

Supplementary for MICCAI 2014 paper titled: “Splines for diffeomorphic image regression”

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Abstract. This document contains additional material supplementary to the main article. It contains the derivations of the variations of the energy functional presented in the main article. In particular, we cover the details for deriving the Euler-Lagrange equations for the relaxation problem on Diffeomorphisms as well as discuss the derivation for its shooting extension. We also provide additional results such as the visualizations for the estimated initial conditions that could not be included in the main article due to space constraints.

A Euler-Lagrange for relaxation problem

We solve the Euler-Lagrange equation in the context of regression problem. The energy takes the form,

$$E(g, m, v, u, I(0)) = \frac{1}{2\sigma^2} \sum_{i=1}^N \|I(0) \circ g^{-1}(t_i) - J_i\|_{L^2} + \frac{1}{2} \int_0^1 \|u(t)\|_{\mathfrak{g}}^2 dt \quad (1)$$

The corresponding constrained energy minimization problem is,

$$\begin{aligned} & \underset{g, m, v, u, I(0)}{\text{minimize}} && E(g, m, v, u, I(0)) \\ & \text{subject to control} && u(t) - \dot{m}(t) - \text{ad}_{v(t)}^* m(t) = 0 \\ & \text{subject to right action} && \dot{g}(t) = v \circ g(t) \\ & \text{subject to image evolution} && I(t) = I(0) \circ g^{-1}(t) \\ & \text{subject to momenta duality} && v(t) = K \star m(t) \end{aligned} \quad (2)$$

The right action and the image evolution constraint above can be combined to write image evolution constraint as an image advection,

$$\begin{aligned} & \underset{m, v, u, I}{\text{minimize}} && E(m, v, u, I) \\ & \text{subject to control} && u(t) - \dot{m}(t) - \text{ad}_{v(t)}^* m(t) = 0 \\ & \text{subject to image advection} && \dot{I}(t) + DI(t) \cdot v(t) = 0 \\ & \text{subject to momenta duality} && v(t) - K \star m(t) = 0 \end{aligned} \quad (3)$$

$DI(t)$ represents the Jacobian of $I(t)$ and,

$$E(m, v, I) = \frac{1}{2\sigma^2} \sum_{i=1}^N \|I(t_i) - J_i\|_{L^2} + \frac{1}{2} \int_0^1 \|u(t)\|_{\mathfrak{g}}^2 dt \quad (4)$$

The unconstrained Lagrangian takes the form,

$$E(m, v, I, \lambda_1, \lambda_2, \lambda_3) = \frac{1}{2\sigma^2} \sum_{i=1}^N \|I(t_i) - J_i\|_{L^2} + \frac{1}{2} \int_0^1 \|u\|_{\mathfrak{g}}^2 dt \quad (5)$$

$$+ \int_0^1 \langle \lambda_1, u - \dot{m} - \text{ad}_v^* m \rangle_{L^2} dt \quad (6)$$

$$+ \int_0^1 \langle \lambda_2, \dot{I} + DI \cdot v \rangle_{L^2} dt \quad (7)$$

$$+ \int_0^1 \langle \lambda_3, v - K \star m \rangle_{L^2} dt \quad (8)$$

A.1 Variations:

In what follows, unless specified, all inner products correspond to L^2 pairing. Computing variations of E with respect to adjoint variables will give us the dynamic constraints back. Computing variations of E with respect to all state variables give,

$$\delta_m E = -\langle \lambda_1(1), \delta m(1) \rangle + \langle \lambda_1(0), \delta m(0) \rangle \quad (9)$$

$$+ \int_0^1 \langle \dot{\lambda}_1, \delta m \rangle dt - \int_0^1 \langle \text{ad}_v \lambda_1, \delta m \rangle dt - \int_0^1 \langle K \star \lambda_3, \delta m \rangle dt \quad (10)$$

$$\delta_v E = \int_0^1 \langle \text{ad}_{\lambda_1}^* m, \delta v \rangle dt + \int_0^1 \langle \lambda_2 DI, \delta v \rangle + \int_0^1 \langle \lambda_3, \delta v \rangle dt \quad (11)$$

$$\delta_u E = \int_0^1 \langle K \star u, \delta u \rangle dt + \int_0^1 \langle \lambda_1, \delta u \rangle dt \quad (12)$$

$$\delta_I E = \frac{1}{\sigma^2} \sum_{i=1}^N \langle \delta I(t_i), I(t_i) - J_i \rangle + \langle \lambda_2(1), \delta I(1) \rangle - \langle \lambda_2(0), \delta I(0) \rangle \quad (13)$$

$$- \int_0^1 \langle \dot{\lambda}_2, \delta I \rangle - \int_0^1 \langle \nabla \cdot (\lambda_2 v), \delta I \rangle \quad (14)$$

