

Patient-Specific Finite Element Modeling of Idiopathic Scoliosis by Optimization Method

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Abstract

The main goal of the present study is to develop a method to construct patient-specific finite element model of idiopathic scoliosis from X-rays CT images by morphing a normal finite element model of spine. Firstly, to construct patient-specific finite element model, surface of CT image was extracted by image processing method. Extracted surface was then given as zero equivalent surface in voxel and defined over 3D signed distance image. Within the region of finite element model, parametric shape fitting problem was solved to find the least integration value of 3D signed distance image function and determined the skeletal shape of vertebrae. Then, the density of finite element spine model was defined as design variable and finite element model was assumed as elastic body. Nonparametric shape fitting problem was solved by determining the least value of sum of square error analysis for nodes of normal finite element spine model and previously determined vertebrae in parametric shape fitting problem before complete patient-specific finite element spine model was obtained. As results, density, displacement from the normal finite element model and strain of the patient finite element model were obtained from clinical X-rays CT image data using the developed computer program. Moreover, the effect of force weight, α was also investigated to improve the fitting results. The results showed that effect of α played a significant role in order to acquire better results.

Keywords: *Idiopathic Scoliosis, Patient-specific modeling, Shape fitting problem, H^1 gradient method*

1. Introduction

Idiopathic scoliosis is a three-dimensional deviation of the spine and rib cage, which develops in most cases during adolescence and accounting for more than 80% of idiopathic cases [?], which can lead to functional impairment. The deformity involves a lateral deviation of the spine from the middle in the coronal plane, rotation in the axial plane and decreased curvature in the thoracic area in the sagittal plane. The scoliotic deformity is usually quantified radio-graphically using the Cobb angle [?], a two-dimensional parameter measured in the frontal plane that only suffices for a superficial description of the scoliosis. Bracing or casting is preferred as a treatment when progressive scoliosis is diagnosed at early stage (Cobb angle 20° - 35°) while surgery is required at skeletal maturity in severe scoliosis case (Cobb angle higher than 45°) [?]. Patient-specific model can be used in both treatments. This model can help to better understand the mechanism of bracing [?] and to optimal the bracing or casting treatment whereas can help surgeons plan surgical intervention and optimized surgical treatment outcomes [?]. To study scoliosis pathomechanics and treatments, it is important to assess the geometric deformity and to analyze the material properties and stresses within the spine [?]. Finite element modeling has been used in spine research since about 50 years ago [?] to study the outcomes of scoliotic surgery, the etiology of scoliosis, biomechanics of scoliosis progression and biomechanics of bracing [?]. In this study, focus is given on etiological study of idiopathic scoliosis. Basically, there are 2 approaches in etiological investigation using finite element model in idiopathic scoliosis. Firstly, etiological investigation based on hypotheses in which the cause of scoliosis is presumed as buckling phenomenon in growth of vertebrae. In this approach, buckling analysis is conducted to replicate the deformity of spine [?, ?]. Secondly, etiological investigation based on finite element analysis of deformed shape in patient's spine model. This approach is suitably used when the first one fails to replicate the deformity in spine model. For example, in case of shape information of patient model is known, hypotheses can be constructed from the mapping of normal spine model to patient model and its strain. In this study, second approach is employed. The main goal is to construct the patient-specific finite element spine model and conduct the strain analysis to investigate the etiology of idiopathic scoliosis. Therefore, in this paper, focus is given on construction of patient-specific finite element spine model using both parametric and nonparametric optimization method.

2. Methodology

In this study, 2 steps of optimization problem namely parametric shape fitting problem and density type nonparametric shape fitting problem are introduced to construct the patient-specific finite element modeling from X-rays CT images.

