Variational Feature Extraction in Scientific Visualization – Derivations

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1 PRELIMINARIES

In this paper, we describe feature curves and surfaces as parametric functions $\mathbf{f}(\mathbf{x}) : \mathbb{X} \to \mathbb{R}^m$ that minimize a functional $\mathcal{F}[\mathbf{f}(\mathbf{x})]$:

$$\mathcal{F}[\mathbf{f}(\mathbf{x})] = \int_{\mathbb{X}} \mathcal{L}\left(\mathbf{f}(\mathbf{x}'), \nabla\mathbf{f}(\mathbf{x}')\right) \mathrm{d}\mathbf{x}'. \tag{1}$$

The unknown functions $\mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}), \dots, f_m(\mathbf{x}))^{\mathrm{T}}$ have m components (i.e., the features are located in an m-dimensional space) and they are defined over the n-dimensional parameter domain $\mathbb{X} \subseteq \mathbb{R}^n$, with $\mathbf{x} = (x_1, \dots, x_n)^{\mathrm{T}} \in \mathbb{X}$. The function $\mathcal{L}$ that is integrated over the parameter domain is called the *Lagrangian*, and it measures what is to be minimized over the parameter domain. The first-order partial derivatives of the unknown function are placed column-wise in the Jacobian matrix $\nabla\mathbf{f}(\mathbf{x}) \in \mathbb{R}^{m\times n}$:

$$\nabla\mathbf{f}(\mathbf{x}) = \begin{pmatrix} \frac{\partial f_1(\mathbf{x})}{\partial x_1} & \dots & \frac{\partial f_1(\mathbf{x})}{\partial x_n} \\ \vdots & & \vdots \\ \frac{\partial f_m(\mathbf{x})}{\partial x_1} & \dots & \frac{\partial f_m(\mathbf{x})}{\partial x_n} \end{pmatrix} = \begin{pmatrix} f_{1,1}(\mathbf{x}) & \dots & f_{1,n}(\mathbf{x}) \\ \vdots & & \vdots \\ f_{m,1}(\mathbf{x}) & \dots & f_{m,n}(\mathbf{x}) \end{pmatrix} \tag{2}$$

where $f_{i,j}(\mathbf{x}) := \frac{\partial f_i(\mathbf{x})}{\partial x_j}$ is a shorthand notation. The following derivations utilize two fundamental identities.

Dirac Identity. Differentiating a function $f(\mathbf{x}')$ at $\mathbf{x}'$ with respect to the same function $f(\mathbf{x})$ at $\mathbf{x}$ gives zero everywhere, except for when $\mathbf{x}' = \mathbf{x}$, i.e., it gives a Dirac delta:

$$\frac{\delta f(\mathbf{x}')}{\delta f(\mathbf{x})} = \delta(\mathbf{x}', \mathbf{x}) \qquad \text{with} \qquad \delta(\mathbf{x}', \mathbf{x}) = \begin{cases} \infty & \mathbf{x}' = \mathbf{x} \\ 0 & \mathbf{x}' \neq \mathbf{x} \end{cases} \tag{3}$$

Intuitively, one may think of the case where $f(\mathbf{x}')$ is a height surface, parameterized by $\mathbf{x}'$. Varying the height $f(\mathbf{x})$ will only change the surface at $\mathbf{x}' = \mathbf{x}$. Elsewhere, no change occurs.

Sifting Property. The other important property is the *sifting* property of the Dirac delta function:

$$\int_{\mathbb{X}} f(\mathbf{x}')\, \delta(\mathbf{x}', \mathbf{x})\, \mathrm{d}\mathbf{x}' = f(\mathbf{x}). \tag{4}$$

Since the Dirac delta $\delta(\mathbf{x}', \mathbf{x})$ is zero for all locations except at $\mathbf{x}' = \mathbf{x}$, the integral vanishes to one location. At this location, the product of the infinite $\delta(\mathbf{x}', \mathbf{x})$ and the infinitesimal $\mathrm{d}\mathbf{x}'$ gives 1.

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2 GENERAL RECIPE

In the following, we describe the general cookbook recipe for the differentiation of functionals, which leads to the well-known Euler-Lagrange equations [Gelfand and Fomin 1963]. Taking the functional derivative of Eq. (1) with respect to the vector-valued function $\mathbf{f}(\mathbf{x})$ is done component-wise with the partials placed in columns:

$$\frac{\delta\mathcal{F}[\mathbf{f}(\mathbf{x})]}{\delta\mathbf{f}(\mathbf{x})} = \left(\frac{\delta\mathcal{F}[\mathbf{f}(\mathbf{x})]}{\delta f_1(\mathbf{x})}, \dots, \frac{\delta\mathcal{F}[\mathbf{f}(\mathbf{x})]}{\delta f_m(\mathbf{x})}\right). \tag{5}$$

For each component f_i, the differentiation proceeds as follows:

$$\frac{\delta\mathcal{F}[\mathbf{f}(\mathbf{x})]}{\delta f_i(\mathbf{x})} = \frac{\delta}{\delta f_i(\mathbf{x})} \int_{\mathbb{X}} \mathcal{L}(\mathbf{f}(\mathbf{x}'), \nabla\mathbf{f}(\mathbf{x}'))\, \mathrm{d}\mathbf{x}' \tag{6}$$

$$= \int_{\mathbb{X}} \frac{\partial\mathcal{L}}{\partial f_i(\mathbf{x}')} \frac{\delta f_i(\mathbf{x}')}{\delta f_i(\mathbf{x})} + \sum_{j=1}^{n} \frac{\partial\mathcal{L}}{\partial f_{i,j}(\mathbf{x}')} \frac{\delta f_{i,j}(\mathbf{x}')}{\delta f_i(\mathbf{x})}\, \mathrm{d}\mathbf{x}' \tag{7}$$

$$= \int_{\mathbb{X}} \frac{\partial\mathcal{L}}{\partial f_i(\mathbf{x}')} \frac{\delta f_i(\mathbf{x}')}{\delta f_i(\mathbf{x})} + \sum_{j=1}^{n} \frac{\partial\mathcal{L}}{\partial f_{i,j}(\mathbf{x}')} \frac{\partial}{\partial x'_j} \frac{\delta f_i(\mathbf{x}')}{\delta f_i(\mathbf{x})}\, \mathrm{d}\mathbf{x}' \tag{8}$$

$$= \int_{\mathbb{X}} \frac{\partial\mathcal{L}}{\partial f_i(\mathbf{x}')} \frac{\delta f_i(\mathbf{x}')}{\delta f_i(\mathbf{x})} - \sum_{j=1}^{n} \frac{\partial}{\partial x'_j} \frac{\partial\mathcal{L}}{\partial f_{i,j}(\mathbf{x}')} \frac{\delta f_i(\mathbf{x}')}{\delta f_i(\mathbf{x})}\, \mathrm{d}\mathbf{x}' \tag{9}$$

$$= \int_{\mathbb{X}} \left(\frac{\partial\mathcal{L}}{\partial f_i(\mathbf{x}')} - \sum_{j=1}^{n} \frac{\partial}{\partial x'_j} \frac{\partial\mathcal{L}}{\partial f_{i,j}(\mathbf{x}')}\right) \frac{\delta f_i(\mathbf{x}')}{\delta f_i(\mathbf{x})}\, \mathrm{d}\mathbf{x}' \tag{10}$$

$$= \int_{\mathbb{X}} \left(\frac{\partial\mathcal{L}}{\partial f_i(\mathbf{x}')} - \sum_{j=1}^{n} \frac{\partial}{\partial x'_j} \frac{\partial\mathcal{L}}{\partial f_{i,j}(\mathbf{x}')}\right) \delta(\mathbf{x}', \mathbf{x})\, \mathrm{d}\mathbf{x}' \tag{11}$$

$$= \frac{\partial\mathcal{L}}{\partial f_i(\mathbf{x})} - \sum_{j=1}^{n} \frac{\partial}{\partial x_j} \frac{\partial\mathcal{L}}{\partial f_{i,j}(\mathbf{x})} \tag{12}$$

Assuming differentiability, the step from Eq. (6) to Eq. (7) moves the derivative into the integral and applies the chain rule to the differentiation of $\mathcal{L}$. From all the terms in $\mathbf{f}(\mathbf{x}')$ and $\nabla\mathbf{f}(\mathbf{x}')$ only the i'th component of $\mathbf{f}(\mathbf{x}')$ and the i'th row of $\nabla\mathbf{f}(\mathbf{x}')$ depend on f_i, which means $\mathcal{L}$ has $n+1$ arguments that depend on f_i. The application of the chain rule therefore requires the partial differentiation and the summation over these $n+1$ terms.