At the optimum the above must vanish. This results in the following adjoint system,

$$\dot{\lambda}_1 - \text{ad}_v \lambda_1 - K \star \lambda_3 = 0 \quad (15)$$

$$\text{ad}_{\lambda_1}^* m + \lambda_2 DI + \lambda_3 = 0 \quad (16)$$

$$K \star u + \lambda_1 = 0 \quad (17)$$

$$-\dot{\lambda}_2 - \nabla \cdot (\lambda_2 v) = 0 \quad (18)$$

with jumps in λ_2 as $\lambda_2(t_i^+) - \lambda_2(t_i^-) = \frac{1}{\sigma^2}(I(t_i) - J_i)$ at measurements, $t = t_i$. The boundary conditions are,

$$\delta_{m(0)} = \lambda_1(0) \quad (19)$$

$$\delta_{m(1)} = -\lambda_1(1) \quad (20)$$

We eliminate λ_1 from the above equations using $\lambda_1 = -K \star u$, to get,

$$-K \star (\dot{u} + \lambda_3) + \text{ad}_v K \star u = 0 \quad (21)$$

$$-\text{ad}_{K \star u}^* m + \lambda_2 DI + \lambda_3 = 0 \quad (22)$$

$$-\dot{\lambda}_2 - \nabla \cdot (\lambda_2 v) = 0 \quad (23)$$

The above elimination uses the fact that the kernel, K , is independent of time.

Further, we eliminate λ_3 using $\lambda_3 = \text{ad}_{K \star u}^* m - \lambda_2 DI$ and apply K^{-1} throughout, to get,

$$\dot{u} - \lambda_2 DI + \text{ad}_{K \star u}^* m - K^{-1} \text{ad}_v K \star u = 0 \quad (24)$$

$$-\dot{\lambda}_2 - \nabla \cdot (\lambda_2 v) = 0 \quad (25)$$

We write the above in \mathfrak{g} instead of in \mathfrak{g}^* . For this define, $f \in \mathfrak{g}$ which is dual to u , such that, $f = K \star u$. The adjoint system takes the form,

$$\dot{f} - K \star \lambda_2 DI + K \star \text{ad}_f^* m - \text{ad}_v f = 0 \quad (26)$$

$$-\dot{\lambda}_2 - \nabla \cdot (\lambda_2 v) = 0 \quad (27)$$

And since the conjugate operator, ad_X^\dagger is $\text{ad}_X^\dagger = K \star \text{ad}_X^* L$, we write,

$$\dot{f} - K \star \lambda_2 DI + \text{ad}_f^\dagger v - \text{ad}_v f = 0 \quad (28)$$

$$-\dot{\lambda}_2 - \nabla \cdot (\lambda_2 v) = 0 \quad (29)$$

B Euler-Lagrange for shooting problem

Let, J_i , for $i = 1 \dots N$, denote N measured images at timepoints, $t_i \in (0, 1)$. Let us assume there are no measurements at the end points, i.e., neither at $t = 0$, nor at $t = 1$. Let $t_c \in (0, 1)$, for $c = 1 \dots C$, denote C data-independent fixed control locations. The control locations also implicitly define $C + 1$ intervals or partitions in $(0, 1)$. Let us denote these intervals as \mathcal{I}_c , for $c = 1 \dots (C + 1)$.

For regression on such a data configuration, the least-squares energy takes the form,

$$E(I) = \frac{1}{2\sigma^2} \sum_{c=1}^{C+1} \sum_{i \in \mathcal{I}_c} \|I(t_i) - J_i\|_{L^2} \quad (30)$$

Note, the L^2 metric on images here can be replaced with the metric on G . Here we will keep this simpler, and derive it for the L^2 metric.

We first write the constrained energy minimization problem as,

$$\begin{array}{ll}
\underset{I}{\text{minimize}} & E(I) \\
\text{subject to velocity evolution} & \dot{v} - f + \text{ad}_v^\dagger v = 0 \\
\text{subject to force evolution} & \dot{f} - K \star PDI + \text{ad}_f^\dagger v - \text{ad}_v f = 0 \\
\text{subject to P evolution} & \dot{P} + \nabla \cdot (Pv) = 0 \\
\text{subject to image advection} & \dot{I} + DI \cdot v = 0 \\
\text{subject to continuity of } v, f, \text{ and } I \text{ at } C \text{ joins} &
\end{array} \left. \vphantom{\begin{array}{l} \\ \\ \\ \\ \\ \end{array}} \right\} \text{Within each interval, } \mathcal{I}_c \tag{31}$$

Notice we could also write the energy minimization problem in terms of duals of v, f ,

$$\begin{array}{ll}
\underset{I}{\text{minimize}} & E(I) \\
\text{subject to momenta evolution} & \dot{m} - u + \text{ad}_v^* m = 0 \\
\text{subject to control evolution} & \dot{u} - PDI + \text{ad}_f^* m - K^{-1} \text{ad}_v f = 0 \\
\text{subject to P evolution} & \dot{P} + \nabla \cdot (Pv) = 0 \\
\text{subject to image advection} & \dot{I} + DI \cdot v = 0 \\
\text{subject to momenta duality} & v - K \star m = 0 \\
\text{subject to control duality} & f - K \star u = 0 \\
\text{subject to continuity of } m, u, \text{ and } I \text{ at } C \text{ joins} &
\end{array} \left. \vphantom{\begin{array}{l} \\ \\ \\ \\ \\ \\ \end{array}} \right\} \text{Within each interval, } \mathcal{I}_c \tag{32}$$

The above avoids the ad^\dagger conjugate operator but uses additional duality conditions. For this derivation, let us use (32) instead of (31).