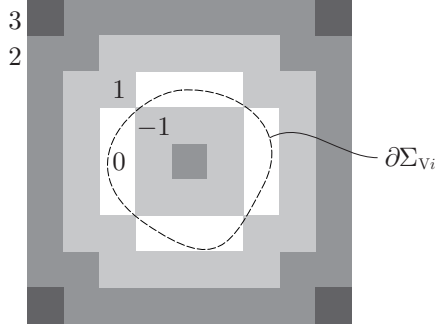


Figure 1. Assignment of signed distance d_i from voxel data

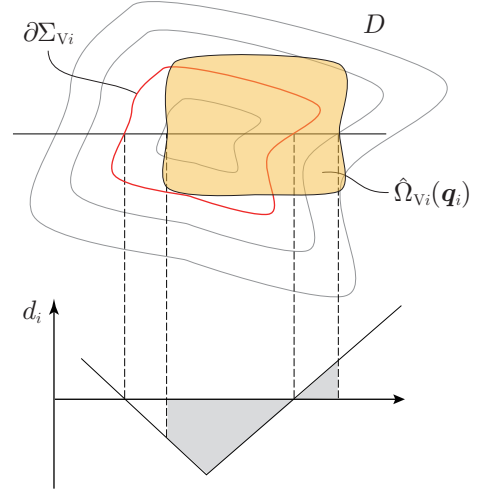


Figure 2. Image of parametric shape fitting problem

2.1. Parametric shape fitting problem

Let us define notations for a CT image and a normal spine finite-element model in the following way.

- (1) Let $D \subset \mathbb{R}^3$ be the domain of the X-rays CT images. $\mathcal{V} = \{C2, \dots, C7, T1, \dots, T12, L1, \dots, L5\}$ and $\mathcal{I} = \{C2-C3, \dots, L4-L5\}$ denote the sets of overall numbers of vertebrae and inter-vertebral disks while $\mathcal{V}_0 \subset \mathcal{V}$ and $\mathcal{I}_0 \subset \mathcal{I}$ be the sets of numbers of vertebrae and inter-vertebral disks that obtained from CT images.
- (2) With respect to $i \in \mathcal{V}_0$, a boundary of i -th vertebra is extracted from CT image by filtering technique [?] and set as $\partial\Sigma_{V_i} \in \mathbb{R}^3$.
- (3) With respect to $i \in \mathcal{V}_0$, let

$$d_i(\mathbf{x}) = \begin{cases} \inf_{\mathbf{y} \in \partial\Sigma_{V_i}} \|\mathbf{x} - \mathbf{y}\|_{\mathbb{R}^3} & \text{for } \mathbf{x} \in D \setminus \Sigma_{V_i} \\ -\inf_{\mathbf{y} \in \partial\Sigma_{V_i}} \|\mathbf{x} - \mathbf{y}\|_{\mathbb{R}^3} & \text{for } \mathbf{x} \in \Sigma_{V_i} \end{cases}$$

be a signed distance function from $\partial\Sigma_{V_i}$. In this study, the signed distance function is assumed to be given as a distribution of integer as shown in Figure ??.

- (4) With respect to $i \in \mathcal{V}_0$ and $j \in \mathcal{I}$, let $\Omega_{V_{0i}} \in \mathbb{R}^3$ be a domain of i -th vertebra in a normal spine finite-element model, and $\Omega_{I_{0j}}$ be a domain of j -th inter-vertebral disk.
- (5) Let Ω_0 ($\bar{\Omega}_0 = (\cup_{i \in \mathcal{V}} \bar{\Omega}_{V_{0i}}) \cup (\cup_{j \in \mathcal{I}} \bar{\Omega}_{I_{0j}})$) be the total domain of a normal spine finite-element model.
- (6) With respect to $i \in \mathcal{V}_0$, let $\mathbf{q}_i \in \mathbb{R}^9$ be the parameters of parametric deformation consisting of transformation \mathbf{q}_{iT} , rotation \mathbf{q}_{iR} and scaling $\Omega_{V_{0i}}$ defined as

