf{x} - \mathbf{p}_i)}{\|\mathbf{x} - \mathbf{p}_i\|^2} \cdot \nabla[\|\mathbf{x} - \mathbf{p}_i\|] \right)
\end{aligned}$$

$$= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + \mathbf{z}_i(\mathbf{x}) + \phi'(\|\mathbf{x} - \mathbf{p}_i\|) \left( \frac{\nabla [\beta_i * (\mathbf{x} - \mathbf{p}_i)]}{\|\mathbf{x} - \mathbf{p}_i\|} - \frac{\beta_i * (\mathbf{x} - \mathbf{p}_i)}{\|\mathbf{x} - \mathbf{p}_i\|^2} \cdot \nabla [\|\mathbf{x} - \mathbf{p}_i\|] \right)$$

The expression  $\nabla [\beta_i * (\mathbf{x} - \mathbf{p}_i)]$  can be easily developed component by component:

$$\nabla [\beta_i * (\mathbf{x} - \mathbf{p}_i)] = \begin{pmatrix} \frac{\partial(\beta_{i,x_0} \cdot (x_0 - p_{i,x_0}) + \dots + \beta_{i,x_n} \cdot (x_n - p_{i,x_n}))}{\partial x_0} \\ \vdots \\ \frac{\partial(\beta_{i,x_0} \cdot (x_0 - p_{i,x_0}) + \dots + \beta_{i,x_n} \cdot (x_n - p_{i,x_n}))}{\partial x_n} \end{pmatrix} = \beta_i$$

$$\begin{aligned} \nabla f(\mathbf{x}) &= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + \mathbf{z}_i(\mathbf{x}) + \phi'(\|\mathbf{x} - \mathbf{p}_i\|) \left( \frac{\beta_i}{\|\mathbf{x} - \mathbf{p}_i\|} - \frac{\beta_i * (\mathbf{x} - \mathbf{p}_i)}{\|\mathbf{x} - \mathbf{p}_i\|^2} \cdot \nabla [\|\mathbf{x} - \mathbf{p}_i\|] \right) \\ &= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + \mathbf{z}_i(\mathbf{x}) + \phi'(\|\mathbf{x} - \mathbf{p}_i\|) \left( \frac{\beta_i}{\|\mathbf{x} - \mathbf{p}_i\|} - \frac{\beta_i * \nabla [\|\mathbf{x} - \mathbf{p}_i\|]}{\|\mathbf{x} - \mathbf{p}_i\|} \cdot \nabla [\|\mathbf{x} - \mathbf{p}_i\|] \right) \end{aligned}$$

To get more compact expression we rename the norm as follow:

$$l_i(\mathbf{x}) = \|\mathbf{x} - \mathbf{p}_i\|$$

If we want to express the gradient under a matrix product form  $\nabla f = A \cdot \begin{pmatrix} \alpha_i \\ \beta_i \end{pmatrix}$  we need to factorize by  $\beta_i$ :

$$\begin{aligned} \nabla f(\mathbf{x}) &= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + \phi''(l_i(\mathbf{x})) \nabla [\|\mathbf{x} - \mathbf{p}_i\|] \cdot (\beta_i * \nabla [\|\mathbf{x} - \mathbf{p}_i\|]) + \phi'(l_i(\mathbf{x})) \left( \frac{\beta_i}{l_i(\mathbf{x})} - \frac{\beta_i * \nabla [\|\mathbf{x} - \mathbf{p}_i\|]}{l_i(\mathbf{x})} \cdot \nabla [\|\mathbf{x} - \mathbf{p}_i\|] \right) \\ &= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + \phi''(l_i(\mathbf{x})) \nabla [\|\mathbf{x} - \mathbf{p}_i\|] \cdot (\beta_i * \nabla [\|\mathbf{x} - \mathbf{p}_i\|]) + \phi'(l_i(\mathbf{x})) \frac{\beta_i}{l_i(\mathbf{x})} - \phi'(l_i(\mathbf{x})) \frac{\beta_i * \nabla [\|\mathbf{x} - \mathbf{p}_i\|]}{l_i(\mathbf{x})} \cdot \nabla [\|\mathbf{x} - \mathbf{p}_i\|] \\ &= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + \phi'(l_i(\mathbf{x})) \frac{\beta_i}{l_i(\mathbf{x})} + (\beta_i * \nabla [\|\mathbf{x} - \mathbf{p}_i\|]) \left( \phi''(l_i(\mathbf{x})) \nabla [\|\mathbf{x} - \mathbf{p}_i\|] - \phi'(l_i(\mathbf{x})) \cdot \frac{\nabla [\|\mathbf{x} - \mathbf{p}_i\|]}{l_i(\mathbf{x})} \right) \\ &= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + \underbrace{\frac{\phi'(l_i(\mathbf{x}))}{l_i(\mathbf{x})}}_{b_i(\mathbf{x})} \beta_i + (\beta_i * (\mathbf{x} - \mathbf{p}_i)) \left( \phi''(l_i(\mathbf{x})) \frac{\nabla [\|\mathbf{x} - \mathbf{p}_i\|]}{l_i(\mathbf{x})} - \phi'(l_i(\mathbf{x})) \cdot \frac{\nabla [\|\mathbf{x} - \mathbf{p}_i\|]}{(l_i(\mathbf{x}))^2} \right) \\ &= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + b_i(\mathbf{x}) \beta_i + (\beta_i * (\mathbf{x} - \mathbf{p}_i)) \cdot \frac{\nabla [\|\mathbf{x} - \mathbf{p}_i\|]}{l_i(\mathbf{x})} \left( \phi''(l_i(\mathbf{x})) - \frac{\phi'(l_i(\mathbf{x}))}{l_i(\mathbf{x})} \right) \\ &= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + b_i(\mathbf{x}) \beta_i + (\beta_i * (\mathbf{x} - \mathbf{p}_i)) \cdot (\mathbf{x} - \mathbf{p}_i) \underbrace{\frac{1}{(l_i(\mathbf{x}))^2} \left( \phi''(l_i(\mathbf{x})) - \frac{\phi'(l_i(\mathbf{x}))}{l_i(\mathbf{x})} \right)}_{c_i(\mathbf{x})} \\ &= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + \beta_i b_i(\mathbf{x}) + (\beta_i * (\mathbf{x} - \mathbf{p}_i)) \cdot (\mathbf{x} - \mathbf{p}_i) c_i(\mathbf{x}) \end{aligned}$$

