# Deformable 2D-3D Registration of Vascular Structures in a One View Scenario

## Supplementary Material

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October 31, 2008

## A Derivative of the Difference Measure

The Difference Measure driving the registration is defined as

$$D = \frac{1}{n}\sum_{i=1}^{n} \|\mathbf{x}_i - f(\mathbf{X}_i + \varphi_i)\|^2 \ . \tag{1}$$

Here, $\mathbf{X}_i$ and $\mathbf{x}_i$ are corresponding 3D and 2D points, and $f : \mathbb{R}^3 \to \mathbb{R}^2$ is a projection function defined by

$$f(\mathbf{X}) = (\mathbf{p}_1^\top \hat{\mathbf{X}} / \mathbf{p}_3^\top \hat{\mathbf{X}}, \mathbf{p}_2^\top \hat{\mathbf{X}} / \mathbf{p}_3^\top \hat{\mathbf{X}})^\top \ . \tag{2}$$

In the above equation, $\mathbf{p}_1^\top$, $\mathbf{p}_2^\top$ and $\mathbf{p}_3^\top$ constitute the row vectors of the projection matrix $\mathbf{P} \in \mathbb{R}^{3\times4}$, and $\hat{\mathbf{X}} = [\mathbf{X}^\top, 1]^\top$ is the homogeneous 4-vector of the 3D point $\mathbf{X}$.

The derivative of $D$ with respect to $\varphi_k$ is derived in the following way. Where convenient, we will use $\mathbf{Y}_i = \mathbf{X}_i + \varphi_i$.

$$\begin{aligned}
\frac{\partial D}{\partial \varphi_k} &= \frac{1}{n}\sum_{i=1}^{n} \|\mathbf{x}_i - f(\mathbf{X}_i + \varphi_i)\|^2 && (3)\\
&= \frac{1}{n}\sum_{i=1}^{n} \|\mathbf{x}_i - f(\mathbf{Y}_i)\|^2 && (4)\\
&= \frac{1}{n}\sum_{i=1}^{n} \langle \mathbf{x}_i - f(\mathbf{Y}_i), \mathbf{x}_i - f(\mathbf{Y}_i)\rangle && (5)\\
&= \frac{1}{n}\sum_{i=1}^{n} 2\cdot(\mathbf{x}_i - f(\mathbf{Y}_i))^\top \left(\frac{\partial(\mathbf{x}_i - f(\mathbf{Y}_i))}{\varphi_k}\right) && (6)\\
&= \frac{1}{n}\sum_{i=1}^{n} 2\cdot(\mathbf{x}_i - f(\mathbf{Y}_i))^\top \left(\frac{\partial(\mathbf{x}_i)}{\partial\varphi_k} - \frac{\partial(f(\mathbf{Y}_i))}{\partial\varphi_k}\right) && (7)\\
&= \frac{1}{n}\sum_{i=1}^{n} 2\cdot(\mathbf{x}_i - f(\mathbf{Y}_i))^\top \left(-\frac{\partial f(\mathbf{Y}_i)}{\partial\varphi_k}\right) && (8)\\
&= \frac{-2}{n}\sum_{i=1}^{n} (\mathbf{x}_i - f(\mathbf{Y}_i))^\top \left(\frac{\partial f(\mathbf{Y}_i)}{\partial\varphi_k}\right) && (9)
\end{aligned}$$

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The derivative $\frac{\partial f(\mathbf{Y}_i)}{\partial \varphi_k}$ from Equation (9) is computed as follows.