The step from Eq. (7) to Eq. (8) is a change in notation in the second term, where the partial derivative operator $\frac{\partial}{\partial x'_j}$ is taken out via $f_{i,j}(\mathbf{x}') = \frac{\partial}{\partial x'_j} f_i(\mathbf{x}')$, cf. the notation below Eq. (2).

The goal is to factor out $\frac{\delta f_i(\mathbf{x}')}{\delta f_i(\mathbf{x})}$, which, however, is not yet possible, since the summands in the second term in Eq. (8) would end on a dangling partial derivative operator $\frac{\partial}{\partial x'_j}$. To move the partial derivative $\frac{\partial}{\partial x'_j}$ to the front, integration by parts $\int u(x)\, v'(x)\, \mathrm{d}x =$

$[u(x)\, v(x)]_{x_0}^{x_1} - \int u'(x)\, v(x)\, \mathrm{d}x$ is utilized for each dimension:

$$\int_{\mathbb{X}} \underbrace{\frac{\partial \mathcal{L}}{\partial f_{i,j}(\mathbf{x}')}}_{u} \underbrace{\frac{\partial}{\partial x'_j} \frac{\delta f_i(\mathbf{x}')}{\delta f_i(\mathbf{x})}}_{v'} \mathrm{d}\mathbf{x}' = \Bigg[\underbrace{\frac{\partial \mathcal{L}}{\partial f_{i,j}(\mathbf{x}')}}_{u} \underbrace{\frac{\delta f_i(\mathbf{x}')}{\delta f_i(\mathbf{x})}}_{v} \Bigg]_{\mathbf{x}_0}^{\mathbf{x}_1} \tag{13}$$

$$- \int_{\mathbb{X}} \underbrace{\frac{\partial}{\partial x'_j} \frac{\partial \mathcal{L}}{\partial f_{i,j}(\mathbf{x}')}}_{u'} \underbrace{\frac{\delta f_i(\mathbf{x}')}{\delta f_i(\mathbf{x})}}_{v} \mathrm{d}\mathbf{x}' \tag{14}$$

The right-hand side of Eq. (13) is zero, since function variations are by definition not performed on the domain boundaries, i.e., $\frac{\delta f_i(\mathbf{x}_0)}{\delta f_i(\mathbf{x})} = \frac{\delta f_i(\mathbf{x}_1)}{\delta f_i(\mathbf{x})} = 0$. Substituting Eq. (14) into Eq. (8) gives Eq. (9).

The step from Eq. (9) to Eq. (10) factors out the derivative $\frac{\delta f_i(\mathbf{x}')}{\delta f_i(\mathbf{x})}$. Applying the Dirac identity from Eq. (3) leads to Eq. (11) .

By the sifting property from Eq. (4) the integral vanishes, which leads to Eq. (12).

Euler-Lagrange equation. The Euler-Lagrange equations state that the functional derivatives $\frac{\delta \mathcal{F}[\mathbf{f}(\mathbf{x})]}{\delta \mathbf{f}(\mathbf{x})}$ must vanish, i.e., for all f_i:

$$\frac{\delta \mathcal{F}[\mathbf{f}(\mathbf{x})]}{\delta f_i(\mathbf{x})} = \frac{\partial \mathcal{L}}{\partial f_i(\mathbf{x})} - \sum_{j=1}^{n} \frac{\partial}{\partial x_j} \frac{\partial \mathcal{L}}{\partial f_{i,j}(\mathbf{x})} = 0 \tag{15}$$

Then, with Eq. (5) a gradient descent can be applied:

$$\frac{\partial \mathbf{f}(\mathbf{x})}{\partial t} = - \frac{\delta \mathcal{F}[\mathbf{f}(\mathbf{x})]}{\delta \mathbf{f}(\mathbf{x})}^{\mathrm{T}} \tag{16}$$

Note that the functional derivative $\frac{\delta \mathcal{F}[\mathbf{f}(\mathbf{x})]}{\delta \mathbf{f}(\mathbf{x})}$ contained the partials in its columns, cf. Eq. (5). Thus, the functional derivative is transposed to align the dimensions with the components of $\mathbf{f}(\mathbf{x})$.

3 DERIVATIONS OF FUNDAMENTAL FEATURES

In the following, we derive the functional derivatives for all fundamental features and regularizers used in the paper. The general procedure is probably clear to the reader after the first one or two features. However, we want to formally derive every single term, since we want to be as clear as possible on the shape of the various vector-valued operators. In addition, we think that further examples give more pointers to interested readers on how their own feature definitions could be derived.

3.1 Isocontours

For an m-dimensional scalar field $s(\mathbf{y}) : \mathbb{Y} \to \mathbb{R}$, the n-dimensional isocontour $\mathbf{f}(\mathbf{x}) = \big(f_1(x_1, \ldots, x_n), \ldots, f_m(x_1, \ldots, x_n)\big)^{\mathrm{T}}$ with $n = m-1$ minimizes for isovalue c_0 the following squared norm:

$$\mathcal{F}^i = \int_{\mathbb{X}} \underbrace{\frac{1}{2} \| s(\mathbf{f}(\mathbf{x})) - c_0 \|^2}_{\mathcal{M}^i} \mathrm{d}\mathbf{x} \tag{17}$$

Differentiation results in the following functional derivatives:

$$\frac{\delta \mathcal{F}^i}{\delta f_i(\mathbf{x})} = \frac{\delta}{\delta f_i(\mathbf{x})} \int_{\mathbb{X}} \frac{1}{2} \| s(\mathbf{f}(\mathbf{x}')) - c_0 \|^2 \mathrm{d}\mathbf{x}' \tag{18}$$

$$= \int_{\mathbb{X}} (s(\mathbf{f}(\mathbf{x}')) - c_0) \cdot \frac{\partial s(\mathbf{f}(\mathbf{x}'))}{\partial f_i(\mathbf{x}')} \cdot \frac{\delta f_i(\mathbf{x}')}{\delta f_i(\mathbf{x})} \mathrm{d}\mathbf{x}' \tag{19}$$

$$= \int_{\mathbb{X}} (s(\mathbf{f}(\mathbf{x}')) - c_0) \cdot \frac{\partial s(\mathbf{f}(\mathbf{x}'))}{\partial f_i(\mathbf{x}')} \cdot \delta(\mathbf{x}', \mathbf{x})\, \mathrm{d}\mathbf{x}' \tag{20}$$

$$= (s(\mathbf{f}(\mathbf{x})) - c_0) \cdot \frac{\partial s(\mathbf{f}(\mathbf{x}))}{\partial f_i(\mathbf{x})} \tag{21}$$

Similar to the general recipe in Section 2, the integrand in Eq. (18) was differentiated with the chain rule, the Dirac identity of Eq. (3) is applied to Eq. (19), and the sifting property of Eq. (4) is used in Eq. (20) to arrive at Eq. (21). By reshaping the individual functional derivatives for $f_i(\mathbf{x})$ into a vector of $\mathbf{f}(\mathbf{x})$ by Eq. (5), we get:

$$\frac{\delta \mathcal{F}^i}{\delta \mathbf{f}(\mathbf{x})} = (s(\mathbf{f}(\mathbf{x})) - c_0) \cdot \frac{\partial s(\mathbf{f}(\mathbf{x}))}{\partial \mathbf{f}(\mathbf{x})} \tag{22}$$

where the first derivative of $s(\mathbf{y})$ is evaluated at the feature $\mathbf{f}(\mathbf{x})$:

$$\frac{\partial s(\mathbf{f}(\mathbf{x}))}{\partial \mathbf{f}(\mathbf{x})} = \left(\frac{\partial s(\mathbf{y})}{\partial y_1}, \ldots, \frac{\partial s(\mathbf{y})}{\partial y_m} \right)_{|\mathbf{y}=\mathbf{f}(\mathbf{x})} = \nabla s(\mathbf{f}(\mathbf{x}))^{\mathrm{T}} \tag{23}$$

Note that Eq. (22) gives a row vector, cf. Eq. (5). This will be the case for all vectorial representations of functional derivatives in the remainder of this document.