The unconstrained Lagrangian takes the form,

$$\begin{aligned}
E(m, u, P, I, v, f, \lambda_m, \lambda_u, \lambda_P, \lambda_I, \lambda_f, \lambda_v) &= \frac{1}{2\sigma^2} \sum_{c=1}^{C+1} \sum_{i \in \mathcal{I}_c} \|I(t_i) - J_i\|_{L^2}^2 \\
&+ \sum_{c=1}^{C+1} \int_0^1 \langle \lambda_{m_c}, \dot{m}_c - u_c + \text{ad}_{v_c}^* m_c \rangle_{L^2} dt \\
&+ \sum_{c=1}^{C+1} \int_0^1 \langle \lambda_{u_c}, \dot{u}_c - P_c D I_c + \text{ad}_{f_c}^* m_c - K^{-1} \text{ad}_{v_c} f_c \rangle_{L^2} dt \\
&+ \sum_{c=1}^{C+1} \int_0^1 \langle \lambda_{P_c}, \dot{P}_c + \nabla \cdot (P_c v_c) \rangle_{L^2} dt \\
&+ \sum_{c=1}^{C+1} \int_0^1 \langle \lambda_{I_c}, \dot{I}_c + D I_c \cdot v_c \rangle_{L^2} dt \\
&+ \sum_{c=1}^{C+1} \int_0^1 \langle \lambda_{v_c}, v_c - K \star m_c \rangle_{L^2} dt \\
&+ \sum_{c=1}^{C+1} \int_0^1 \langle \lambda_{f_c}, f_c - K \star u_c \rangle_{L^2} dt \\
&+ \text{subject to continuity of } m, u, \text{ and } I \text{ at } C \text{ joins}
\end{aligned}$$

B.1 Variations

We discuss each piece of this optimization separately and combine the result in the end of this section. It is easy to first derive it without the data terms. The unconstrained Lagrangian takes the form,

$$\begin{aligned}
E(m, u, P, I, v, f, \lambda_m, \lambda_u, \lambda_P, \lambda_I, \lambda_v, \lambda_f) &= + \int_0^1 \langle \lambda_m, \dot{m} - u + \text{ad}_v^* m \rangle_{L^2} dt \\
&+ \int_0^1 \langle \lambda_u, \dot{u} - P D I + \text{ad}_f^* m - K^{-1} \text{ad}_v f \rangle_{L^2} dt \\
&+ \int_0^1 \langle \lambda_P, \dot{P} + \nabla \cdot (P v) \rangle_{L^2} dt \\
&+ \int_0^1 \langle \lambda_I, \dot{I} + D I \cdot v \rangle_{L^2} dt \\
&+ \int_0^1 \langle \lambda_v, v - K \star m \rangle_{L^2} dt \\
&+ \int_0^1 \langle \lambda_f, f - K \star u \rangle_{L^2} dt
\end{aligned}$$

We write the variations with respect to all the primals as:

$$\begin{aligned}
\delta_m E &= \langle \lambda_m(1), \delta m(1) \rangle - \langle \lambda_m(0), \delta m(0) \rangle \\
&\quad - \int_0^1 \langle \dot{\lambda}_m, \delta m \rangle dt + \int_0^1 \langle \text{ad}_v \lambda_m, \delta m \rangle dt + \int_0^1 \langle \text{ad}_f \lambda_u, \delta m \rangle dt - \int_0^1 \langle K \star \lambda_v, \delta m \rangle dt \\
\delta_u E &= \langle \lambda_u(1), \delta u(1) \rangle - \langle \lambda_u(0), \delta u(0) \rangle \\
&\quad - \int_0^1 \langle \lambda_m, \delta u \rangle dt - \int_0^1 \langle \dot{\lambda}_u, \delta u \rangle dt - \int_0^1 \langle K \star \lambda_f, \delta u \rangle dt \\
\delta_P E &= \langle \lambda_P(1), \delta P(1) \rangle - \langle \lambda_P(0), \delta P(0) \rangle \\
&\quad - \int_0^1 \langle DI \cdot \lambda_u, \delta P \rangle dt - \int_0^1 \langle \dot{\lambda}_P, \delta P \rangle dt - \int_0^1 \langle D\lambda_P \cdot v, \delta P \rangle dt \\
\delta_I E &= \langle \lambda_I(1), \delta I(1) \rangle - \langle \lambda_I(0), \delta I(0) \rangle \\
&\quad - \int_0^1 \langle \dot{\lambda}_I, \delta I \rangle dt - \int_0^1 \langle \nabla \cdot (\lambda_I v), \delta I \rangle dt + \int_0^1 \langle \nabla \cdot (P\lambda_u), \delta I \rangle dt \\
\delta_v E &= - \int_0^1 \langle \text{ad}_{\lambda_m}^* m, \delta v \rangle dt + \int_0^1 \langle \text{ad}_f^* K^{-1} \lambda_u, \delta v \rangle dt + \int_0^1 \langle \lambda_I DI, \delta v \rangle dt + \int_0^1 \langle \lambda_v, \delta v \rangle dt \\
\delta_f E &= - \int_0^1 \langle \text{ad}_{\lambda_u}^* m, \delta f \rangle dt - \int_0^1 \langle \text{ad}_v^* K^{-1} \lambda_u, \delta f \rangle dt + \int_0^1 \langle \lambda_f, \delta f \rangle dt
\end{aligned}$$