$$\mathbf{q}_i = \begin{pmatrix} \mathbf{q}_{iT} \\ \mathbf{q}_{iR} \\ \mathbf{q}_{iS} \end{pmatrix} \text{ where } \mathbf{q}_{iT} = \begin{pmatrix} q_{i1} \\ q_{i2} \\ q_{i3} \end{pmatrix}, \mathbf{q}_{iR} = \begin{pmatrix} q_{i4} \\ q_{i5} \\ q_{i6} \end{pmatrix}, \mathbf{q}_{iS} = \begin{pmatrix} q_{i7} \\ q_{i8} \\ q_{i9} \end{pmatrix}.$$

Using \mathbf{q}_i , the parametric mapping is defined by

$$\omega_i(\mathbf{q}_i)(\mathbf{x}) = \mathbf{S}(\mathbf{q}_{iT}) \mathbf{R}(\mathbf{q}_{iR}) \mathbf{T}(\mathbf{q}_{iT}) \mathbf{x}. \quad (1)$$

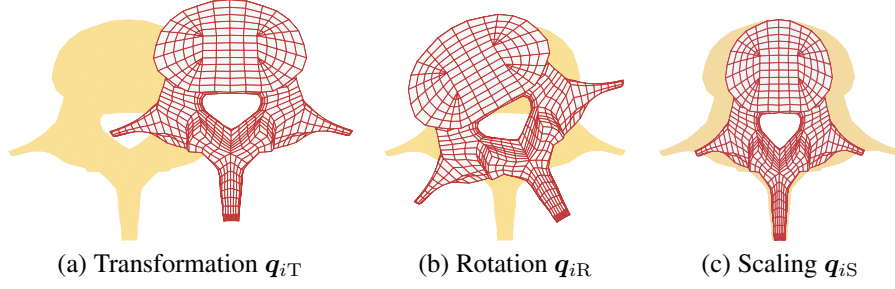


Figure 3. Parametric shape fitting problem

Putting $\omega_i(q_i)(x) = y$ and using the homogeneous coordinate system, Eq. (??) is given by

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ 1 \end{pmatrix} = \begin{pmatrix} q_7 & 0 & 0 & 0 \\ 0 & q_8 & 0 & 0 \\ 0 & 0 & q_9 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \times \begin{pmatrix} \cos q_6 & -\sin q_6 & 0 & 0 \\ \sin q_6 & \cos q_6 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos q_5 & 0 & \sin q_5 & 0 \\ 0 & 1 & 0 & 0 \\ -\sin q_5 & 0 & \cos q_5 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos q_4 & -\sin q_4 & 0 \\ 0 & \sin q_4 & \cos q_4 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \times \begin{pmatrix} 1 & 0 & 0 & q_1 \\ 0 & 1 & 0 & q_2 \\ 0 & 0 & 1 & q_3 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ 1 \end{pmatrix}.$$

Based on the definitions above, we formulate a parametric shape fitting problem in the following way.

Problem 1 (Parametric shape fitting problem) With respect to $i \in \mathcal{V}_0$, let $\omega_i(q_i)$ be defined by Eq. (??) and $\hat{\Omega}_{V_i}(q_i)$ denote $\omega_i(q_i)(\Omega_{V_{0i}})$. Find $\hat{\Omega}_{V_i}(q_i)$ such that

$$\min_{q_i \in \mathbb{R}^9} \left\{ f_{Pi} = \int_{\hat{\Omega}_{V_i}(q_i)} d_i dx \right\}.$$

To solve Problem ??, the following numerical scheme can be considered.

- (1) Find the voxels including $\partial\Sigma_{V_i}$ by the outline extraction treatment from a CT image.
- (2) Put $d_i = 0$ for the voxels including $\partial\Sigma_{V_i}$. Put $d_i = 1$ for the next voxels in outside, and $d_i = -1$ for the next voxels in innerside. Put $d_i = 2$ for the next voxels in outside, and $d_i = -2$. In the same manner, put the values of d_i for the all voxels in D .
- (3) Compute the gradient of f_{Pi} by using finite differences with respect to small variations of each element of q_i .
- (4) With the gradient, find the minimum point of Problem ?? by the gradient method.