$$\begin{aligned}
\frac{\partial f(\mathbf{Y}_i)}{\partial \varphi_k} &= \frac{\partial f(\mathbf{X}_i + \varphi_i)}{\partial \varphi_k} && (10)\\
&= \frac{\partial f(\mathbf{X}_i + \varphi_i)}{\partial (\mathbf{X}_i + \varphi_i)} \frac{\partial (\mathbf{X}_i + \varphi_i)}{\partial \varphi_k} && (11)\\
&= \frac{\partial f(\mathbf{Y}_i)}{\partial \mathbf{Y}_i} \frac{\partial (\mathbf{X}_i + \varphi_i)}{\partial \varphi_k} && (12)\\
&= \frac{\partial f(\mathbf{Y}_i)}{\partial \mathbf{Y}_i} \left( \frac{\partial \mathbf{X}_i}{\partial \varphi_k} + \frac{\partial \varphi_i}{\partial \varphi_k} \right) && (13)\\
&= \frac{\partial f(\mathbf{Y}_i)}{\partial \mathbf{Y}_i} \frac{\partial \varphi_i}{\partial \varphi_k} && (14)\\
&= \frac{\partial f(\mathbf{Y}_i)}{\partial \mathbf{Y}_i} \delta_{i,k} && (15)
\end{aligned}$$

Here, the symbol $\delta_{i,k}$ is used for a matrix from $\mathbb{R}^{3\times 3}$, which is the identity for $i = k$ and zero otherwise.

By substituting the Equation (15) into (9) we get the following equation,

$$\frac{\partial D}{\partial \varphi_k} = \frac{-2}{n} (\mathbf{x}_k - f(\mathbf{Y}_k))^\top \left( \frac{\partial f(\mathbf{Y}_k)}{\partial \mathbf{Y}_k} \right) , \tag{16}$$

since all summands for $i \neq k$ evaluate to zero.

The only remaining unknown term is the derivative $\frac{\partial f(\mathbf{X})}{\partial \mathbf{X}}$, which can be derived as follows.

$$\frac{\partial f(\mathbf{X})}{\partial \mathbf{X}} = \begin{bmatrix} \frac{\partial f_1}{\partial \mathbf{X}} \\ \frac{\partial f_2}{\partial \mathbf{X}} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial \mathbf{X}_1} & \frac{\partial f_1}{\partial \mathbf{X}_2} & \frac{\partial f_1}{\partial \mathbf{X}_3} \\ \frac{\partial f_2}{\partial \mathbf{X}_1} & \frac{\partial f_2}{\partial \mathbf{X}_2} & \frac{\partial f_2}{\partial \mathbf{X}_3} \end{bmatrix} . \tag{17}$$

We use the definition of $f$ as

$$f = \begin{bmatrix} \frac{\mathbf{p}_1^\top \hat{\mathbf{X}}}{\mathbf{p}_3^\top \hat{\mathbf{X}}} \\ \frac{\mathbf{p}_2^\top \hat{\mathbf{X}}}{\mathbf{p}_3^\top \hat{\mathbf{X}}} \end{bmatrix} = \begin{bmatrix} \frac{\mathbf{p}_{11}\mathbf{X}_1 + \mathbf{p}_{12}\mathbf{X}_2 + \mathbf{p}_{13}\mathbf{X}_3 + \mathbf{p}_{14}}{\mathbf{p}_{31}\mathbf{X}_1 + \mathbf{p}_{32}\mathbf{X}_2 + \mathbf{p}_{33}\mathbf{X}_3 + \mathbf{p}_{34}} \\ \frac{\mathbf{p}_{21}\mathbf{X}_1 + \mathbf{p}_{22}\mathbf{X}_2 + \mathbf{p}_{23}\mathbf{X}_3 + \mathbf{p}_{24}}{\mathbf{p}_{31}\mathbf{X}_1 + \mathbf{p}_{32}\mathbf{X}_2 + \mathbf{p}_{33}\mathbf{X}_3 + \mathbf{p}_{34}} \end{bmatrix} . \tag{18}$$

We will employ in the following the notation from either the left or the right hand side, depending which is more convenient.