Now the problem is how do we factorize  $\beta_i$  while it is bound with a dot product with  $((\mathbf{x} - \mathbf{p}_i) \cdot c_i(\mathbf{x}))$  and with a component wise product with  $b_i(\mathbf{x})$  at the same time. The trick here, is to express the two sort of product with a more general matrix product of corresponding dimension ( $n \times n$ ) in order to factorize it:

$$\begin{aligned} \nabla f(\mathbf{x}) &= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + \underbrace{\begin{pmatrix} b_i(\mathbf{x}) & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & b_i(\mathbf{x}) \end{pmatrix}}_{\mathbf{B}_i(\mathbf{x})} \beta_i + (\mathbf{x} - \mathbf{p}_i) \otimes (\mathbf{x} - \mathbf{p}_i) c_i(\mathbf{x}) \beta_i \\ &= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + \mathbf{B}_i(\mathbf{x}) \beta_i + \underbrace{\begin{pmatrix} (x_0 - p_{i,x_0})(x_0 - p_{i,x_0}) c_i(\mathbf{x}) & \dots & (x_n - p_{i,x_n})(x_0 - p_{i,x_0}) c_i(\mathbf{x}) \\ \vdots & \ddots & \vdots \\ (x_0 - p_{i,x_0})(x_n - p_{i,x_n}) c_i(\mathbf{x}) & \dots & (x_n - p_{i,x_n})(x_n - p_{i,x_n}) c_i(\mathbf{x}) \end{pmatrix}}_{\mathbf{C}_i(\mathbf{x})} \beta_i \\ &= \sum_i^N \alpha_i \mathbf{a}_i(\mathbf{x}) + (\mathbf{B}_i(\mathbf{x}) + \mathbf{C}_i(\mathbf{x})) \beta_i \end{aligned}$$

## 4 MATRIX REPRESENTATION

To be easier to read, developments will be done for  $n = 3$ . Generalizing to a  $\mathbb{R}^n$  space is done easily because so far we kept  $f$  and  $\nabla f$  as general as possible without setting  $n$ .

Finding the HRBF weights is done by developing the following system with a LU decomposition:

$$\begin{pmatrix} f(\mathbf{p}_i) \\ \nabla f(\mathbf{p}_i) \end{pmatrix} = \begin{pmatrix} c \\ \mathbf{n}_i \end{pmatrix}$$

If we develop according to the interpolated points:

$$\begin{pmatrix} f(\mathbf{p}_0) \\ \vdots \\ f(\mathbf{p}_N) \\ \nabla f(\mathbf{p}_0) \\ \vdots \\ \nabla f(\mathbf{p}_N) \end{pmatrix} = \begin{pmatrix} c \\ \vdots \\ c \\ \mathbf{n}_0 \\ \vdots \\ \mathbf{n}_N \end{pmatrix}$$

