FOCUS Curve Transition Objective Function

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April 15, 2021

General

A functions that describes how fast one curve transitions to another curve is given in (1). This function can be used as a general coil complexity metric and is motivated by the Frenet-Serret equations.

$$c = \sqrt{\left(\frac{\partial \kappa}{\partial s}\right)^2 + (\kappa\tau)^2} \tag{1}$$

$$\frac{\partial \boldsymbol{r}}{\partial s} = \hat{\boldsymbol{t}} \tag{2}$$

$$\frac{\partial^2 \boldsymbol{r}}{\partial s^2} = \kappa \hat{\boldsymbol{n}} \tag{3}$$

$$\frac{\partial^3 \boldsymbol{r}}{\partial s^3} = \frac{\partial \kappa}{\partial s}\hat{\boldsymbol{n}} + \kappa\left(\tau\hat{\boldsymbol{b}} - \kappa\hat{\boldsymbol{t}}\right) \tag{4}$$

A circular curve has $\tau = 0$, $\frac{\partial \kappa}{\partial s} = 0$, and $\kappa \neq 0$. We want to penalize only the terms that a circle does not have.

$$\hat{\boldsymbol{t}} \times \frac{\partial^3 \boldsymbol{r}}{\partial s^3} = \frac{\partial \kappa}{\partial s}\hat{\boldsymbol{b}} - \kappa\tau\hat{\boldsymbol{n}} \tag{5}$$

$$c = \left|\hat{\boldsymbol{t}} \times \frac{\partial^3 \boldsymbol{r}}{\partial s^3}\right| \tag{6}$$

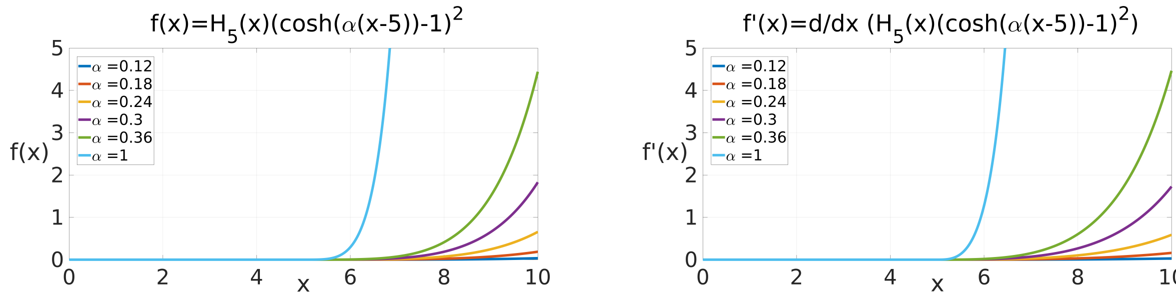
FOCUS can optimize for c through the objective function given in (7). This objective function can constrain the coil's maximum c by using the penalty functions p_1 and p_2 and it can optimize for an average c quantity. A coil is parameterized as $\boldsymbol{r}(\zeta)$ with $\zeta \in [0, 2\pi]$.

$$f_c = \frac{1}{N_c}\sum_{i=1}^{N_c}\frac{1}{L_i}\int_0^{2\pi}\left(p_{1,2}(c_i, c_0) + \sigma c_i^{\gamma}\right)\left|\boldsymbol{r_i}'\right| d\zeta \tag{7}$$

$$c_0 \geq 0 \qquad \sigma \geq 0 \qquad \gamma \geq 1$$

$$p_1(c, c_0) = H_{c_0}(c)\left(\cosh(\alpha(c - c_0)) - 1\right)^2 \tag{8}$$

$$\alpha \geq 0 \qquad c_0 \geq 0$$



(a) (b)

Figure 1: The function p_1 is plotted in (a) where the variable c is changed to x and the value of c_0 is set to 5. Multiple values of the penalty function variable, α are plotted. The derivative is plotted in (b).

$$p_2(c, c_0) = H_{c_0}(c)\left(\alpha(c - c_0)\right)^{\beta} \tag{9}$$

$$\alpha \geq 0 \qquad c_0 \geq 0 \qquad \beta \geq 2$$

$$H_{c_0}(c) \equiv H(c - c_0) = \begin{cases} 0, & c < c_0 \\ \frac{1}{2}, & c = c_0 \\ 1, & c > c_0 \end{cases} \tag{10}$$