For the single elements of the derivative $\frac{\partial f(\mathbf{X})}{\partial \mathbf{X}}$ (Equation (17)), by the application of the quotient rule, we finally get

$$\begin{aligned}
\frac{\partial f_1(\mathbf{X})}{\partial \mathbf{X}_1} &= \frac{p_{11} \cdot \mathbf{p}_3^\top \hat{\mathbf{X}} - \mathbf{p}_1^\top \hat{\mathbf{X}} \cdot p_{31}}{(\mathbf{p}_3^\top \hat{\mathbf{X}})^2} && (19)\\
\frac{\partial f_1(\mathbf{X})}{\partial \mathbf{X}_2} &= \frac{p_{12} \cdot \mathbf{p}_3^\top \hat{\mathbf{X}} - \mathbf{p}_1^\top \hat{\mathbf{X}} \cdot p_{32}}{(\mathbf{p}_3^\top \hat{\mathbf{X}})^2} && (20)\\
\frac{\partial f_1(\mathbf{X})}{\partial \mathbf{X}_3} &= \frac{p_{13} \cdot \mathbf{p}_3^\top \hat{\mathbf{X}} - \mathbf{p}_1^\top \hat{\mathbf{X}} \cdot p_{33}}{(\mathbf{p}_3^\top \hat{\mathbf{X}})^2} && (21)\\
\frac{\partial f_2(\mathbf{X})}{\partial \mathbf{X}_1} &= \frac{p_{21} \cdot \mathbf{p}_3^\top \hat{\mathbf{X}} - \mathbf{p}_2^\top \hat{\mathbf{X}} \cdot p_{31}}{(\mathbf{p}_3^\top \hat{\mathbf{X}})^2} && (22)\\
\frac{\partial f_2(\mathbf{X})}{\partial \mathbf{X}_2} &= \frac{p_{22} \cdot \mathbf{p}_3^\top \hat{\mathbf{X}} - \mathbf{p}_2^\top \hat{\mathbf{X}} \cdot p_{32}}{(\mathbf{p}_3^\top \hat{\mathbf{X}})^2} && (23)\\
\frac{\partial f_2(\mathbf{X})}{\partial \mathbf{X}_3} &= \frac{p_{23} \cdot \mathbf{p}_3^\top \hat{\mathbf{X}} - \mathbf{p}_2^\top \hat{\mathbf{X}} \cdot p_{33}}{(\mathbf{p}_3^\top \hat{\mathbf{X}})^2} && (24)\\
& && (25)
\end{aligned}$$

In the summary, by using $\mathbf{Y}_i = \mathbf{X}_i + \varphi_i$, we can write the gradient of $D$ as

$$\frac{\partial D}{\partial \varphi_k} = -\frac{2}{n} (\mathbf{x}_k - f(\mathbf{Y}_k))^\top \mathbf{J}_k , \tag{26}$$

where $\mathbf{J}_k \in \mathbb{R}^{2\times 3}$ denotes $\frac{\partial f(\mathbf{Y}_k)}{\partial \mathbf{Y}_k}$, which is the Jacobian of $f$ with respect to $\varphi_k$, and is given by

$$\mathbf{J}_k = \frac{1}{(\mathbf{p}_3^\top \hat{\mathbf{Y}}_k)^2} \begin{bmatrix} p_{11}\mathbf{p}_3^\top \hat{\mathbf{Y}}_k - p_{31}\mathbf{p}_1^\top \hat{\mathbf{Y}}_k & p_{21}\mathbf{p}_3^\top \hat{\mathbf{Y}}_k - p_{31}\mathbf{p}_2^\top \hat{\mathbf{Y}}_k \\ p_{12}\mathbf{p}_3^\top \hat{\mathbf{Y}}_k - p_{32}\mathbf{p}_1^\top \hat{\mathbf{Y}}_k & p_{22}\mathbf{p}_3^\top \hat{\mathbf{Y}}_k - p_{32}\mathbf{p}_2^\top \hat{\mathbf{Y}}_k \\ p_{13}\mathbf{p}_3^\top \hat{\mathbf{Y}}_k - p_{33}\mathbf{p}_1^\top \hat{\mathbf{Y}}_k & p_{23}\mathbf{p}_3^\top \hat{\mathbf{Y}}_k - p_{33}\mathbf{p}_2^\top \hat{\mathbf{Y}}_k \end{bmatrix}^\top \tag{27}$$

where $p_{ij}$ denote the entries of the projection matrix $\mathbf{P}$.