2.2. Nonparametric shape fitting problem of density type

Using the solution $\hat{\Omega}_{V_i}(q_i)$ of Problem ?? with respect to all $i \in \mathcal{V}_0$, we consider a problem finding a mapping $i + u : \Omega_0 \rightarrow \mathbb{R}^3$ such that $(i + u)(\Omega_{V_{0i}})$ approaches $\hat{\Omega}_{V_i}(q_i)$. Here, i and u denotes the identity mapping and displacement. In this study, we formulate an elastic problem with finite deformation in which a traction in proportion to the distance of each point on $\partial\Omega_0$ to the corresponding point on $\partial\hat{\Omega}_{V_i}(q_i)$ acts, and define a minimization problem of a norm of the distance by controlling a density of elastic modulus defined at each point in $\Omega_{V_{0i}}$.

This idea can be formulated as a topology optimization problem of density type [?] in the following way. Let $\mathcal{V}_0 \subset \mathcal{V}$ be the set of the numbers of vertebrae for which the solution q_i of Problem ?? is obtained. With respect to $i \in \mathcal{V}_0$, we construct a problem finding the finite deformation $u : \Omega_0 \rightarrow \mathbb{R}^3$ of the normal model approaches the parametric deformation $u_{0i} = \omega_i(q_i) - i$ as a state determination problem in a topology optimization problem. Figure ?? shows the deformations u and u_{0i} .

Here, we assume the following hypotheses.

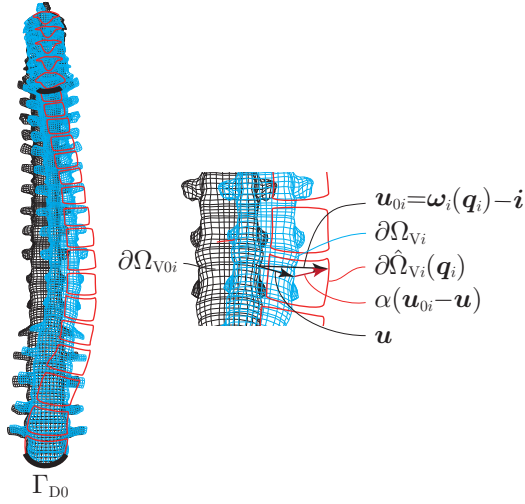


Figure 4. Nonparametric fitting problem

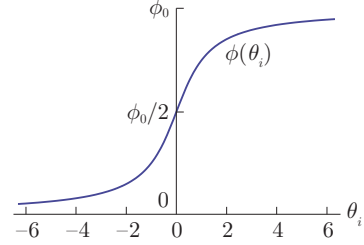


Figure 5. Relationship between θ and ϕ

- (1) Suppose that the spine finite-element model is a hyper-elastic body of Saint Venant-Kirchhoff model (the second Piola-Kirchhoff stress is in proportion to Green-Lagrange strain).
- (2) Set a design variable $\boldsymbol{\theta} = (\theta_1, \theta_2, \theta_3)^T$ as an arbitrary element of

$$X = H^1(\Omega_0; \mathbb{R}^3) \quad (2)$$

and density

$$\phi(\theta_i) = \phi_0 \frac{\tanh \theta_i + 1}{2} \quad (3)$$

with respect to $i \in \{1, 2, 3\}$, where ϕ_0 is a positive number denoting the maximum value of density. Figure ?? shows the $\phi(\theta_i)$.

- (3) Let $\bar{\Omega}_0 \cap_{i \in \mathcal{V}_0} \bar{\Sigma}_{Vi}$ be a fixed boundary Γ_{D0} .