At the optimum, the above must vanish. This results in the following adjoint system:

$$-\dot{\lambda}_m + \text{ad}_v \lambda_m + \text{ad}_f \lambda_u - K \star \lambda_v = 0 \quad (33)$$

$$-\lambda_m - \dot{\lambda}_u - K \star \lambda_f = 0 \quad (34)$$

$$-DI \cdot \lambda_u - \dot{\lambda}_P - D\lambda_P \cdot v = 0 \quad (35)$$

$$-\dot{\lambda}_I - \nabla \cdot (\lambda_I v) + \nabla \cdot (P\lambda_u) = 0 \quad (36)$$

$$-\text{ad}_{\lambda_m}^* m + \text{ad}_f^* K^{-1} \lambda_u + \lambda_I DI + \lambda_v = 0 \quad (37)$$

$$-\text{ad}_{\lambda_u}^* m - \text{ad}_v^* K^{-1} \lambda_u + \lambda_f = 0 \quad (38)$$

The boundary conditions are,

$$\delta_{m(0)} E = -\lambda_m(0) \quad (39)$$

$$\delta_{m(1)} E = \lambda_m(1) \quad (40)$$

$$\delta_{u(0)} E = -\lambda_u(0) \quad (41)$$

$$\delta_{u(1)} E = \lambda_u(1) \quad (42)$$

$$\delta_{P(0)} E = -\lambda_P(0) \quad (43)$$

$$\delta_{P(1)} E = \lambda_P(1) \quad (44)$$

$$\delta_{I(0)} E = -\lambda_I(0) \quad (45)$$

$$\delta_{I(1)} E = \lambda_I(1) \quad (46)$$

We eliminate some variables from the above adjoint system. First we use, $\lambda_f = \text{ad}_{\lambda_u}^* m + \text{ad}_v^* K^{-1} \lambda_u$,

$$-\dot{\lambda}_m + \text{ad}_v \lambda_m + \text{ad}_f \lambda_u - K \star \lambda_v = 0 \quad (47)$$

$$-\lambda_m - \dot{\lambda}_u - \text{ad}_{\lambda_u}^\dagger v - \text{ad}_v^\dagger \lambda_u = 0 \quad (48)$$

$$-DI \cdot \lambda_u - \dot{\lambda}_P - D\lambda_P \cdot v = 0 \quad (49)$$

$$-\dot{\lambda}_I - \nabla \cdot (\lambda_I v) + \nabla \cdot (P\lambda_u) = 0 \quad (50)$$

$$-\text{ad}_{\lambda_m}^* m + \text{ad}_f^* K^{-1} \lambda_u + \lambda_I DI + \lambda_v = 0 \quad (51)$$

Next we use, $\lambda_v = \text{ad}_{\lambda_m}^* m - \text{ad}_f^* K^{-1} \lambda_u - \lambda_I DI$, and rearrange the terms to get,

$$\dot{\lambda}_m + \text{ad}_{\lambda_m} v + \text{ad}_{\lambda_m}^\dagger v - \text{ad}_f \lambda_u - \text{ad}_f^\dagger \lambda_u - K \star \lambda_I DI = 0 \quad (52)$$

$$\dot{\lambda}_u + \lambda_m + \text{ad}_{\lambda_u}^\dagger v + \text{ad}_v^\dagger \lambda_u = 0 \quad (53)$$

$$\dot{\lambda}_P + DI \cdot \lambda_u + D\lambda_P \cdot v = 0 \quad (54)$$

$$\dot{\lambda}_I + \nabla \cdot (\lambda_I v) - \nabla \cdot (P\lambda_u) = 0 \quad (55)$$

For dynamics and data fit constraints: We have presented the variations for the similar energy functional as above but in the general case of single interval without any data. The data fit constraints results in jumps in the backward integration of the adjoint variable, λ_{Ic} .

For continuity constraints: We derive the variations of the energy functional for the joins and study the continuity of the adjoint system in the interval $(0, 1)$. We first rewrite the above functional here as,

$$E = + \text{fit of the data within each interval, } \mathcal{I}_c \quad (56)$$

$$+ \text{dynamics within each interval, } \mathcal{I}_c \quad (57)$$

$$+ \sum_{c=1}^C \langle \alpha_{mc}, m_c(t_c) - m_{c+1}(t_c) \rangle_{L^2} \quad (58)$$

$$+ \sum_{c=1}^C \langle \alpha_{uc}, u_c(t_c) - u_{c+1}(t_c) \rangle_{L^2} \quad (59)$$

$$+ \sum_{c=1}^C \langle \alpha_{Ic}, I_c(t_c) - I_{c+1}(t_c) \rangle_{L^2} \quad (60)$$

We write the variations with respect to all the primals at joins as:

$$\delta_{m_c(t_c)}E = \lambda_{m_c}(t_c) + \alpha_m \quad (61)$$

$$\delta_{m_{c+1}(t_c)}E = -\lambda_{m_{c+1}}(t_c) - \alpha_m \quad (62)$$

$$\delta_{u_c(t_c)}E = \lambda_{u_c}(t_c) + \alpha_u \quad (63)$$

$$\delta_{u_{c+1}(t_c)}E = -\lambda_{u_{c+1}}(t_c) - \alpha_u \quad (64)$$

$$\delta_{I_c(t_c)}E = \lambda_{I_c}(t_c) + \alpha_I \quad (65)$$

$$\delta_{I_{c+1}(t_c)}E = -\lambda_{I_{c+1}}(t_c) + \alpha_I \quad (66)$$

Equating all the above variations to zero and eliminating variables, we get,

$$\lambda_{m_c}(t_c) = \lambda_{m_{c+1}}(t_c) \quad (67)$$

$$\lambda_{u_c}(t_c) = \lambda_{u_{c+1}}(t_c) \quad (68)$$

$$\lambda_{I_c}(t_c) = \lambda_{I_{c+1}}(t_c) \quad (69)$$

This means that λ_{m_c} , λ_{u_c} and λ_{I_c} are continuous at the boundaries of the control point locations.