# B Derivative of the Length Preservation Term

The length preserving cost function is defined as

$$S_L = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{d_i^-(\mathbf{0})-d_i^-(\varphi)}{d_i^-(\mathbf{0})}\right|^2+\left|\frac{d_i^+(\mathbf{0})-d_i^+(\varphi)}{d_i^+(\mathbf{0})}\right|^2 , \tag{28}$$

The terms $d_i^-(\varphi)$ and $d_i^+(\varphi)$ are defined by

$$d_i^-(\varphi) = \|\mathbf{Y}_i-\mathbf{Y}_{i-1}\|^2 \text{ , and} \tag{29}$$
$$d_i^+(\varphi) = \|\mathbf{Y}_i-\mathbf{Y}_{i+1}\|^2 . \tag{30}$$

We once again set $\mathbf{Y}_i = \mathbf{X}_i + \varphi_i$ where convenient.

The derivative of $S_L$ with respect to $\varphi_k$ can be derived in the following way.

$$\begin{aligned}
\frac{\partial S_L}{\partial \varphi_k} &= \frac{\partial}{\partial \varphi_k}\left(\frac{1}{n}\sum_{i=1}^{n}\left|\frac{d_i^-(\mathbf{0})-d_i^-(\varphi)}{d_i^-(\mathbf{0})}\right|^2+\left|\frac{d_i^+(\mathbf{0})-d_i^+(\varphi)}{d_i^+(\mathbf{0})}\right|^2\right) && (31)\\
&= \frac{1}{n}\sum_{i=1}^{n} 2\cdot\left(\frac{d_i^-(\mathbf{0})-d_i^-(\varphi)}{d_i^-(\mathbf{0})}\right)\cdot\frac{\partial}{\partial \varphi_k}\left(\frac{d_i^-(\mathbf{0})-d_i^-(\varphi)}{d_i^-(\mathbf{0})}\right) && (32)\\
&\quad +2\cdot\left(\frac{d_i^+(\mathbf{0})-d_i^+(\varphi)}{d_i^+(\mathbf{0})}\right)\cdot\frac{\partial}{\partial \varphi_k}\left(\frac{d_i^+(\mathbf{0})-d_i^+(\varphi)}{d_i^+(\mathbf{0})}\right) && (33)\\
&= \frac{2}{n}\sum_{i=1}^{n}\left(\frac{d_i^-(\mathbf{0})-d_i^-(\varphi)}{d_i^-(\mathbf{0})}\right)\cdot\frac{\partial}{\partial \varphi_k}\left(-d_i^-(\varphi)\right) && (34)\\
&\quad +\left(\frac{d_i^+(\mathbf{0})-d_i^+(\varphi)}{d_i^+(\mathbf{0})}\right)\cdot\frac{\partial}{\partial \varphi_k}\left(-d_i^+(\varphi)\right) && (35)\\
&= \frac{2}{n}\sum_{i=1}^{n}\left(\frac{d_i^-(\mathbf{0})-d_i^-(\varphi)}{d_i^-(\mathbf{0})}\right)\cdot\left(-\frac{\partial d_i^-(\varphi)}{\partial \varphi_k}\right) && (36)\\
&\quad +\left(\frac{d_i^+(\mathbf{0})-d_i^+(\varphi)}{d_i^+(\mathbf{0})}\right)\cdot\left(-\frac{\partial d_i^+(\varphi)}{\partial \varphi_k}\right) && (37)\\
&= \frac{-2}{n}\sum_{i=1}^{n}\left(\frac{d_i^-(\mathbf{0})-d_i^-(\varphi)}{d_i^-(\mathbf{0})}\right)\cdot\frac{\partial d_i^-(\varphi)}{d\varphi_k} && (38)\\
&\quad +\left(\frac{d_i^+(\mathbf{0})-d_i^+(\varphi)}{d_i^+(\mathbf{0})}\right)\cdot\frac{\partial d_i^+(\varphi)}{d\varphi_k} . && (39)
\end{aligned}$$