Using design variable $\boldsymbol{\theta} \in X$, we define a finite elastic deformation problem in the following way. Let $\mathbf{y} = \mathbf{i} + \mathbf{u} : \Omega_0 \rightarrow \mathbb{R}^3$ be a mapping of a finite elastic deformation, where \mathbf{i} and \mathbf{u} denotes the identity mapping and finite elastic deformation respectively. We assume the linear space of \mathbf{u} as

$$U = \{ \mathbf{u} \in H^1(\Omega_0; \mathbb{R}^d) \mid \mathbf{u} = \mathbf{0} \text{ on } \Gamma_{D0} \} \quad (4)$$

and the admissible set of \mathbf{u} as

$$\mathcal{S} = U \cap W^{1,\infty}(\Omega_0; \mathbb{R}^d). \quad (5)$$

Denoting a deformation gradient as

$$\mathbf{F}(\mathbf{u}) = \left(\frac{\partial y_i}{\partial x_j} \right)_{ij} = (\nabla \mathbf{y}^T)^T = \mathbf{I} + (\nabla \mathbf{u}^T)^T,$$

Green-Lagrange strain is defined by

$$\mathbf{E}(\mathbf{u}) = (e_{ij}(\mathbf{u}))_{ij} = \frac{1}{2} (\mathbf{F}(\mathbf{u}) \mathbf{F}^T(\mathbf{u}) - \mathbf{I}) = \mathbf{E}_L(\mathbf{u}) + \frac{1}{2} \mathbf{E}_B(\mathbf{u}, \mathbf{u}), \quad (6)$$

where

$$\mathbf{E}_L(\mathbf{u}) = \frac{1}{2} (\nabla \mathbf{u}^T + (\nabla \mathbf{u}^T)^T), \quad (7)$$

$$\mathbf{E}_B(\mathbf{u}, \mathbf{v}) = \frac{1}{2} (\nabla \mathbf{u}^T (\nabla \mathbf{v}^T)^T + \nabla \mathbf{v}^T (\nabla \mathbf{u}^T)^T). \quad (8)$$

With respect to $\mathbf{E}(\mathbf{u})$, we can compute the eigen values $\lambda_1(\mathbf{u}), \lambda_2(\mathbf{u}), \lambda_3(\mathbf{u}) \in \mathbb{R}$ and eigen vectors $\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3 \in \mathbb{R}^3$ which satisfies

$$\mathbf{\Lambda}(\mathbf{u}) = \begin{pmatrix} \lambda_1(\mathbf{u}) & 0 & 0 \\ 0 & \lambda_2(\mathbf{u}) & 0 \\ 0 & 0 & \lambda_3(\mathbf{u}) \end{pmatrix} = \mathbf{T}^T \mathbf{E}(\mathbf{u}) \mathbf{T}, \quad (9)$$

$$\mathbf{E}(\mathbf{u}) = \mathbf{T} \mathbf{\Lambda}(\mathbf{u}) \mathbf{T}^T, \quad (10)$$

where $\mathbf{T} = (\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3) \in \mathbb{R}^{3 \times 3}$. In this study, we assume the second Piola-Kirchhoff stresses is given by

$$\mathbf{S}(\boldsymbol{\theta}, \mathbf{u}) = \mathbf{T} \boldsymbol{\Phi}^p(\boldsymbol{\theta}) \mathbf{C}_0 \mathbf{\Lambda}(\mathbf{u}) \mathbf{T}^T, \quad (11)$$

and the first Piola-Kirchhoff stresses is defined by

$$\mathbf{\Pi}(\boldsymbol{\theta}, \mathbf{u}) = \mathbf{S}(\boldsymbol{\theta}, \mathbf{u}) \mathbf{F}(\mathbf{u}). \quad (12)$$

Here, we used $\mathbf{C}_0 : \Omega_0 \rightarrow \mathbb{R}^{d \times d \times d \times d}$ as the stiffness of the normal spine model, and

$$\boldsymbol{\Phi}(\boldsymbol{\theta}) = \text{diag}(\phi(\theta_1), \phi(\theta_2), \phi(\theta_3)) = \begin{pmatrix} \phi(\theta_1) & 0 & 0 \\ 0 & \phi(\theta_2) & 0 \\ 0 & 0 & \phi(\theta_3) \end{pmatrix}. \quad (13)$$

p is a positive constant to control the nonlinearity between the density and the stiffness for which 3 is used as a default.