Gradient computation using backward integration We summarize the optimization here. The gradients with respect to the initial conditions are,

$$\delta_{m_1(0)}E = -\lambda_{m_1}(0) \quad (70)$$

$$\delta_{u_1(0)}E = -\lambda_{u_1}(0) \quad (71)$$

$$\delta_{P_1(0)}E = -\lambda_{P_1}(0) \quad (72)$$

$$\delta_{I_1(0)}E = -\lambda_{I_1}(0) \quad (73)$$

We compute the gradients by integrating the adjoint system of equations within each interval backward in time,

$$\dot{\lambda}_{m_c} + \text{ad}_{\lambda_{m_c}} v_c + \text{ad}_{\lambda_{m_c}}^\dagger v_c - \text{ad}_{f_c} \lambda_{u_c} - \text{ad}_{f_c}^\dagger \lambda_{u_c} - K \star \lambda_{I_c} D I_c = 0 \quad (74)$$

$$\dot{\lambda}_{u_c} + \lambda_{m_c} + \text{ad}_{\lambda_{u_c}}^\dagger v_c + \text{ad}_{v_c}^\dagger \lambda_{u_c} = 0 \quad (75)$$

$$\dot{\lambda}_{P_c} + D I_c \cdot \lambda_{u_c} + D \lambda_{P_c} \cdot v_c = 0 \quad (76)$$

$$\dot{\lambda}_{I_c} + \nabla \cdot (\lambda_{I_c} v_c) - \nabla \cdot (P_c \lambda_{u_c}) = 0 \quad (77)$$

All variables start from zero as their initial conditions for this backward integration.

Note 1. true for non-periodic case only We add jumps in λ_I as $\lambda_{I_c}(t_i^+) - \lambda_{I_c}(t_i^-) = \frac{1}{\sigma^2}(I_c(t_i) - J_i)$ at measurements, $t = t_i$. We ensure the continuity of λ_{m_c} , λ_{u_c} , and λ_{I_c} at the joins. However, λ_{P_c} starts from zero at every join.

The accumulated $\lambda_{P_{c+1}}$ is used to update the $P_c(t_k)$ as per the gradient,

$$\delta_{P_{c+1}(t_c)}E = -\lambda_{P_{c+1}}(t_c) \quad (78)$$

Note this is the ‘data independent’ control that we motivated our formulation with. This determines the initial condition of the forward system for each interval and needs to be estimated by gradient descent.

C Supplementary results

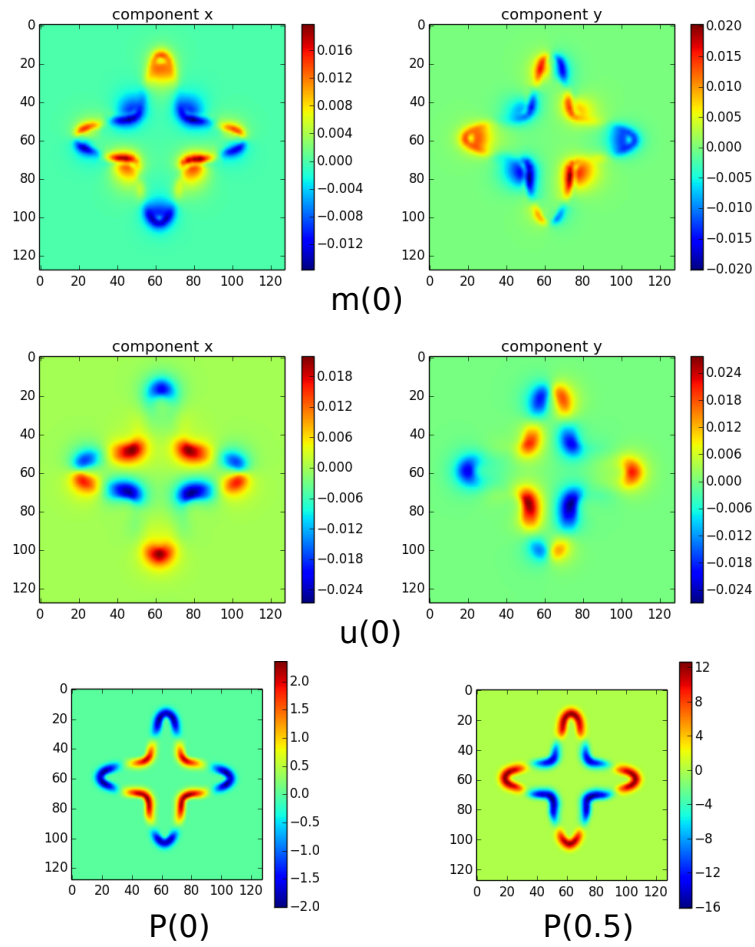


Fig. 1: Estimated states for regression using splines with one control for synthetic data. Top row: initial momenta at $t=0$. Middle row: initial acceleration or control at $t=0$. Bottom left: jerk at $t=0$, and bottom right: jerk at $t=0.5$.