The terms $\frac{\partial d_i^-(\varphi)}{\partial \varphi_k}$ and $\frac{\partial d_i^+(\varphi)}{\partial \varphi_k}$ are only non-zero for $i = k$, $i = k-1$, and $i = k+1$, so that we get

$$\begin{aligned}
\frac{\partial S_L}{\partial \varphi_k} &= -\frac{2}{n}\left(\left(\frac{d_k^-(\mathbf{0})-d_k^-(\varphi)}{d_k^-(\mathbf{0})}\right)\cdot\frac{\partial d_k^-(\varphi)}{\partial \varphi_k}\right. && (40)\\
&\quad \left.+\left(\frac{d_k^+(\mathbf{0})-d_k^+(\varphi)}{d_k^+(\mathbf{0})}\right)\cdot\frac{\partial d_k^+(\varphi)}{\partial \varphi_k}\right) && (41)\\
&\quad -\frac{2}{n}\left(\left(\frac{d_{k-1}^-(\mathbf{0})-d_{k-1}^-(\varphi)}{d_{k-1}^-(\mathbf{0})}\right)\cdot\frac{\partial d_{k-1}^-(\varphi)}{\partial \varphi_k}\right. && (42)\\
&\quad \left.+\left(\frac{d_{k-1}^+(\mathbf{0})-d_{k-1}^+(\varphi)}{d_{k-1}^+(\mathbf{0})}\right)\cdot\frac{\partial d_{k-1}^+(\varphi)}{\partial \varphi_k}\right) && (43)\\
&\quad -\frac{2}{n}\left(\left(\frac{d_{k+1}^-(\mathbf{0})-d_{k+1}^-(\varphi)}{d_{k+1}^-(\mathbf{0})}\right)\cdot\frac{\partial d_{k+1}^-(\varphi)}{\partial \varphi_k}\right. && (44)\\
&\quad \left.+\left(\frac{d_{k+1}^+(\mathbf{0})-d_{k+1}^+(\varphi)}{d_{k+1}^+(\mathbf{0})}\right)\cdot\frac{\partial d_{k+1}^+(\varphi)}{\partial \varphi_k}\right) . && (45)
\end{aligned}$$

By defining

$$w_i^- = \frac{d_i^-(\mathbf{0}) - d_i^-(\varphi)}{d_i^-(\mathbf{0})} \quad \text{and} \quad w_i^+ = \frac{d_i^+(\mathbf{0}) - d_i^+(\varphi)}{d_i^+(\mathbf{0})} \;, \tag{46}$$

we can further simplify the expression. We take advantage of $\frac{\partial d_{k-1}^-(\varphi)}{\partial \varphi_k} = 0$ and $\frac{\partial d_{k+1}^+(\varphi)}{\partial \varphi_k} = 0$. We also use the facts that $d_{k-1}^+ = d_k^-$ and $d_{k+1}^- = d_k^+$, and thus $w_{i+1}^- = w_i^+$ and $w_{i-1}^+ = w_i^-$, and get