Using the notations, a finite elastic deformation problem approaches $\hat{\Omega}_{V_i}(\mathbf{q}_i)$ is formulated in the following way.

Problem 2 (Finite elastic deformation problem) *With respect to $i \in \mathcal{V}_0$, let $\mathbf{u}_{0i} = \boldsymbol{\omega}_i(\mathbf{q}_i) - \mathbf{i}$ is given by the solution \mathbf{q}_i of Problem ?? . Let $\alpha : \cup_{i \in \mathcal{V}_0} \Omega_{V0i} \rightarrow \mathbb{R}$ be a positive real valued function denoting a weight. For $\boldsymbol{\theta} \in X$, find $\mathbf{u} \in \mathcal{S}$ such that*

$$\begin{aligned} \nabla^T \mathbf{\Pi}(\boldsymbol{\theta}, \mathbf{u}) &= \mathbf{0}_{\mathbb{R}^3}^T \quad \text{in } \Omega_0 \\ \mathbf{\Pi}^T(\boldsymbol{\theta}, \mathbf{u}) \boldsymbol{\nu} &= \alpha(\mathbf{u}_{0i} - \mathbf{u}) \quad \text{on } \cup_{i \in \mathcal{V}_0} \partial \Omega_{V0i} \\ \mathbf{\Pi}^T(\boldsymbol{\theta}, \mathbf{u}) \boldsymbol{\nu} &= \mathbf{0}_{\mathbb{R}^3} \quad \text{on } \partial \Omega_0 \setminus (\cup_{i \in \mathcal{V}_0} \partial \Omega_{V0i}) \\ \mathbf{u} &= \mathbf{0} \quad \text{on } \Gamma_{D0}. \end{aligned}$$

The weak form of Problem ?? can be expressed in the following way. We now define the Lagrange function with respect to Problem ?? as

$$\mathcal{L}_M(\boldsymbol{\theta}, \mathbf{u}, \mathbf{v}) = \int_{\Omega_0} (\nabla^T \mathbf{\Pi}(\boldsymbol{\theta}, \mathbf{u}))^T \cdot \mathbf{v} \, dx + \int_{\cup_{i \in \mathcal{V}_0} \partial \Omega_{V0i}} \alpha(\mathbf{u}_{0i} - \mathbf{u}) \cdot \mathbf{v} \, d\gamma, \quad (14)$$

where $\mathbf{v} \in U$ is the Lagrange multiplier. We can rewrite the first term of the right-hand side in Eq. (??) as

$$\begin{aligned} \int_{\Omega_0} (\nabla^T \mathbf{\Pi}(\boldsymbol{\theta}, \mathbf{u}))^T \cdot \mathbf{v} \, dx &= \int_{\Omega_0} \left\{ \nabla \cdot (\mathbf{\Pi}^T(\boldsymbol{\theta}, \mathbf{u}) \mathbf{v}) - \mathbf{\Pi}^T(\boldsymbol{\theta}, \mathbf{u}) \cdot (\nabla \mathbf{v}^T)^T \right\} dx \\ &= \int_{\partial \Omega_0} (\mathbf{\Pi}^T(\boldsymbol{\theta}, \mathbf{u}) \mathbf{v}) \cdot \boldsymbol{\nu} \, d\gamma - \int_{\Omega_0} \mathbf{\Pi}^T(\boldsymbol{\theta}, \mathbf{u}) \cdot \mathbf{F}'[\mathbf{v}] \, dx, \end{aligned} \quad (15)$$

where

$$\mathbf{F}'[\mathbf{v}] = \frac{\partial \mathbf{v}}{\partial \mathbf{x}^T} = (\nabla \mathbf{v}^T)^T.$$