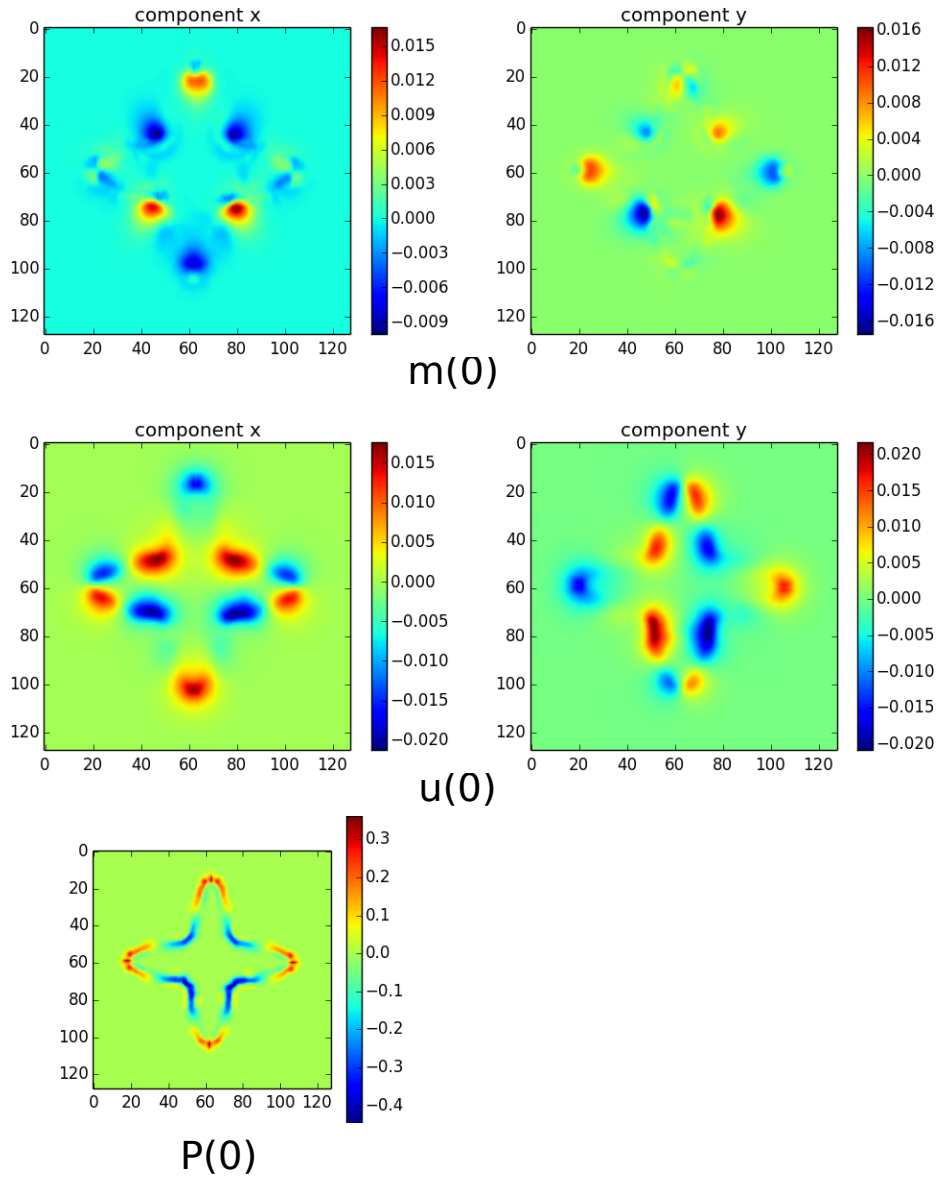


Fig. 2: Estimated states for regression using splines without control for synthetic data. Top row: initial momenta at $t=0$. Middle row: initial acceleration or control at $t=0$. Bottom left: jerk at $t=0$.