$$\begin{aligned}
\frac{\partial S_L}{\partial \varphi_k} &= -\frac{2}{n}\left(w_k^- \cdot \frac{\partial d_k^-(\varphi)}{\partial \varphi_k} + w_k^+ \cdot \frac{\partial d_k^+(\varphi)}{\partial \varphi_k}\right) && (47)\\
&\quad -\frac{2}{n}\left(w_{k-1}^- \cdot \frac{\partial d_{k-1}^-(\varphi)}{\partial \varphi_k} + w_{k-1}^+ \cdot \frac{\partial d_{k-1}^+(\varphi)}{\partial \varphi_k}\right) && (48)\\
&\quad -\frac{2}{n}\left(w_{k+1}^- \cdot \frac{\partial d_{k+1}^-(\varphi)}{\partial \varphi_k} + w_{k+1}^+ \cdot \frac{\partial d_{k+1}^+(\varphi)}{\partial \varphi_k}\right) && (49)\\
&= -\frac{2}{n}\left(w_k^- \cdot \frac{\partial d_k^-(\varphi)}{\partial \varphi_k} + w_k^+ \cdot \frac{\partial d_k^+(\varphi)}{\partial \varphi_k}\right) && (50)\\
&\quad -\frac{2}{n}\left(+w_{k-1}^+ \cdot \frac{\partial d_{k-1}^+(\varphi)}{\partial \varphi_k} + w_{k+1}^- \cdot \frac{\partial d_{k+1}^-(\varphi)}{\partial \varphi_k}\right) && (51)\\
&= -\frac{2}{n}\left(w_k^- \cdot \frac{\partial d_k^-(\varphi)}{\partial \varphi_k} + w_k^+ \cdot \frac{\partial d_k^+(\varphi)}{\partial \varphi_k}\right) && (52)\\
&\quad -\frac{2}{n}\left(w_k^- \cdot \frac{\partial d_k^-(\varphi)}{\partial \varphi_k} + w_k^+ \cdot \frac{\partial d_k^+(\varphi)}{\partial \varphi_k}\right) && (53)\\
&= -\frac{4}{n}\left(w_k^- \cdot \frac{\partial d_k^-(\varphi)}{\partial \varphi_k} + w_k^+ \cdot \frac{\partial d_k^+(\varphi)}{\partial \varphi_k}\right) \;. && (54)
\end{aligned}$$

In order to compute the derivatives of the single terms in Equation (54) , we give the detailed version of the terms, that is

$$\begin{aligned}
d_i^-(\varphi) &= \|(\mathbf{X}_i + \varphi_i) - (\mathbf{X}_{i-1} + \varphi_{i-1})\|^2 && (55)\\
&= ((\mathbf{X}_i + \varphi_i) - (\mathbf{X}_{i-1} + \varphi_{i-1}))^\top && (56)\\
&\quad ((\mathbf{X}_i + \varphi_i) - (\mathbf{X}_{i-1} + \varphi_{i-1})) && (57)\\
&= (\mathbf{X}_i + \varphi_i)^\top (\mathbf{X}_i + \varphi_i) && (58)\\
&\quad -2(\mathbf{X}_i + \varphi_i)^\top (\mathbf{X}_{i-1} + \varphi_{i-1}) && (59)\\
&\quad +(\mathbf{X}_{i-1} + \varphi_{i-1})^\top (\mathbf{X}_{i-1} + \varphi_{i-1}) && (60)\\
&= \mathbf{X}_i^\top \mathbf{X}_i + 2\mathbf{X}_i^\top \varphi_i + {\varphi_i}^\top \varphi_i && (61)\\
&\quad -2(\mathbf{X}_i^\top \mathbf{X}_{i-1} + \varphi_i^\top \mathbf{X}_{i-1} + \mathbf{X}_i^\top \varphi_{i-1} + \varphi_i^\top \varphi_{i-1}) && (62)\\
&\quad +\mathbf{X}_{i-1}^\top \mathbf{X}_{i-1} + 2\mathbf{X}_{i-1}^\top \varphi_{i-1} + \varphi_{i-1}^\top \varphi_{i-1} && (63)\\
&= \mathbf{X}_i^\top \mathbf{X}_i + 2\mathbf{X}_i^\top \varphi_i + \varphi_i^\top \varphi_i && (64)\\
&\quad -2\mathbf{X}_i^\top \mathbf{X}_{i-1} - 2\varphi_i^\top \mathbf{X}_{i-1} - 2\mathbf{X}_i^\top \varphi_{i-1} - 2\varphi_i^\top \varphi_{i-1} && (65)\\
&\quad +\mathbf{X}_{i-1}^\top \mathbf{X}_{i-1} + 2\mathbf{X}_{i-1}^\top \varphi_{i-1} + \varphi_{i-1}^\top \varphi_{i-1} \;, && (66)
\end{aligned}$$