3.2 Critical Lines

Critical lines describe the path of a critical point through space-time. Given a 2-dimensional, time-dependent vector field $\mathbf{v}(\mathbf{y}, t) : \mathbb{Y} \times \mathbb{R} \to \mathbb{R}^2$ with $\mathbf{v}(\mathbf{y}, t) = (u(y_1, y_2, t), v(y_1, y_2, t))^{\mathrm{T}}$ a 1-dimensional critical line in space-time $\mathbf{f}(x) = \big(f_1(x), \ldots, f_3(x)\big)^{\mathrm{T}}$ (where $f_3(x)$ is the time coordinate) is the minimizer of the functional:

$$\mathcal{F}^c = \int_{\mathbb{X}} \underbrace{\frac{1}{2} \| \mathbf{v}(\mathbf{f}(x)) \|^2}_{\mathcal{M}^c} \mathrm{d}x \tag{24}$$

which has the following functional derivatives:

$$\frac{\delta \mathcal{F}^c}{\delta f_i(x)} = \frac{\delta}{\delta f_i(x)} \int_{\mathbb{X}} \frac{1}{2} \| \mathbf{v}(\mathbf{f}(x')) \|^2 \mathrm{d}x' \tag{25}$$

$$= \int_{\mathbb{X}} \mathbf{v}(\mathbf{f}(x'))^{\mathrm{T}} \cdot \frac{\partial \mathbf{v}(\mathbf{f}(x'))}{\partial f_i(x')} \cdot \frac{\delta f_i(x')}{\delta f_i(x)} \mathrm{d}x' \tag{26}$$

$$= \int_{\mathbb{X}} \mathbf{v}(\mathbf{f}(x'))^{\mathrm{T}} \cdot \frac{\partial \mathbf{v}(\mathbf{f}(x'))}{\partial f_i(x')} \cdot \delta(x', x)\, \mathrm{d}x' \tag{27}$$

$$= \mathbf{v}(\mathbf{f}(x))^{\mathrm{T}} \cdot \frac{\partial \mathbf{v}(\mathbf{f}(x))}{\partial f_i(x)} \tag{28}$$

When reshaping the functional derivative into a vector, we get:

$$\frac{\delta \mathcal{F}^c}{\delta \mathbf{f}(x)} = \mathbf{v}(\mathbf{f}(x))^{\mathrm{T}} \cdot \frac{\partial \mathbf{v}(\mathbf{f}(x))}{\partial \mathbf{f}(x)} \tag{29}$$

where the Jacobian of the vector field is evaluated at the feature:

$$\frac{\partial \mathbf{v}(\mathbf{f}(x))}{\partial \mathbf{f}(x)} = \begin{pmatrix} \frac{\partial u(\mathbf{y},t)}{\partial y_1} & \frac{\partial u(\mathbf{y},t)}{\partial y_2} & \frac{\partial u(\mathbf{y},t)}{\partial t} \\ \frac{\partial v(\mathbf{y},t)}{\partial y_1} & \frac{\partial v(\mathbf{y},t)}{\partial y_2} & \frac{\partial v(\mathbf{y},t)}{\partial t} \end{pmatrix}_{|(\mathbf{y},t)=\mathbf{f}(x)} \tag{30}$$

3.3 Parallel Vector Lines

The parallel vectors operator [Peikert and Roth 1999] is a very important tool, since many of the commonly used feature definitions can be formulated with it. Given are two 3-dimensional vector fields $\mathbf{v}_1(\mathbf{y}), \mathbf{v}_2(\mathbf{y}) : \mathbb{Y} \to \mathbb{R}^3$. The parallel vectors operator locates curves $\mathbf{f}(x)$ along which the two vector fields are parallel, which minimize the following functional:

$$\mathcal{F}^{pv} = \int_{\mathbb{X}} \underbrace{\frac{1}{2} \left\| \mathbf{v}_1(\mathbf{f}(x)) \times \mathbf{v}_2(\mathbf{f}(x)) \right\|^2}_{\mathcal{M}^{pv}} \mathrm{d}x \tag{31}$$

To minimize this functional, the following functional derivatives have to vanish:

$$\frac{\delta \mathcal{F}^{pv}}{\delta f_i(x)} = \frac{\delta}{\delta f_i(x)} \int_{\mathbb{X}} \frac{1}{2} \left\| \mathbf{v}_1(\mathbf{f}(x')) \times \mathbf{v}_2(\mathbf{f}(x')) \right\|^2 \mathrm{d}x' \tag{32}$$

$$= \int_{\mathbb{X}} (\mathbf{v}_1(\mathbf{f}(x')) \times \mathbf{v}_2(\mathbf{f}(x')))^{\mathrm{T}} \left(\frac{\partial \mathbf{v}_1(\mathbf{f}(x'))}{\partial f_i(x')} \times \mathbf{v}_2(\mathbf{f}(x')) \right. \tag{33}$$

$$\left. + \mathbf{v}_1(\mathbf{f}(x')) \times \frac{\partial \mathbf{v}_2(\mathbf{f}(x'))}{\partial f_i(x')} \right) \cdot \frac{\delta f_i(x')}{\delta f_i(x)} \mathrm{d}x' \tag{34}$$

$$= \int_{\mathbb{X}} (\mathbf{v}_1(\mathbf{f}(x')) \times \mathbf{v}_2(\mathbf{f}(x')))^{\mathrm{T}} \left(\frac{\partial \mathbf{v}_1(\mathbf{f}(x'))}{\partial f_i(x')} \times \mathbf{v}_2(\mathbf{f}(x')) \right. \tag{35}$$

$$\left. + \mathbf{v}_1(\mathbf{f}(x')) \times \frac{\partial \mathbf{v}_2(\mathbf{f}(x'))}{\partial f_i(x')} \right) \cdot \delta(x', x) \, \mathrm{d}x' \tag{36}$$

$$= (\mathbf{v}_1(\mathbf{f}(x)) \times \mathbf{v}_2(\mathbf{f}(x)))^{\mathrm{T}} \left(\frac{\partial \mathbf{v}_1(\mathbf{f}(x))}{\partial f_i(x)} \times \mathbf{v}_2(\mathbf{f}(x)) \right. \tag{37}$$

$$\left. + \mathbf{v}_1(\mathbf{f}(x)) \times \frac{\partial \mathbf{v}_2(\mathbf{f}(x))}{\partial f_i(x)} \right) \tag{38}$$

Following the general recipe in Section 2, the integrand is differentiated with the chain rule, the Dirac identity of Eq. (3) is applied, and the sifting property of Eq. (4) is used to remove the integral. When reshaping the functional derivatives into a vector, we get:

$$\frac{\delta \mathcal{F}^{pv}}{\delta \mathbf{f}(x)} = (\mathbf{v}_1 \times \mathbf{v}_2)^{\mathrm{T}} \cdot \begin{pmatrix} (\frac{\partial \mathbf{v}_1}{\partial y_1} \times \mathbf{v}_2 + \mathbf{v}_1 \times \frac{\partial \mathbf{v}_2}{\partial y_1})^{\mathrm{T}} \\ \vdots \\ (\frac{\partial \mathbf{v}_1}{\partial y_m} \times \mathbf{v}_2 + \mathbf{v}_1 \times \frac{\partial \mathbf{v}_2}{\partial y_m})^{\mathrm{T}} \end{pmatrix}^{\mathrm{T}}_{|\mathbf{y}=\mathbf{f}(x)} \tag{39}$$

where we dropped the dependencies for brevity, i.e., $\mathbf{v}_1 := \mathbf{v}_1(\mathbf{y})$ and $\mathbf{v}_2 := \mathbf{v}_2(\mathbf{y})$.

3.4 Ridge Lines

Given is a three-dimensional scalar field $s(\mathbf{y}) : \mathbb{Y} \to \mathbb{R}$ with the gradient vector $\nabla s(\mathbf{y})$ (which is a column vector) and the Hessian matrix $\mathbf{H}(\mathbf{y})$, which has at each location $\mathbf{y}$ the real-valued, sorted eigenvalues $\lambda_1(\mathbf{y}) \leq \lambda_2(\mathbf{y}) \leq \lambda_3(\mathbf{y})$ and the corresponding eigenvectors $\mathbf{c}_1(\mathbf{y}), \mathbf{c}_2(\mathbf{y}), \mathbf{c}_3(\mathbf{y})$, i.e., $\mathbf{H}(\mathbf{y})\mathbf{c}_i(\mathbf{y}) = \lambda_i(\mathbf{y})\mathbf{c}_i(\mathbf{y})$ for all $i \in \{1, 2, 3\}$. The ridge line criterion of Eberly [1996] requires that the eigenvectors $\mathbf{c}_1$ and $\mathbf{c}_2$ are both orthogonal to the gradient, i.e., $\nabla s(\mathbf{y})^{\mathrm{T}}\mathbf{c}_1 = \nabla s(\mathbf{y})^{\mathrm{T}}\mathbf{c}_2 = 0$ and that the corresponding eigenvalues are negative, i.e., $\lambda_1 \leq \lambda_2 < 0$. Due to the orthogonality of the eigenvectors, ridge lines can be equivalently found by searching for locations at which the eigenvector $\mathbf{c}_3$ corresponding to the largest eigenvalue λ_3 is parallel to the gradient ∇s. Thus, the 1-dimensional ridge line $\mathbf{f}(x) = \left(f_1(x), \ldots, f_3(x)\right)^{\mathrm{T}}$ minimizes the functional:

$$\mathcal{F}^{rl} = \int_{\mathbb{X}} \underbrace{\frac{1}{2} \left\| \nabla s(\mathbf{f}(x)) \times \mathbf{c}_3(\mathbf{f}(x)) \right\|^2}_{\mathcal{M}^{rl}} \mathrm{d}x \tag{40}$$

$$s.t. \quad \lambda_1(\mathbf{f}(x)) \leq \lambda_2(\mathbf{f}(x)) < 0. \tag{41}$$