Moreover, considering $\mathbf{S}(\boldsymbol{\theta}, \mathbf{u}) = \mathbf{S}^T(\boldsymbol{\theta}, \mathbf{u})$, we obtain

$$\begin{aligned} - \int_{\Omega_0} \mathbf{\Pi}^T(\boldsymbol{\theta}, \mathbf{u}) \cdot \mathbf{F}'[\mathbf{v}] \, dx &= - \int_{\Omega_0} (\mathbf{S}(\boldsymbol{\theta}, \mathbf{u}) \mathbf{F}^T(\mathbf{u}))^T \cdot \mathbf{F}'[\mathbf{v}] \, dx \\ &= - \int_{\Omega_0} \mathbf{S}(\boldsymbol{\theta}, \mathbf{u}) \cdot (\mathbf{F}^T(\mathbf{u}) \mathbf{F}'[\mathbf{v}]) \, dx = - \int_{\Omega_0} \mathbf{S}(\boldsymbol{\theta}, \mathbf{u}) \cdot \mathbf{E}'(\mathbf{u})[\mathbf{v}] \, dx, \end{aligned} \quad (16)$$

where

$$\mathbf{E}'(\mathbf{u})[\mathbf{v}] = \frac{1}{2} (\mathbf{F}'^T[\mathbf{v}] \mathbf{F}(\mathbf{u}) + \mathbf{F}^T(\mathbf{u}) \mathbf{F}'[\mathbf{v}]) = \mathbf{E}_L(\mathbf{v}) + \mathbf{E}_B(\mathbf{u}, \mathbf{v}).$$

Then, using Eq. (??) and Eq. (??), Eq. (??) can be rewritten as

$$\mathcal{L}_M(\boldsymbol{\theta}, \mathbf{u}, \mathbf{v}) = - \int_{\Omega_0} \mathbf{S}(\boldsymbol{\theta}, \mathbf{u}) \cdot \mathbf{E}'(\mathbf{u})[\mathbf{v}] \, dx + \int_{\cup_{i \in \mathcal{V}_0} \partial\Omega_{V0i}} \alpha (\mathbf{u}_{0i} - \mathbf{u}) \cdot \mathbf{v} \, d\gamma. \quad (17)$$

Using $\mathcal{L}_M(\boldsymbol{\theta}, \mathbf{u}, \mathbf{v})$, we can write the weak form of Problem ?? as

$$\mathcal{L}_M(\boldsymbol{\theta}, \mathbf{u}, \mathbf{v}) = 0 \quad (18)$$

for all $\mathbf{v} \in U$. Numerical solutions of Problem ?? can be obtained by the finite-element method based on Eq. (??).

With respect to the design variable $\boldsymbol{\theta} \in X$, we call the solution $\mathbf{u} \in U$ of the state determination problem (Problem ??) the state variable. Using this variable, we define a cost function for the nonparametric shape fitting problem by

$$f_N(\boldsymbol{\theta}, \mathbf{u}) = \int_{\cup_{i \in \mathcal{V}_0} \partial\Omega_{V0i}} \alpha \|\mathbf{u}_{0i} - \mathbf{u}\|_{\mathbb{R}^3}^2 \, d\gamma. \quad (19)$$

Using f_N , we formulate a nonparametric shape fitting problem of density type in the following way.