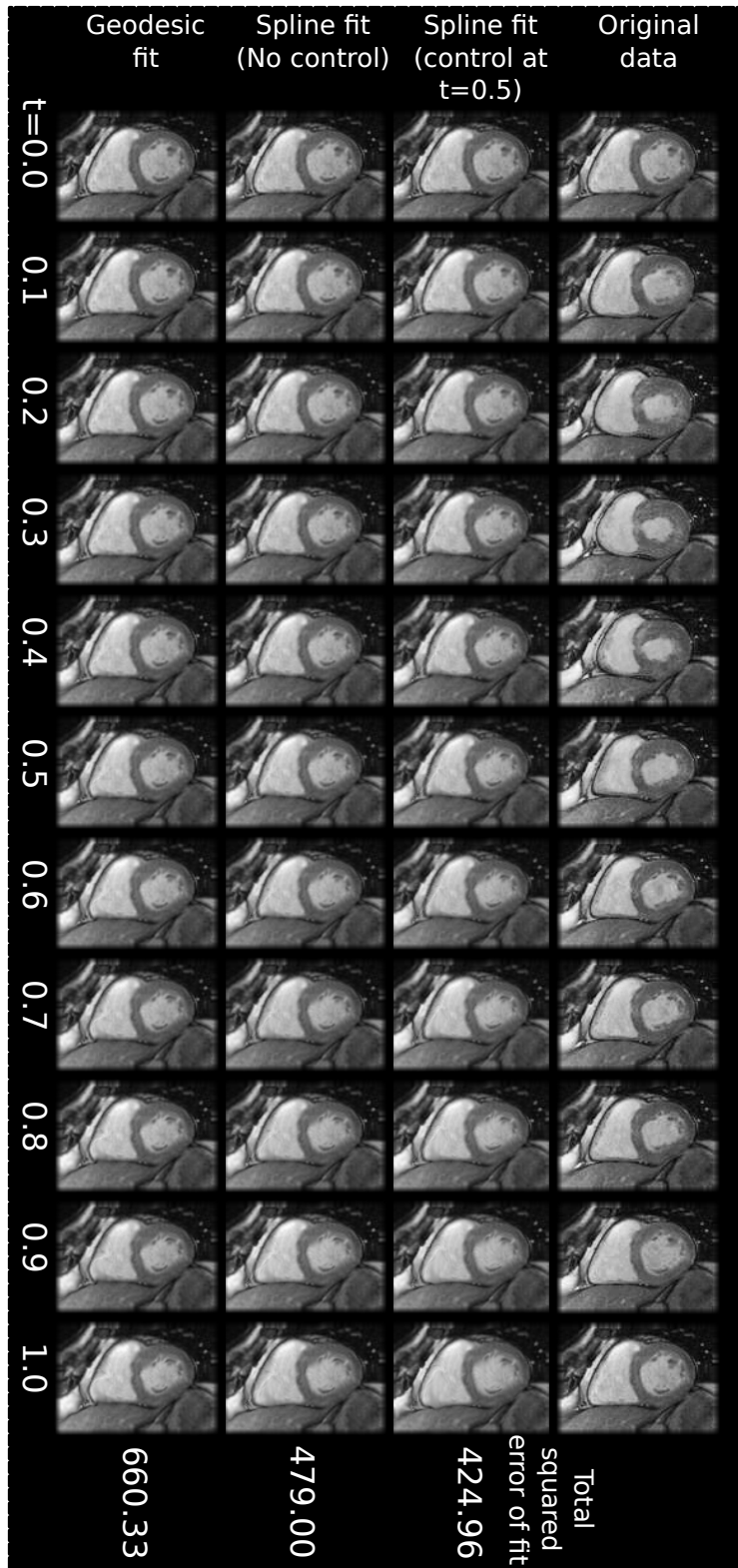


Fig. 3: Full-page version of spline regression results on cardiac MRI breathing data.