The norm of cross product of two vectors vanishes to zero if the two vectors are parallel. The functional has the following functional derivatives:

$$\frac{\delta \mathcal{F}^{rl}}{\delta f_i(x)} = \frac{\delta}{\delta f_i(x)} \int_{\mathbb{X}} \frac{1}{2} \left\| \nabla s(\mathbf{f}(x')) \times \mathbf{c}_3(\mathbf{f}(x')) \right\|^2 \mathrm{d}x' \tag{42}$$

$$= \int_{\mathbb{X}} (\nabla s(\mathbf{f}(x')) \times \mathbf{c}_3(\mathbf{f}(x')))^{\mathrm{T}} \left(\frac{\partial \nabla s(\mathbf{f}(x'))}{\partial f_i(x')} \times \mathbf{c}_3(\mathbf{f}(x')) \right. \tag{43}$$

$$\left. + \nabla s(\mathbf{f}(x')) \times \frac{\partial \mathbf{c}_3(\mathbf{f}(x'))}{\partial f_i(x')} \right) \cdot \frac{\delta f_i(x')}{\delta f_i(x)} \mathrm{d}x' \tag{44}$$

$$= \int_{\mathbb{X}} (\nabla s(\mathbf{f}(x')) \times \mathbf{c}_3(\mathbf{f}(x')))^{\mathrm{T}} \left(\frac{\partial \nabla s(\mathbf{f}(x'))}{\partial f_i(x')} \times \mathbf{c}_3(\mathbf{f}(x')) \right. \tag{45}$$

$$\left. + \nabla s(\mathbf{f}(x')) \times \frac{\partial \mathbf{c}_3(\mathbf{f}(x'))}{\partial f_i(x')} \right) \cdot \delta(x', x) \, \mathrm{d}x' \tag{46}$$

$$= (\nabla s(\mathbf{f}(x)) \times \mathbf{c}_3(\mathbf{f}(x)))^{\mathrm{T}} \left(\frac{\partial \nabla s(\mathbf{f}(x))}{\partial f_i(x)} \times \mathbf{c}_3(\mathbf{f}(x)) \right. \tag{47}$$

$$\left. + \nabla s(\mathbf{f}(x)) \times \frac{\partial \mathbf{c}_3(\mathbf{f}(x))}{\partial f_i(x)} \right) \tag{48}$$

As in the general recipe in Section 2, the integrand was differentiated with the chain rule, the Dirac identity of Eq. (3) was applied, and the sifting property of Eq. (4) was used. When reshaping the functional derivative into a row vector, we get:

$$\frac{\delta \mathcal{F}^{rl}}{\delta \mathbf{f}(x)} = (\nabla s \times \mathbf{c}_3)^{\mathrm{T}} \cdot \begin{pmatrix} (\frac{\partial \nabla s}{\partial y_1} \times \mathbf{c}_3 + \nabla s \times \frac{\partial \mathbf{c}_3}{\partial y_1})^{\mathrm{T}} \\ \vdots \\ (\frac{\partial \nabla s}{\partial y_m} \times \mathbf{c}_3 + \nabla s \times \frac{\partial \mathbf{c}_3}{\partial y_m})^{\mathrm{T}} \end{pmatrix}^{\mathrm{T}}_{|\mathbf{y}=\mathbf{f}(x)} \tag{49}$$

For notational convenience we dropped the dependencies, i.e., $\nabla s := \nabla s(\mathbf{y})$ and $\mathbf{c}_3 := \mathbf{c}_3(\mathbf{y})$. Valley lines of a scalar field $s(\mathbf{y})$ are analogously found as ridge lines of the negated scalar field $-s(\mathbf{y})$. In a two-dimensional domain ($m = 2$), the parallel vectors may either be lifted by appending a zero, or the ridge line may be searched as locations where the dot product of the gradient and the eigenvector with smallest eigenvalue vanish. A vanishing dot product is also the minimizer for ridge surfaces, as introduced next.

3.5 Ridge Surfaces

Given is a three-dimensional scalar field $s(\mathbf{y}) : \mathbb{Y} \to \mathbb{R}$ with the gradient vector $\nabla s(\mathbf{y})$ and the Hessian matrix $\mathbf{H}(\mathbf{y})$, which has at each location $\mathbf{y}$ the real-valued, sorted eigenvalues $\lambda_1(\mathbf{y}) \leq \lambda_2(\mathbf{y}) \leq \lambda_3(\mathbf{y})$ and the corresponding eigenvectors $\mathbf{c}_1(\mathbf{y}), \mathbf{c}_2(\mathbf{y}), \mathbf{c}_3(\mathbf{y})$, i.e., $\mathbf{H}(\mathbf{y})\mathbf{c}_i(\mathbf{y}) = \lambda_i(\mathbf{y})\mathbf{c}_i(\mathbf{y})$ for all $i \in \{1, 2, 3\}$. Following Eberly [1996], a ridge surface is characterized by locations at which the eigenvector $\mathbf{c}_1(\mathbf{y})$ to the smallest eigenvalue $\lambda_1(\mathbf{y})$ is orthogonal to the gradient $\nabla s(\mathbf{y})$ and where the corresponding eigenvalue is negative, i.e., $\lambda_1(\mathbf{y}) < 0$. The 2-dimensional ridge surface

$\mathbf{f}(x_1, x_2) = \left(f_1(x_1, x_2), \ldots, f_3(x_1, x_2)\right)^{\mathrm{T}}$ minimizes the functional:

$$\mathcal{F}^{rs} = \int_{\mathbb{X}} \underbrace{\frac{1}{2} \left\| \nabla s(\mathbf{f}(\mathbf{x}))^{\mathrm{T}} \mathbf{c}_1(\mathbf{f}(\mathbf{x})) \right\|^2}_{\mathcal{M}^{rs}} \mathrm{d}x \quad (50)$$

$$s.t. \quad \lambda_1(\mathbf{f}(\mathbf{x})) < 0. \quad (51)$$

which has the following functional derivatives:

$$\frac{\delta \mathcal{F}^{rs}}{\delta f_i(\mathbf{x})} = \frac{\delta}{\delta f_i(\mathbf{x})} \int_{\mathbb{X}} \frac{1}{2} \left\| \nabla s(\mathbf{f}(\mathbf{x}'))^{\mathrm{T}} \mathbf{c}_1(\mathbf{f}(\mathbf{x}')) \right\|^2 \mathrm{d}\mathbf{x}' \quad (52)$$

$$= \int_{\mathbb{X}} \left(\nabla s(\mathbf{f}(\mathbf{x}'))^{\mathrm{T}} \mathbf{c}_1(\mathbf{f}(\mathbf{x}')) \right) \left(\frac{\partial \nabla s(\mathbf{f}(\mathbf{x}'))}{\partial f_i(\mathbf{x}')}^{\mathrm{T}} \mathbf{c}_1(\mathbf{f}(\mathbf{x}')) \quad (53)$$

$$+ \nabla s(\mathbf{f}(\mathbf{x}'))^{\mathrm{T}} \frac{\partial \mathbf{c}_1(\mathbf{f}(\mathbf{x}'))}{\partial f_i(\mathbf{x}')} \right) \cdot \frac{\delta f_i(\mathbf{x}')}{\delta f_i(\mathbf{x})} \mathrm{d}\mathbf{x}' \quad (54)$$

$$= \int_{\mathbb{X}} \left(\nabla s(\mathbf{f}(\mathbf{x}'))^{\mathrm{T}} \mathbf{c}_1(\mathbf{f}(\mathbf{x}')) \right) \left(\frac{\partial \nabla s(\mathbf{f}(\mathbf{x}'))}{\partial f_i(\mathbf{x}')}^{\mathrm{T}} \mathbf{c}_1(\mathbf{f}(\mathbf{x}')) \quad (55)$$

$$+ \nabla s(\mathbf{f}(\mathbf{x}'))^{\mathrm{T}} \frac{\partial \mathbf{c}_1(\mathbf{f}(\mathbf{x}'))}{\partial f_i(\mathbf{x}')} \right) \cdot \delta(\mathbf{x}', \mathbf{x}) \, \mathrm{d}\mathbf{x}' \quad (56)$$

$$= \left(\nabla s(\mathbf{f}(\mathbf{x}))^{\mathrm{T}} \mathbf{c}_1(\mathbf{f}(\mathbf{x})) \right) \left(\frac{\partial \nabla s(\mathbf{f}(\mathbf{x}))}{\partial f_i(\mathbf{x})}^{\mathrm{T}} \mathbf{c}_1(\mathbf{f}(\mathbf{x})) \quad (57)$$

$$+ \nabla s(\mathbf{f}(\mathbf{x}))^{\mathrm{T}} \frac{\partial \mathbf{c}_1(\mathbf{f}(\mathbf{x}))}{\partial f_i(\mathbf{x})} \right) \quad (58)$$