First Derivatives

First derivatives of (7) are now given. Let λ_j be an optimization variable that defines the position of the j-th coil, $\boldsymbol{r_j}$ where $j \in \{1, 2, ..., N_c\}$. The coil length functional, L and its derivatives can be found in the length objective function documentation.

$$\frac{\partial f_c}{\partial \lambda_j} = \frac{-1}{N_c L_j^2}\frac{\partial L_j}{\partial \lambda_j}\int_0^{2\pi}\left(p_{1,2} + \sigma c_j^{\gamma}\right)\left|\boldsymbol{r_j}'\right| d\zeta + \frac{1}{N_c L_j}\int_0^{2\pi}\left(\frac{\partial p_{1,2}}{\partial c_j} + \sigma\gamma c_j^{\gamma-1}\right)\frac{\partial c_j}{\partial \lambda_j}\left|\boldsymbol{r_j}'\right| d\zeta + \frac{1}{N_c L_j}\int_0^{2\pi}\left(p_{1,2} + \sigma c_j^{\gamma}\right)\left|\boldsymbol{r_j}'\right|^{-1}\boldsymbol{r_j}' \cdot \frac{\partial \boldsymbol{r_j}'}{\partial \lambda_j} d\zeta \tag{11}$$

$$\frac{\partial p_1}{\partial c} = H_{c_0}(c)\, 2\alpha\left(\cosh(\alpha(c - c_0)) - 1\right)\sinh(\alpha(c - c_0)) \tag{12}$$

$$\frac{\partial p_2}{\partial c} = H_{c_0}(c)\beta\alpha\left(\alpha(c - c_0)\right)^{\beta - 1} \tag{13}$$

$$\frac{\partial c}{\partial \lambda} = \left(\left(\frac{\partial \kappa}{\partial s}\right)^2 + (\kappa\tau)^2\right)^{-1/2}\left(\frac{\partial \kappa}{\partial s}\frac{\partial^2 \kappa}{\partial \lambda\, \partial s} + \kappa\tau\frac{\partial(\kappa\tau)}{\partial \lambda}\right) \tag{14}$$

$$\kappa = \frac{|\boldsymbol{r}' \times \boldsymbol{r}''|}{|\boldsymbol{r}'|^3} \tag{15}$$

$$\tau = \frac{\boldsymbol{r}''' \cdot (\boldsymbol{r}' \times \boldsymbol{r}'')}{|\boldsymbol{r}' \times \boldsymbol{r}''|^2} \tag{16}$$

$$\kappa\tau = \frac{\boldsymbol{r}''' \cdot (\boldsymbol{r}' \times \boldsymbol{r}'')}{|\boldsymbol{r}'|^3 \, |\boldsymbol{r}' \times \boldsymbol{r}''|} \tag{17}$$

$$\frac{\partial \kappa}{\partial s} = \kappa' |\boldsymbol{r}'|^{-1} \tag{18}$$

$$\kappa = \frac{|\boldsymbol{r}' \times \boldsymbol{r}''|}{|\boldsymbol{r}'|^3} = \frac{|\boldsymbol{\omega}|}{|\boldsymbol{r}'|^3} \tag{19}$$

$$\kappa' = \left|\boldsymbol{r}'\right|^{-3} \hat{\boldsymbol{\omega}} \cdot \boldsymbol{\omega}' - 3\,|\boldsymbol{\omega}| \left|\boldsymbol{r}'\right|^{-5} \boldsymbol{r}' \cdot \boldsymbol{r}'' \tag{20}$$

$$\frac{\partial \kappa}{\partial s} = \left|\boldsymbol{r}'\right|^{-4} \hat{\boldsymbol{\omega}} \cdot \boldsymbol{\omega}' - 3\,|\boldsymbol{\omega}| \left|\boldsymbol{r}'\right|^{-6} \boldsymbol{r}' \cdot \boldsymbol{r}'' \tag{21}$$