and in a completely analogue manner we get

$$\begin{aligned}
d_i^+(\varphi) &= \mathbf{X}_i^\top \mathbf{X}_i + 2\mathbf{X}_i^\top \varphi_i + \varphi_i^\top \varphi_i && (67)\\
&\quad -2\mathbf{X}_i^\top \mathbf{X}_{i+1} - 2\varphi_i^\top \mathbf{X}_{i+1} - 2\mathbf{X}_i^\top \varphi_{i+1} - 2\varphi_i^\top \varphi_{i+1} && (68)\\
&\quad +\mathbf{X}_{i+1}^\top \mathbf{X}_{i+1} + 2\mathbf{X}_{i+1}^\top \varphi_{i+1} + \varphi_{i+1}^\top \varphi_{i+1} && (69)
\end{aligned}$$

For the single terms from Equation (54), we now get

$$\begin{aligned}
\frac{\partial}{\partial \varphi_k}\left(d_k^-(\varphi)\right) &= 2\mathbf{X}_k^\top + 2\varphi_k^\top - 2\mathbf{X}_{k-1}^\top - 2\varphi_{k-1}^\top && (70)\\
&= 2(\mathbf{Y}_k - \mathbf{Y}_{k-1})^\top \;. && (71)
\end{aligned}$$

$$\frac{\partial}{\partial \varphi_k}\left(d_k^+(\varphi)\right) = 2\mathbf{X}_k^\top + 2\varphi_k^\top - 2\mathbf{X}_{k+1}^\top - 2\varphi_{k+1}^\top \tag{72}$$

$$= 2(\mathbf{Y}_k - \mathbf{Y}_{k+1})^\top \ . \tag{73}$$

Finally, we get

$$\frac{\partial S_L}{\partial \varphi_k} = \frac{-8}{n}\left(w_k^-(\mathbf{Y}_k - \mathbf{Y}_{k-1}) + w_k^+(\mathbf{Y}_k - \mathbf{Y}_{k+1})\right)^\top \ . \tag{74}$$

# C Analytical Derivative of the TPS-parameterized Diffusion Energy

We employ the Thin-Plate Spline model $\varphi_{\mathrm{TPS}}$ to represent a continuous version of the displacement function, which is explicitly represented at the graph nodes by the vectors $\varphi_i$

$$\varphi_{\mathrm{TPS}}(\mathbf{X}) = \begin{bmatrix} \left(a_0^{(x_1)} + {A^{(x_1)}}^\top \mathbf{X} + \sum_{k=1}^n \omega_k^{(x_1)} \|\mathbf{X}_k - \mathbf{X}\|\right) - \mathbf{X}^{(x_1)} \\ \left(a_0^{(x_2)} + {A^{(x_2)}}^\top \mathbf{X} + \sum_{k=1}^n \omega_k^{(x_2)} \|\mathbf{X}_k - \mathbf{X}\|\right) - \mathbf{X}^{(x_2)} \\ \left(a_0^{(x_3)} + {A^{(x_3)}}^\top \mathbf{X} + \sum_{k=1}^n \omega_k^{(x_3)} \|\mathbf{X}_k - \mathbf{X}\|\right) - \mathbf{X}^{(x_3)} \end{bmatrix}, \tag{75}$$

with $A^{(x_k)} = \left[a_1^{(x_k)}, a_2^{(x_k)}, a_3^{(x_k)}\right]^\top$, where the scalar values $a_i$ and the vectors $\omega_k$ constitute the parameters of the TPS, which are computed to match the $n$ given displacement values at the nodes of the graph, located at points $\mathbf{X}_k$.