The derivation is analogous to the derivation for ridge lines, but with a dot product instead of a cross product. When reshaping the functional derivative into a vector, we get:

$$\frac{\delta \mathcal{F}^{rs}}{\delta \mathbf{f}(\mathbf{x})} = \left(\nabla s^{\mathrm{T}} \mathbf{c}_1 \right) \cdot \begin{pmatrix} \frac{\partial \nabla s}{\partial y_1}^{\mathrm{T}} \mathbf{c}_1 + \nabla s^{\mathrm{T}} \frac{\partial \mathbf{c}_1}{\partial y_1} \\ \vdots \\ \frac{\partial \nabla s}{\partial y_m}^{\mathrm{T}} \mathbf{c}_1 + \nabla s^{\mathrm{T}} \frac{\partial \mathbf{c}_1}{\partial y_m} \end{pmatrix}^{\mathrm{T}}_{|\mathbf{y}=\mathbf{f}(\mathbf{x})} \quad (59)$$

where we dropped the dependencies for brevity, i.e., $\nabla s := \nabla s(\mathbf{y})$ and $\mathbf{c} := \mathbf{c}_1(\mathbf{y})$. Valley surfaces of a scalar field $s(\mathbf{y})$ are analogously found as ridge surfaces of the negated scalar field $-s(\mathbf{y})$.

3.6 Vortex Corelines and Bifurcation Lines

Based on the parallel vectors operator, vortex corelines and bifurcation lines can be defined as locations where the velocity and the acceleration are parallel [Roth 2000; Sujudi and Haimes 1995]. Since this is another example for a parallel vectors based feature, we abbreviate the notation, since the derivation follows directly the parallel vectors derivation. Given is a 3-dimensional steady vector field $\mathbf{v}(\mathbf{y}) : \mathbb{Y} \to \mathbb{R}^3$, 1-dimensional vortex corelines and bifurcation lines $\mathbf{f}(x_1, \ldots, x_n) = \left(f_1(x), \ldots, f_3(x)\right)^{\mathrm{T}}$ minimize:

$$\mathcal{F}^{v} = \int_{\mathbb{X}} \underbrace{\frac{1}{2} \left\| \mathbf{v}(\mathbf{f}(x)) \times \nabla \mathbf{v}(\mathbf{f}(x)) \, \mathbf{v}(\mathbf{f}(x)) \right\|^2}_{\mathcal{M}^{v}} \mathrm{d}x \quad (60)$$

Depending on whether vortex corelines or bifurcation lines are searched, additional requirements are demanded for the eigenvalues.

The following functional derivatives can be derived:

$$\frac{\delta \mathcal{F}^{v}}{\delta f_i(x)} = \frac{\delta}{\delta f_i(x)} \int_{\mathbb{X}} \frac{1}{2} \left\| \mathbf{v}(\mathbf{f}(x')) \times \nabla \mathbf{v}(\mathbf{f}(x')) \, \mathbf{v}(\mathbf{f}(x')) \right\|^2 \mathrm{d}x' \quad (61)$$

$$= \int_{\mathbb{X}} (\mathbf{v} \times (\nabla \mathbf{v})\mathbf{v})^{\mathrm{T}} \left(\frac{\partial \mathbf{v}}{\partial f_i} \times ((\nabla \mathbf{v})\mathbf{v}) \quad (62)$$

$$+ \mathbf{v} \times \left(\frac{\partial \nabla \mathbf{v}}{\partial f_i} \mathbf{v} + (\nabla \mathbf{v}) \frac{\partial \mathbf{v}}{\partial f_i} \right) \right) \cdot \frac{\delta f_i(x')}{\delta f_i(x)} \mathrm{d}x' \quad (63)$$

$$= \int_{\mathbb{X}} (\mathbf{v} \times (\nabla \mathbf{v})\mathbf{v})^{\mathrm{T}} \left(\frac{\partial \mathbf{v}}{\partial f_i} \times ((\nabla \mathbf{v})\mathbf{v}) \quad (64)$$

$$+ \mathbf{v} \times \left(\frac{\partial \nabla \mathbf{v}}{\partial f_i} \mathbf{v} + (\nabla \mathbf{v}) \frac{\partial \mathbf{v}}{\partial f_i} \right) \right) \cdot \delta(x', x) \, \mathrm{d}x' \quad (65)$$

$$= (\mathbf{v} \times (\nabla \mathbf{v})\mathbf{v})^{\mathrm{T}} \left(\frac{\partial \mathbf{v}}{\partial f_i} \times ((\nabla \mathbf{v})\mathbf{v}) + \mathbf{v} \times \left(\frac{\partial \nabla \mathbf{v}}{\partial f_i} \mathbf{v} + (\nabla \mathbf{v}) \frac{\partial \mathbf{v}}{\partial f_i} \right) \right) \quad (66)$$

Reshaping the functional derivatives into a row vector gives the following expression:

$$\frac{\delta \mathcal{F}^{v}}{\delta \mathbf{f}(x)} = (\mathbf{v} \times (\nabla \mathbf{v})\mathbf{v})^{\mathrm{T}} \quad (67)$$

$$\cdot \begin{pmatrix} (\frac{\partial \mathbf{v}}{\partial y_1} \times ((\nabla \mathbf{v})\mathbf{v}) + \mathbf{v} \times (\frac{\partial \nabla \mathbf{v}}{\partial y_1} \mathbf{v} + (\nabla \mathbf{v}) \frac{\partial \mathbf{v}}{\partial y_1}))^{\mathrm{T}} \\ \vdots \\ (\frac{\partial \mathbf{v}}{\partial y_m} \times ((\nabla \mathbf{v})\mathbf{v}) + \mathbf{v} \times (\frac{\partial \nabla \mathbf{v}}{\partial y_m} \mathbf{v} + (\nabla \mathbf{v}) \frac{\partial \mathbf{v}}{\partial y_m}))^{\mathrm{T}} \end{pmatrix}^{\mathrm{T}}_{|\mathbf{y}=\mathbf{f}(x)} \quad (68)$$

where we again dropped the dependencies for brevity, i.e., $\mathbf{v} := \mathbf{v}(\mathbf{y})$.

3.7 Jacobi Sets

Jacobi sets are curves along which two gradient fields align [Edelsbrunner and Harer 2002]. Given two 3-dimensional scalar fields $s_1(\mathbf{y}), s_2(\mathbf{y}) : \mathbb{Y} \to \mathbb{R}$, a 1-dimensional Jacobi set is a curve $\mathbf{f}(x) = \left(f_1(x), \ldots, f_3(x)\right)^{\mathrm{T}}$, which is defined by:

$$\mathcal{F}^{j} = \int_{\mathbb{X}} \underbrace{\frac{1}{2} \left\| \nabla s_1(\mathbf{f}(x)) \times \nabla s_2(\mathbf{f}(x)) \right\|^2}_{\mathcal{M}^{j}} \mathrm{d}x \quad (69)$$

which has the following functional derivatives:

$$\frac{\delta \mathcal{F}^{j}}{\delta f_i(x)} = \frac{\delta}{\delta f_i(x)} \int_{\mathbb{X}} \frac{1}{2} \left\| \nabla s_1(\mathbf{f}(x')) \times \nabla s_2(\mathbf{f}(x')) \right\|^2 \mathrm{d}x' \quad (70)$$

$$= \int_{\mathbb{X}} (\nabla s_1(\mathbf{f}(x')) \times \nabla s_2(\mathbf{f}(x')))^{\mathrm{T}} \left(\frac{\partial \nabla s_1(\mathbf{f}(x'))}{\partial f_i(x')} \times \nabla s_2(\mathbf{f}(x')) \quad (71)$$

$$+ \nabla s_1(\mathbf{f}(x')) \times \frac{\partial \nabla s_2(\mathbf{f}(x'))}{\partial f_i(x')} \right) \cdot \frac{\delta f_i(x')}{\delta f_i(x)} \mathrm{d}x' \quad (72)$$

$$= \int_{\mathbb{X}} (\nabla s_1(\mathbf{f}(x')) \times \nabla s_2(\mathbf{f}(x')))^{\mathrm{T}} \left(\frac{\partial \nabla s_1(\mathbf{f}(x'))}{\partial f_i(x')} \times \nabla s_2(\mathbf{f}(x')) \quad (73)$$

$$+ \nabla s_1(\mathbf{f}(x')) \times \frac{\partial \nabla s_2(\mathbf{f}(x'))}{\partial f_i(x')} \right) \cdot \delta(x', x) \, \mathrm{d}x' \quad (74)$$

$$= (\nabla s_1(\mathbf{f}(x)) \times \nabla s_2(\mathbf{f}(x)))^{\mathrm{T}} \left(\frac{\partial \nabla s_1(\mathbf{f}(x))}{\partial f_i(x)} \times \nabla s_2(\mathbf{f}(x)) \right. \tag{75}$$

$$\left. + \nabla s_1(\mathbf{f}(x)) \times \frac{\partial \nabla s_2(\mathbf{f}(x))}{\partial f_i(x)} \right) \tag{76}$$