We have to expand the gradient to see the  $n + 3n$  equations explicitly:

$$\begin{pmatrix} f(\mathbf{p}_1) \\ \vdots \\ f(\mathbf{p}_N) \\ f_x(\mathbf{p}_1) \\ f_y(\mathbf{p}_1) \\ f_z(\mathbf{p}_1) \\ f_x(\mathbf{p}_2) \\ \vdots \\ f_z(\mathbf{p}_N) \end{pmatrix} = \begin{pmatrix} c \\ \vdots \\ c \\ \mathbf{n}_{1,x} \\ \mathbf{n}_{1,y} \\ \mathbf{n}_{1,z} \\ \mathbf{n}_{2,x} \\ \vdots \\ \mathbf{n}_{N,z} \end{pmatrix}$$

The equation system  $\mathbf{A.x} = \mathbf{b}$  entirely developed look like this:

$$\mathbf{A} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_N \\ \beta_{1,x} \\ \beta_{1,y} \\ \beta_{1,z} \\ \vdots \\ \beta_{N,z} \end{pmatrix} = \begin{pmatrix} c \\ \vdots \\ c \\ n_{1,x} \\ n_{1,y} \\ n_{1,z} \\ \vdots \\ n_{N,z} \end{pmatrix}$$

With the matrix  $\mathbf{A}$ :

$$\begin{pmatrix} \phi(l_1(\mathbf{x}_1)) & \dots & \phi(l_N(\mathbf{x}_1)) & e_{1,x}(\mathbf{x}_1) & e_{1,y}(\mathbf{x}_1) & e_{1,z}(\mathbf{x}_1) & \dots & e_{N,z}(\mathbf{x}_1) \\ \phi(l_1(\mathbf{x}_2)) & \dots & \phi(l_N(\mathbf{x}_2)) & e_{1,x}(\mathbf{x}_2) & e_{1,y}(\mathbf{x}_2) & e_{1,z}(\mathbf{x}_2) & \dots & e_{N,z}(\mathbf{x}_2) \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \phi(l_1(\mathbf{x}_N)) & \dots & \phi(l_N(\mathbf{x}_N)) & e_{1,x}(\mathbf{x}_N) & e_{1,y}(\mathbf{x}_N) & e_{1,z}(\mathbf{x}_N) & \dots & e_{N,z}(\mathbf{x}_N) \\ a_1(\mathbf{x}_1) & \dots & a_N(\mathbf{x}_1) & (b_1 + d_{1,x}d_{1,x}.c_1) & d_{1,y}d_{1,x}.c_1 & d_{1,z}d_{1,x}.c_1 & \dots & (b_N + d_{N,z}d_{1,x}.c_N) \\ a_1(\mathbf{x}_1) & \dots & a_N(\mathbf{x}_1) & d_{1,x}d_{1,y}.c_1 & (b_1 + d_{1,y}d_{1,y}.c_1) & d_{1,z}d_{1,y}.c_1 & \dots & (b_N + d_{N,z}d_{1,y}.c_N) \\ a_1(\mathbf{x}_1) & \dots & a_N(\mathbf{x}_1) & d_{1,x}d_{1,z}.c_1 & d_{1,y}d_{1,z}.c_1 & (b_1 + d_{1,z}d_{1,z}.c_1) & \dots & (b_N + d_{N,z}d_{1,z}.c_N) \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ a_1(\mathbf{x}_N) & \dots & a_N(\mathbf{x}_N) & d_{1,x}d_{1,z}.c_1 & d_{1,y}d_{1,z}.c_1 & (b_1 + d_{1,z}d_{1,z}.c_1) & \dots & (b_N + d_{N,z}d_{1,z}.c_N) \end{pmatrix}$$

To be more compact the parameter  $\mathbf{x}_i$  is implicit. Moreover we renamed some expressions:

$$b_i(\mathbf{x}) = b_i$$

$$c_i(\mathbf{x}) = c_i$$

$$\mathbf{d}_i(\mathbf{x}) = \begin{pmatrix} d_{i,x}(\mathbf{x}) \\ d_{i,y}(\mathbf{x}) \\ d_{i,z}(\mathbf{x}) \end{pmatrix} = \mathbf{x} - \mathbf{p}_i$$

$$\mathbf{e}_i(\mathbf{x}) = \begin{pmatrix} e_{i,x}(\mathbf{x}) \\ e_{i,y}(\mathbf{x}) \\ e_{i,z}(\mathbf{x}) \end{pmatrix} = \phi'(\|\mathbf{x} - \mathbf{p}_i\|) \frac{\mathbf{x} - \mathbf{p}_i}{\|\mathbf{x} - \mathbf{p}_i\|} = \phi'(l_i(\mathbf{x})) \cdot \frac{\mathbf{d}_i(\mathbf{x})}{l_i(\mathbf{x})}$$

In practice when filling the matrix, every coefficients of  $\mathbf{A}$  with null division must be set to zero to be ignored.