Next, we give an analytical expression for the derivative of the TPS. This is used for the computation of the Diffusion Energy energy term, as well as for computing the derivative of this energy. Let $\nabla\varphi_{\mathrm{TPS}}^{(x_j)}$ be the gradient of the $x_j$ dimension of $\varphi_{\mathrm{TPS}}$

$$\nabla\varphi_{\mathrm{TPS}}^{(x_j)}(\mathbf{X}) = \begin{bmatrix} a_1^{(x_j)} - \left(\sum_{k=1}^n \omega_k^{(x_j)} \frac{\mathbf{X}_k^{(x_1)} - \mathbf{X}^{(x_1)}}{\|\mathbf{X}_k - \mathbf{X}\|_\epsilon}\right) - \delta_{x_1 j} \\ a_2^{(x_j)} - \left(\sum_{k=1}^n \omega_k^{(x_j)} \frac{\mathbf{X}_k^{(x_2)} - \mathbf{X}^{(x_2)}}{\|\mathbf{X}_k - \mathbf{X}\|_\epsilon}\right) - \delta_{x_2 j} \\ a_3^{(x_j)} - \left(\sum_{k=1}^n \omega_k^{(x_j)} \frac{\mathbf{X}_k^{(x_3)} - \mathbf{X}^{(x_3)}}{\|\mathbf{X}_k - \mathbf{X}\|_\epsilon}\right) - \delta_{x_3 j} \end{bmatrix}. \tag{76}$$

Here, in order to be able to perform the differentiation, an approximation to the second norm is employed $\|\mathbf{X}\|_\epsilon = \sqrt{\mathbf{X}^\top\mathbf{X} + \epsilon}$ with a small positive scalar $\epsilon$. The Kronecker Delta $\delta_{ij}$ equals 1 for $i = j$ and is 0 otherwise.

The analytical form of the Laplace operator for the TPS-parameterized function finally reads

$$\begin{aligned}
\Delta\varphi_{\mathrm{TPS}}^{(x_j)}(\mathbf{X}) &= \sum_{i=1}^{3} \frac{d}{dx_i} \left(\nabla\varphi_{\mathrm{TPS}}^{(x_j)}\right)^{(x_i)} (\mathbf{X}) &(77)\\
&= \sum_{i=1}^{3} \frac{d}{dx_i} \left(a_1^{(x_j)} - \left(\sum_{k=1}^{n} \omega_k^{(x_j)} \frac{\mathbf{X}_k^{(x_i)} - \mathbf{X}^{(x_i)}}{\|\mathbf{X}_k - \mathbf{X}\|_\epsilon}\right) - \delta_{x_i j}\right) &(78)\\
&= -\sum_{i=1}^{3} \frac{d}{dx_i} \left(\sum_{k=1}^{n} \omega_k^{(x_j)} \frac{\mathbf{X}_k^{(x_i)} - \mathbf{X}^{(x_i)}}{\|\mathbf{X}_k - \mathbf{X}\|_\epsilon}\right) &(79)\\
&= -\sum_{i=1}^{3} \sum_{k=1}^{n} \omega_k^{(x_j)} \left(\frac{-1}{\|\mathbf{X}_k - \mathbf{X}\|_\epsilon} + \frac{\left(\mathbf{X}_k^{(x_i)} - \mathbf{X}^{(x_i)}\right)^2}{\sqrt{(\mathbf{X}_k - \mathbf{X})^\top(\mathbf{X}_k - \mathbf{X}) + \epsilon}^{3}}\right). &(80)
\end{aligned}$$