When reshaping the functional derivative into a vector, we get:

$$\frac{\delta \mathcal{F}^j}{\delta \mathbf{f}(x)} = (\nabla s_1 \times \nabla s_2)^{\mathrm{T}} \cdot \begin{pmatrix} (\frac{\partial \nabla s_1}{\partial y_1} \times \nabla s_2 + \nabla s_1 \times \frac{\partial \nabla s_2}{\partial y_1})^{\mathrm{T}} \\ \vdots \\ (\frac{\partial \nabla s_1}{\partial y_m} \times \nabla s_2 + \nabla s_1 \times \frac{\partial \nabla s_2}{\partial y_m})^{\mathrm{T}} \end{pmatrix}^{\mathrm{T}}_{|\mathbf{y}=\mathbf{f}(x)} \tag{77}$$

As before, we dropped the dependencies for notational convenience, i.e., $\nabla s_1 := \nabla s_1(\mathbf{y})$ and $\nabla s_2 := \nabla s_2(\mathbf{y})$.

3.8 Parallel Eigenvector Lines

Next, we describe a feature definition for tensor fields in a variational manner. Given are two three-dimensional tensor fields $\mathbf{S}(\mathbf{y}), \mathbf{T}(\mathbf{y}) : \mathbb{Y} \to \mathbb{R}^{3\times 3}$. The parallel eigenvector operator of Oster et al. [2018b] searches for locations $\mathbf{y}$ at which there is a direction vector $\mathbf{r} \neq \mathbf{0} \in \mathbb{R}^3$, for which the following parallel vector conditions hold:

$$\mathbf{r} \parallel \mathbf{S}(\mathbf{y})\mathbf{r} \parallel \mathbf{T}(\mathbf{y})\mathbf{r}\,. \tag{78}$$

Here, both $\mathbf{y}$ and $\mathbf{r}$ are unknowns. We introduce a 6D feature vector $\mathbf{f}(x) = (\mathbf{g}(x), \mathbf{r}(x))$ where $\mathbf{g}(x)$ is the unknown position and $\mathbf{r}(x)$ is the unknown direction. We can then simply use twice the parallel vectors operator from Section 3.3 and apply an additional regularization that prevents the unknown direction from vanishing:

$$\mathcal{F}^{pe} = \int_{\mathbb{X}} \underbrace{\frac{1}{2}\left(\|\mathbf{S}(\mathbf{g})\mathbf{r} \times \mathbf{r}\|^2 + \|\mathbf{T}(\mathbf{g})\mathbf{r} \times \mathbf{r}\|^2 + \frac{1}{2}\left(\|\mathbf{r}\|^2 - 1\right)^2 \right)}_{\mathcal{M}^{pe}} \mathrm{d}x \tag{79}$$

In the following, we derive the functional derivatives for $\mathbf{g}(x)$ and $\mathbf{r}(x)$ separately. First, we compute the partial of only the $\mathbf{S}$ term with respect to $\mathbf{g}(x)$. The $\mathbf{T}$ term is analogous.

$$\frac{\delta \mathcal{F}^{pe}}{\delta g_i(x)} = \frac{\delta}{\delta g_i(x)} \int_{\mathbb{X}} \frac{1}{2} \left\| \mathbf{S}(\mathbf{g}(x'))\mathbf{r}(x') \times \mathbf{r}(x') \right\|^2 \mathrm{d}x' \tag{80}$$

$$= \int_{\mathbb{X}} (\mathbf{S}(\mathbf{g})\mathbf{r} \times \mathbf{r})^{\mathrm{T}} \left(\frac{\partial \mathbf{S}(\mathbf{g})}{\partial g_i(x')} \mathbf{r} \times \mathbf{r} \right) \cdot \frac{\delta g_i(x')}{\delta g_i(x)} \mathrm{d}x' \tag{81}$$

$$= \int_{\mathbb{X}} (\mathbf{S}(\mathbf{g})\mathbf{r} \times \mathbf{r})^{\mathrm{T}} \left(\frac{\partial \mathbf{S}(\mathbf{g})}{\partial g_i(x')} \mathbf{r} \times \mathbf{r} \right) \cdot \delta(x', x) \, \mathrm{d}x' \tag{82}$$

$$= (\mathbf{S}(\mathbf{g})\mathbf{r} \times \mathbf{r})^{\mathrm{T}} \left(\frac{\partial \mathbf{S}(\mathbf{g})}{\partial g_i(x)} \mathbf{r} \times \mathbf{r} \right) \tag{83}$$

Reshaped into a row vector this gives for the $\mathbf{S}$ term and $\mathbf{T}$ term:

$$\frac{\delta \mathcal{F}^{pe}}{\delta \mathbf{g}(x)} = (\mathbf{S}(\mathbf{g})\mathbf{r} \times \mathbf{r})^{\mathrm{T}} \cdot \left(\frac{\partial \mathbf{S}(\mathbf{y})}{\partial y_1} \mathbf{r} \times \mathbf{r}, \dots, \frac{\partial \mathbf{S}(\mathbf{y})}{\partial y_3} \mathbf{r} \times \mathbf{r} \right)_{|\mathbf{y}=\mathbf{g}(x)} \tag{84}$$

$$+ (\mathbf{T}(\mathbf{g})\mathbf{r} \times \mathbf{r})^{\mathrm{T}} \cdot \left(\frac{\partial \mathbf{T}(\mathbf{y})}{\partial y_1} \mathbf{r} \times \mathbf{r}, \dots, \frac{\partial \mathbf{T}(\mathbf{y})}{\partial y_3} \mathbf{r} \times \mathbf{r} \right)_{|\mathbf{y}=\mathbf{g}(x)} \tag{85}$$

Next, we compute the functional derivative with respect to the unknown direction $\mathbf{r}(x)$, again first only for the $\mathbf{S}$ term.

$$\frac{\delta \mathcal{F}^{pe}}{\delta r_i(x)} = \frac{\delta}{\delta r_i(x)} \int_{\mathbb{X}} \frac{1}{2} \left\| \mathbf{S}(\mathbf{g}(x'))\mathbf{r}(x') \times \mathbf{r}(x') \right\|^2 \mathrm{d}x' \tag{86}$$

$$= \int_{\mathbb{X}} (\mathbf{S}(\mathbf{g})\mathbf{r} \times \mathbf{r})^{\mathrm{T}} \left(\mathbf{S}(\mathbf{g})\mathbf{r} \times \hat{\mathbf{e}}_i + \mathbf{S}(\mathbf{g})\hat{\mathbf{e}}_i \times \mathbf{r} \right) \cdot \frac{\delta r_i(x')}{\delta r_i(x)} \mathrm{d}x' \tag{87}$$

$$= \int_{\mathbb{X}} (\mathbf{S}(\mathbf{g})\mathbf{r} \times \mathbf{r})^{\mathrm{T}} \left(\mathbf{S}(\mathbf{g})\mathbf{r} \times \hat{\mathbf{e}}_i + \mathbf{S}(\mathbf{g})\hat{\mathbf{e}}_i \times \mathbf{r} \right) \cdot \delta(x', x) \, \mathrm{d}x' \tag{88}$$

$$= (\mathbf{S}(\mathbf{g})\mathbf{r} \times \mathbf{r})^{\mathrm{T}} \left(\mathbf{S}(\mathbf{g})\mathbf{r} \times \hat{\mathbf{e}}_i + \mathbf{S}(\mathbf{g})\hat{\mathbf{e}}_i \times \mathbf{r} \right) \tag{89}$$