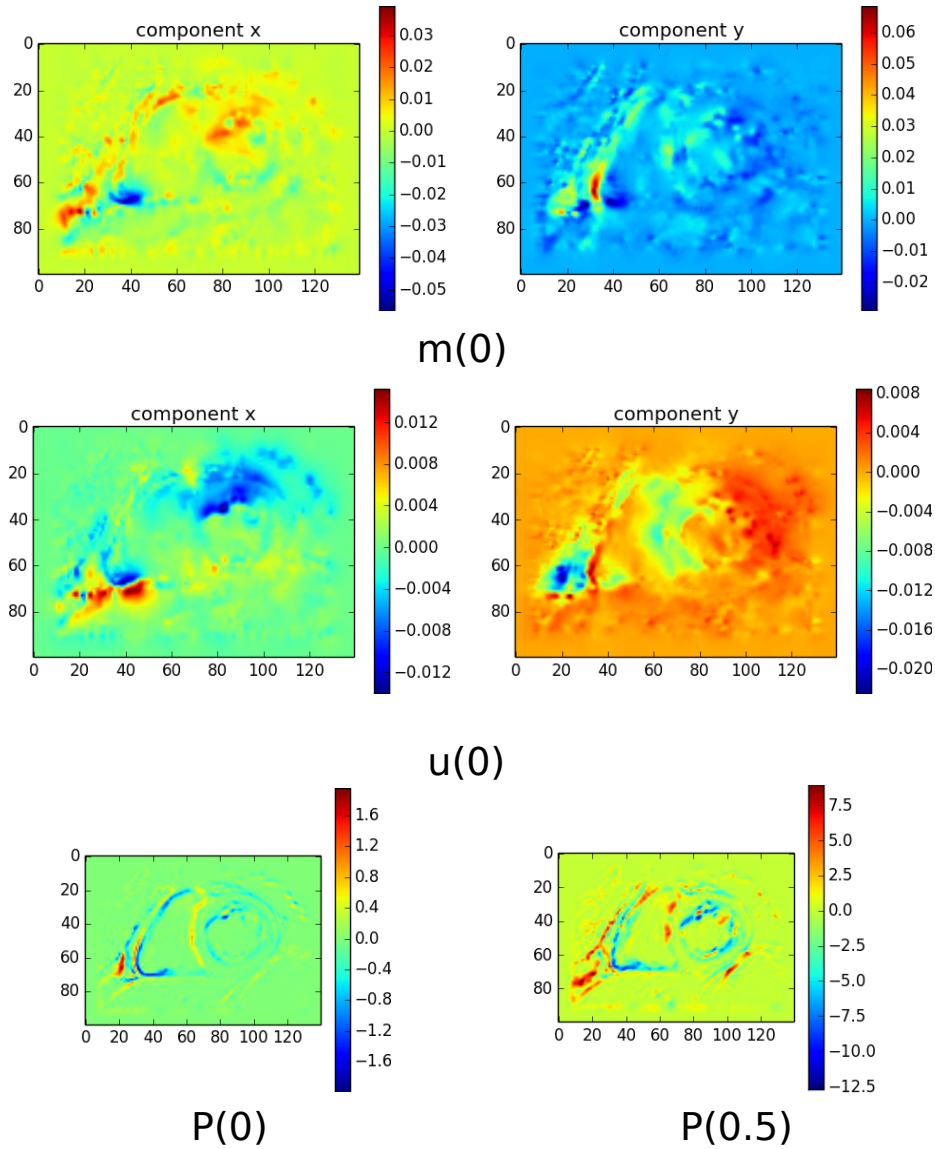


Fig. 4: Estimated states for regression using splines with one control for cardiac data. Top row: initial momenta at $t=0$. Middle row: initial acceleration or control at $t=0$. Bottom left: jerk at $t=0$, and bottom right: jerk at $t=0.5$.

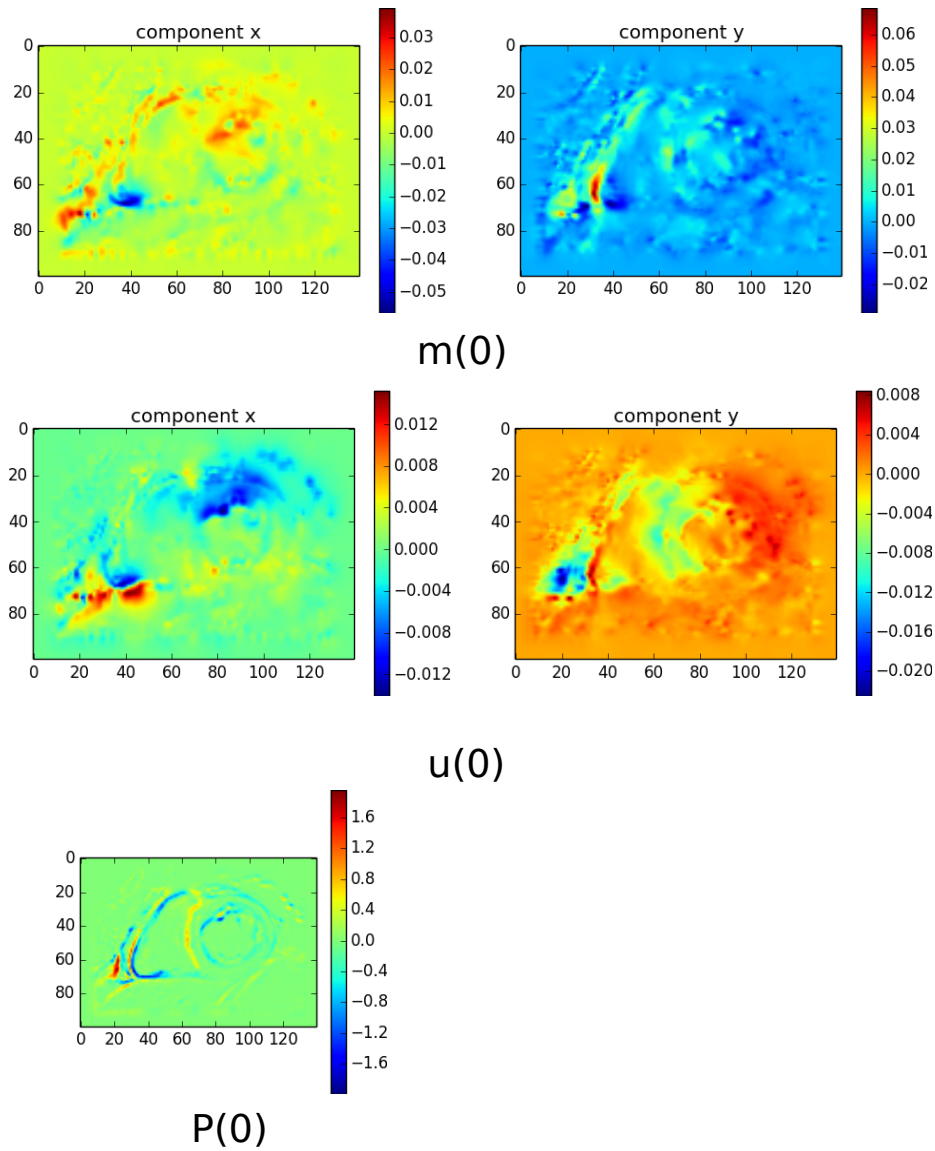


Fig. 5: Estimated states for regression using splines without control for cardiac data. Top row: initial momenta at $t=0$. Middle row: initial acceleration or control at $t=0$. Bottom left: jerk at $t=0$.