$$\begin{aligned} \frac{\partial^2 \kappa}{\partial \lambda\, \partial s} = {} & \left|\boldsymbol{r}'\right|^{-4} \frac{\partial \hat{\boldsymbol{\omega}}}{\partial \lambda} \cdot \boldsymbol{\omega}' + \left|\boldsymbol{r}'\right|^{-4} \hat{\boldsymbol{\omega}} \cdot \frac{\partial \boldsymbol{\omega}'}{\partial \lambda} - 4 \left|\boldsymbol{r}'\right|^{-6} \boldsymbol{r}' \cdot \frac{\partial \boldsymbol{r}'}{\partial \lambda} \hat{\boldsymbol{\omega}} \cdot \boldsymbol{\omega}' - 3 \hat{\boldsymbol{\omega}} \cdot \frac{\partial \boldsymbol{\omega}}{\partial \lambda} \left|\boldsymbol{r}'\right|^{-6} \boldsymbol{r}' \cdot \boldsymbol{r}'' \\ & + 18\,|\boldsymbol{\omega}| \left|\boldsymbol{r}'\right|^{-8} \boldsymbol{r}' \cdot \frac{\partial \boldsymbol{r}'}{\partial \lambda} \boldsymbol{r}' \cdot \boldsymbol{r}'' - 3\,|\boldsymbol{\omega}| \left|\boldsymbol{r}'\right|^{-6} \left(\frac{\partial \boldsymbol{r}'}{\partial \lambda} \cdot \boldsymbol{r}'' + \boldsymbol{r}' \cdot \frac{\partial \boldsymbol{r}''}{\partial \lambda} \right) \end{aligned} \tag{22}$$

$$\tau = \frac{\boldsymbol{\omega} \cdot \boldsymbol{r}'''}{|\boldsymbol{\omega}|^2} = \frac{\hat{\boldsymbol{\omega}} \cdot \boldsymbol{r}'''}{|\boldsymbol{\omega}|} \tag{23}$$

$$\kappa\tau = \frac{\hat{\boldsymbol{\omega}} \cdot \boldsymbol{r}'''}{|\boldsymbol{r}'|^3} \tag{24}$$

$$\frac{\partial (\kappa\tau)}{\partial \lambda} = \frac{\partial \hat{\boldsymbol{\omega}}}{\partial \lambda} \cdot \boldsymbol{r}''' |\boldsymbol{r}'|^{-3} + \hat{\boldsymbol{\omega}} \cdot \frac{\partial \boldsymbol{r}'''}{\partial \lambda} |\boldsymbol{r}'|^{-3} - 3 \hat{\boldsymbol{\omega}} \cdot \boldsymbol{r}''' |\boldsymbol{r}'|^{-5} \boldsymbol{r}' \cdot \frac{\partial \boldsymbol{r}'}{\partial \lambda} \tag{25}$$

$$\frac{\partial \hat{\boldsymbol{\omega}}}{\partial \lambda} = \frac{\partial \boldsymbol{\omega}}{\partial \lambda} |\boldsymbol{\omega}|^{-1} - \boldsymbol{\omega} |\boldsymbol{\omega}|^{-3} \boldsymbol{\omega} \cdot \frac{\partial \boldsymbol{\omega}}{\partial \lambda} \tag{26}$$

$$\frac{\partial \boldsymbol{\omega}}{\partial \lambda} = \frac{\partial \boldsymbol{r}'}{\partial \lambda} \times \boldsymbol{r}'' + \boldsymbol{r}' \times \frac{\partial \boldsymbol{r}''}{\partial \lambda} \tag{27}$$

$$\boldsymbol{\omega}' = \boldsymbol{r}' \times \boldsymbol{r}''' \tag{28}$$

$$\frac{\partial \boldsymbol{\omega}'}{\partial \lambda} = \frac{\partial \boldsymbol{r}'}{\partial \lambda} \times \boldsymbol{r}''' + \boldsymbol{r}' \times \frac{\partial \boldsymbol{r}'''}{\partial \lambda} \tag{29}$$

Notes

The above derivative equations do not use functional derivatives. Functional derivatives for this objective function are very complicated and due to that complexity are not implemented in FOCUS. FOCUS has the above derivatives implemented for a Fourier parameterized coil. There is some development work required if one wants to use a different parameterization.

How to Use

To use this objective functions, a weight, "weight_nis", needs to be set. This variable and all other variables in this section are set in the "*.input" file. No changes to the "*.focus" file are necessary. An integer named "penfun_nis" can be set to 1 or 2 and determines which penalty function is used. The value of c_0 is set by the variable "nis0". The values of α, β, γ, and σ are set by the variables "nis_alpha", "nis_beta", "nis_gamma", and "nis_sigma".