with $\hat{\mathbf{e}}_1 = (1,0,0)^{\mathrm{T}}$, $\hat{\mathbf{e}}_2 = (0,1,0)^{\mathrm{T}}$, $\hat{\mathbf{e}}_3 = (0,0,1)^{\mathrm{T}}$ being the unit basis vectors. Combining the $\mathbf{S}$ term, the $\mathbf{T}$ term, and also the regularizer that prevents a vanishing $\mathbf{r}$ gives:

$$\frac{\delta \mathcal{F}^{pe}}{\delta \mathbf{r}(x)} = (\mathbf{S}(\mathbf{g})\mathbf{r} \times \mathbf{r})^{\mathrm{T}} \cdot \begin{pmatrix} (\mathbf{S}(\mathbf{g})\mathbf{r} \times \hat{\mathbf{e}}_1 + \mathbf{S}(\mathbf{g})\hat{\mathbf{e}}_1 \times \mathbf{r})^{\mathrm{T}} \\ (\mathbf{S}(\mathbf{g})\mathbf{r} \times \hat{\mathbf{e}}_2 + \mathbf{S}(\mathbf{g})\hat{\mathbf{e}}_2 \times \mathbf{r})^{\mathrm{T}} \\ (\mathbf{S}(\mathbf{g})\mathbf{r} \times \hat{\mathbf{e}}_3 + \mathbf{S}(\mathbf{g})\hat{\mathbf{e}}_3 \times \mathbf{r})^{\mathrm{T}} \end{pmatrix}^{\mathrm{T}}_{|\mathbf{y}=\mathbf{g}(x)} \tag{90}$$

$$+ (\mathbf{T}(\mathbf{g})\mathbf{r} \times \mathbf{r})^{\mathrm{T}} \cdot \begin{pmatrix} (\mathbf{T}(\mathbf{g})\mathbf{r} \times \hat{\mathbf{e}}_1 + \mathbf{T}(\mathbf{g})\hat{\mathbf{e}}_1 \times \mathbf{r})^{\mathrm{T}} \\ (\mathbf{T}(\mathbf{g})\mathbf{r} \times \hat{\mathbf{e}}_2 + \mathbf{T}(\mathbf{g})\hat{\mathbf{e}}_2 \times \mathbf{r})^{\mathrm{T}} \\ (\mathbf{T}(\mathbf{g})\mathbf{r} \times \hat{\mathbf{e}}_3 + \mathbf{T}(\mathbf{g})\hat{\mathbf{e}}_3 \times \mathbf{r})^{\mathrm{T}} \end{pmatrix}^{\mathrm{T}}_{|\mathbf{y}=\mathbf{g}(x)} \tag{91}$$

$$+ \mathbf{r}^{\mathrm{T}}(\|\mathbf{r}\|^2 - 1) \tag{92}$$

For brevity, we removed the dependencies $\mathbf{g} := \mathbf{g}(x)$ and $\mathbf{r} := \mathbf{r}(x)$.

3.9 Tensor Corelines

For a symmetric tensor field $\mathbf{S}(\mathbf{y})$ in a three-dimensional domain $\mathbf{y} \in \mathbb{Y} \subseteq \mathbb{R}^3$, Oster et al. [2018a] introduced the concept of tensor corelines. In analogy to the vortex criterion of Sujudi and Haimes [1995] for steady fluid flow, tensor corelines are curves around which hyperstreamlines of the eigenvector field are swirling. These feature curves are obtained with the parallel eigenvectors operator of Section 3.8 when choosing $\mathbf{T}(\mathbf{y}) = \nabla_{\mathbf{r}}\mathbf{S}(\mathbf{y})$ to be the directional derivative of $\mathbf{S}(\mathbf{y})$ in direction $\mathbf{r}$:

$$\mathbf{T}(\mathbf{y}) = \sum_{i=1}^{3} \frac{\partial \mathbf{S}(\mathbf{y})}{\partial y_i} \cdot r_i \qquad \frac{\partial \mathbf{T}(\mathbf{y})}{\partial y_j} = \sum_{i=1}^{3} \frac{\partial^2 \mathbf{S}(\mathbf{y})}{\partial y_i \partial y_j} \cdot r_i \tag{93}$$

4 DERIVATIONS OF REGULARIZERS

In the following, we continue with the derivation of the regularizers, which can be additively applied on top of the feature definitions.

4.1 Proximity

If for each feature point $\mathbf{f}(\mathbf{x})$ a reference position $\mathbf{c}(\mathbf{x}) : \mathbb{X} \to \mathbb{Y}$ is known that the feature should remain close to, the following regularizer can be added:

$$\mathcal{F}^p = \int_{\mathbb{X}} \underbrace{\frac{1}{2}\|\mathbf{f}(\mathbf{x}) - \mathbf{c}(\mathbf{x})\|^2}_{\Gamma^p} \mathrm{d}\mathbf{x} \tag{94}$$

The corresponding functional derivatives are:

$$\frac{\delta \mathcal{F}^p}{\delta f_i(\mathbf{x})} = \frac{\delta}{\delta f_i(\mathbf{x})} \int_{\mathbb{X}} \frac{1}{2} \|\mathbf{f}(\mathbf{x}') - \mathbf{c}(\mathbf{x}')\|^2 \mathrm{d}\mathbf{x}' \tag{95}$$

$$= \int_{\mathbb{X}} (f_i(\mathbf{x}') - c_i(\mathbf{x}')) \cdot \frac{\delta f_i(\mathbf{x}')}{\delta f_i(\mathbf{x})} \,\mathrm{d}\mathbf{x}' \tag{96}$$

$$= \int_{\mathbb{X}} (f_i(\mathbf{x}') - c_i(\mathbf{x}')) \cdot \delta(\mathbf{x}', \mathbf{x}) \,\mathrm{d}\mathbf{x}' \tag{97}$$

$$= f_i(\mathbf{x}) - c_i(\mathbf{x}) \tag{98}$$

A noticeable difference compared to other derivations is that Eq. (96) contains only the i'th component of the vectors, namely $(f_i(\mathbf{x}') - c_i(\mathbf{x}'))$, since $\mathbf{f}(\mathbf{x}')$ is not the argument of a function to which the chain rule gets applied. Conveniently, the functional derivatives can be shaped into a row vector:

$$\frac{\delta \mathcal{F}^p}{\delta \mathbf{f}(\mathbf{x})} = (\mathbf{f}(\mathbf{x}) - \mathbf{c}(\mathbf{x}))^{\mathrm{T}} \tag{99}$$

4.2 Smoothness

For both feature curves and feature surfaces, a smooth solution is obtained when minimizing the Dirichlet energy:

$$\mathcal{F}^s = \int_{\mathbb{X}} \underbrace{\frac{1}{2} \|\nabla \mathbf{f}(\mathbf{x})\|^2}_{\Gamma^s} \,\mathrm{d}\mathbf{x} \tag{100}$$

In this case, the integrand depends on the gradient of $\mathbf{f}$ and not on $\mathbf{f}$ itself. This means, the summation in Eq. (5) comes into play. The functional derivatives are derived as follows:

$$\frac{\delta \mathcal{F}^s}{\delta f_i(\mathbf{x})} = \frac{\delta}{\delta f_i(\mathbf{x})} \int_{\mathbb{X}} \frac{1}{2} \|\nabla \mathbf{f}(\mathbf{x}')\|^2 \mathrm{d}\mathbf{x}' \tag{101}$$

$$= \int_{\mathbb{X}} \sum_{j=1}^{n} f_{i,j}(\mathbf{x}') \cdot \frac{\partial}{\partial x_j'} \frac{\delta f_i(\mathbf{x}')}{\delta f_i(\mathbf{x})} \,\mathrm{d}\mathbf{x}' \tag{102}$$

$$= \int_{\mathbb{X}} - \sum_{j=1}^{n} \frac{\partial}{\partial x_j'} f_{i,j}(\mathbf{x}') \cdot \delta(\mathbf{x}', \mathbf{x}) \,\mathrm{d}\mathbf{x}' \tag{103}$$

$$= - \sum_{j=1}^{n} \frac{\partial}{\partial x_j} f_{i,j}(\mathbf{x}) \tag{104}$$

$$= - \sum_{j=1}^{n} \frac{\partial^2}{\partial x_j^2} f_i(\mathbf{x}) \tag{105}$$

where the step from Eq. (102) to Eq. (103) included integration by parts as in Eqs. (13)–(14). As before, the Dirac identity of Eq. (3) and the sifting property of Eq. (4) are applied. Each functional derivative eventually reduces to a Laplacian, which can be phrased to a component-wise Laplacian to compute the functional derivative in one expression:

$$\frac{\delta \mathcal{F}^s}{\delta \mathbf{f}(\mathbf{x})} = - \left(\sum_{j=1}^{n} \frac{\partial^2}{\partial x_j^2} f_1(\mathbf{x}), \ldots, \sum_{j=1}^{n} \frac{\partial^2}{\partial x_j^2} f_m(\mathbf{x}) \right) = -\nabla^2 \mathbf{f}(\mathbf{x})^{\mathrm{T}} \tag{106}$$

4.3 Flow Alignment

The tangent $\nabla \mathbf{f}(x) = \frac{\mathrm{d}\mathbf{f}(x)}{\mathrm{d}x}$ of a feature curve ($n = 1$) can be aligned with a vector field $\mathbf{v}(\mathbf{y}) : \mathbb{Y} \to \mathbb{R}^m$ by using

$$\mathcal{F}^a = \int_{\mathbb{X}} \underbrace{\frac{1}{2} \|\mathbf{v}(\mathbf{f}(x)) - \nabla \mathbf{f}(x)\|^2}_{\Gamma^a} \,\mathrm{d}x \tag{107}$$

This integrand depends on $\mathbf{f}(x)$ and $\nabla \mathbf{f}(x)$, which means that chain rules are calculated for both, following Eq. (5). This results in the following functional derivatives:

$$\frac{\delta \mathcal{F}^a}{\delta f_i(x)} = \frac{\delta}{\delta f_i(x)} \int_{\mathbb{X}} \frac{1}{2} \|\mathbf{v}(\mathbf{f}(x')) - \nabla \mathbf{f}(x')\|^2 \mathrm{d}x' \tag{108}$$

$$= \int_{\mathbb{X}} (\mathbf{v}(\mathbf{f}(x')) - \nabla \mathbf{f}(x'))^{\mathrm{T}} \cdot \frac{\partial \mathbf{v}(\mathbf{f}(x'))}{\partial f_i(x')} \cdot \frac{\delta f_i(x')}{\delta f_i(x)} \tag{109}$$

$$- \left(v_i(\mathbf{f}(x')) - \frac{\mathrm{d} f_i(x')}{\mathrm{d}x'} \right) \cdot \frac{\mathrm{d}}{\mathrm{d}x'} \frac{\delta f_i(x')}{\delta f_i(x)} \,\mathrm{d}x' \tag{110}$$

$$= \int_{\mathbb{X}} \left(\mathbf{v}(\mathbf{f}(x')) - \nabla \mathbf{f}(x') \right)^{\mathrm{T}} \cdot \frac{\partial \mathbf{v}(\mathbf{f}(x'))}{\partial f_i(x')} \cdot \delta(x', x) \tag{111}$$

$$+ \frac{\mathrm{d}}{\mathrm{d}x'} \left(v_i(\mathbf{f}(x')) - \frac{\mathrm{d} f_i(x')}{\mathrm{d}x'} \right) \cdot \delta(x', x) \,\mathrm{d}x' \tag{112}$$

$$= \int_{\mathbb{X}} \left(\left(\mathbf{v}(\mathbf{f}(x')) - \nabla \mathbf{f}(x') \right)^{\mathrm{T}} \cdot \frac{\partial \mathbf{v}(\mathbf{f}(x'))}{\partial f_i(x')} \right. \tag{113}$$

$$\left. + \frac{\mathrm{d}}{\mathrm{d}x'} \left(v_i(\mathbf{f}(x')) - \frac{\mathrm{d} f_i(x')}{\mathrm{d}x'} \right) \right) \cdot \delta(x', x) \,\mathrm{d}x' \tag{114}$$

$$= (\mathbf{v}(\mathbf{f}(x)) - \nabla \mathbf{f}(x))^{\mathrm{T}} \cdot \frac{\partial \mathbf{v}(\mathbf{f}(x))}{\partial f_i(x)} \tag{115}$$

$$+ \frac{\mathrm{d}}{\mathrm{d}x} \left(v_i(\mathbf{f}(x)) - \frac{\mathrm{d} f_i(x)}{\mathrm{d}x} \right) \tag{116}$$

$$= (\mathbf{v}(\mathbf{f}(x)) - \nabla \mathbf{f}(x))^{\mathrm{T}} \cdot \frac{\partial \mathbf{v}(\mathbf{f}(x))}{\partial f_i(x)} \tag{117}$$

$$+ \frac{\partial v_i(\mathbf{f}(x))}{\partial \mathbf{f}(x)} \frac{\mathrm{d}\mathbf{f}(x)}{\mathrm{d}x} - \frac{\mathrm{d}^2 f_i(x)}{\mathrm{d}x^2} \tag{118}$$

A noteworthy detail is the negative sign in front of Eq. (110), which originates from the application of the chain rule to $-\nabla \mathbf{f}(x')$ in the line before. Reshaped into a vector, we get the following:

$$\frac{\delta \mathcal{F}^a}{\delta \mathbf{f}(\mathbf{x})} = (\mathbf{v}(\mathbf{f}(x)) - \nabla \mathbf{f}(x))^{\mathrm{T}} \cdot \frac{\partial \mathbf{v}(\mathbf{f}(x))}{\partial \mathbf{f}(x)} \tag{119}$$

$$+ \left(\frac{\partial \mathbf{v}(\mathbf{f}(x))}{\partial \mathbf{f}(x)} \nabla \mathbf{f}(x) \right)^{\mathrm{T}} - \nabla^2 \mathbf{f}(x)^{\mathrm{T}} \tag{120}$$

where the Jacobian matrix holds the partial derivatives of the velocity field in the columns, which get evaluated at the feature curve:

$$\frac{\partial \mathbf{v}(\mathbf{f}(x))}{\partial \mathbf{f}(x)} = \begin{pmatrix} \frac{\partial v_1(\mathbf{y})}{\partial y_1} & \cdots & \frac{\partial v_1(\mathbf{y})}{\partial y_n} \\ \vdots & & \vdots \\ \frac{\partial v_m(\mathbf{y})}{\partial y_1} & \cdots & \frac{\partial v_m(\mathbf{y})}{\partial y_n} \end{pmatrix}_{|\mathbf{y}=\mathbf{f}(x)} \tag{121}$$

4.4 Orientation

If a desired tangent vector $\mathbf{v}(x) : \mathbb{X} \to \mathbb{R}^m$ to a feature curve ($n = 1$) is specified along the curve, then the following regularizer applies:

$$\mathcal{F}^o = \int_{\mathbb{X}} \underbrace{\frac{1}{2} \|\mathbf{v}(x) - \nabla \mathbf{f}(x)\|^2}_{\Gamma^o} \, \mathrm{d}\mathbf{x} \tag{122}$$

which requires the computation of the functional derivatives

$$\frac{\delta \mathcal{F}^o}{\delta f_i(x)} = \frac{\delta}{\delta f_i(x)} \int_{\mathbb{X}} \frac{1}{2} \|\mathbf{v}(x') - \nabla \mathbf{f}(x')\|^2 \mathrm{d}x' \tag{123}$$

$$= \int_{\mathbb{X}} -\left(v_i(x') - \frac{\mathrm{d}f_i(x')}{\mathrm{d}x'}\right) \cdot \frac{\mathrm{d}}{\mathrm{d}x'} \frac{\delta f_i(x')}{\delta f_i(x)} \, \mathrm{d}x' \tag{124}$$

$$= \int_{\mathbb{X}} \frac{\mathrm{d}}{\mathrm{d}x'} \left(v_i(x') - \frac{\mathrm{d}f_i(x')}{\mathrm{d}x'}\right) \cdot \delta(x', x) \, \mathrm{d}x' \tag{125}$$

$$= \frac{\mathrm{d}}{\mathrm{d}x} \left(v_i(x) - \frac{\mathrm{d}f_i(x)}{\mathrm{d}x}\right) \tag{126}$$

$$= \frac{\mathrm{d}v_i(x)}{\mathrm{d}x} - \frac{\mathrm{d}^2 f_i(x)}{\mathrm{d}x^2} \tag{127}$$

Integration by parts as in Eqs. (13)–(14), the Dirac identity of Eq. (3), and the sifting property of Eq. (4) were needed in the derivation.

Phrased in vector notation, where $\nabla \mathbf{v}(x) = \frac{\mathrm{d}\mathbf{v}(x)}{\mathrm{d}x}$ is the tangent of $\mathbf{v}(x)$, we arrive at the following expression:

$$\frac{\delta \mathcal{F}^o}{\delta \mathbf{f}(x)} = \left(\nabla \mathbf{v}(x) - \nabla^2 \mathbf{f}(x)\right)^{\mathrm{T}} \tag{128}$$

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