Problem 3 (Nonparametric shape fitting problem of density type) *Let f_N be defined by Eq. (??). Find \mathbf{u} such that*

$$\min_{\boldsymbol{\theta} \in X} \{f_N(\boldsymbol{\theta}, \mathbf{u}) \mid \mathbf{u} \in \mathcal{S}, \text{ Problem ??} \}.$$

The numerical solution of Problem ?? can be obtained by the H^1 gradient method for the topology optimization problem of density type [?]. In the present study, we aim to obtain the numerical solution \mathbf{u} of Problem ?? and to evaluate the Green-Lagrange strain $\mathbf{E}(\mathbf{u})$ with which we expect to investigate the etiology of the idiopathic scoliosis.

In the H^1 gradient method for the topology optimization problem of density type, $\boldsymbol{\theta}$ derivative (the Fréchet derivative with respect to an arbitrary variation of $\boldsymbol{\theta} \in X$) of the cost function f_N . To obtain the $\boldsymbol{\theta}$ derivative of f_N , we use the Lagrange multiplier method (adjoint variable method). Hereafter, letting $\boldsymbol{\vartheta} \in X$ denote an arbitrary variation of $\boldsymbol{\theta}$, we define the Lagrange function with respect to Problem ?? as

$$\mathcal{L}_N(\boldsymbol{\theta}, \mathbf{u}, \mathbf{v}_N) = f_N(\mathbf{u}) + \mathcal{L}_M(\boldsymbol{\theta}, \mathbf{u}, \mathbf{v}_N) \quad (20)$$

for all $(\boldsymbol{\theta}, \mathbf{u}, \mathbf{v}_N) \in X \times \mathcal{S} \times U$, where \mathcal{L}_M is defined in Eq. (??) and \mathbf{v}_N is introduced as the Lagrange multiplier (adjoint variable) with respect to f_N . The total derivative of \mathcal{L}_N with respect to an arbitrary variation $(\boldsymbol{\vartheta}, \mathbf{u}', \mathbf{v}'_N) \in X \times U \times U$ can be written as

$$\mathcal{L}'_N(\boldsymbol{\theta}, \mathbf{u}, \mathbf{v}_N)[\boldsymbol{\vartheta}, \mathbf{u}', \mathbf{v}'_N] = \mathcal{L}_{N\boldsymbol{\theta}}(\boldsymbol{\theta}, \mathbf{u}, \mathbf{v}_N)[\boldsymbol{\vartheta}] + \mathcal{L}_{N\mathbf{u}}(\boldsymbol{\theta}, \mathbf{u}, \mathbf{v}_N)[\mathbf{u}'] + \mathcal{L}_{N\mathbf{v}_N}(\boldsymbol{\theta}, \mathbf{u}, \mathbf{v}_N)[\mathbf{v}'_N]. \quad (21)$$

Here, if \mathbf{u} is the solution of Problem ??, the third term of the right-hand side in Eq. (??) becomes 0. Moreover, if \mathbf{v}_N satisfies

$$\begin{aligned} \mathcal{L}_{N\mathbf{u}}(\boldsymbol{\theta}, \mathbf{u}, \mathbf{v}_N)[\mathbf{u}'] &= - \int_{\Omega_0} (\mathbf{S}_{\mathbf{u}}(\boldsymbol{\theta}, \mathbf{u})[\mathbf{u}'] \cdot \mathbf{E}'(\mathbf{u})[\mathbf{v}_N] + \mathbf{S}(\boldsymbol{\theta}, \mathbf{u}) \cdot \mathbf{E}''(\mathbf{u})[\mathbf{v}_N, \mathbf{u}']) \, dx \\ &\quad + \int_{\cup_{i \in \mathcal{V}_0} \partial\Omega_{V0i}} \alpha \{2(\mathbf{u} - \mathbf{u}_{0i}) - \mathbf{v}\} \cdot \mathbf{u}' \, d\gamma = 0 \end{aligned} \quad (22)$$

for all $\mathbf{u}' \in U$, the second term of the right-hand side in Eq. (??) becomes 0. Here, we used notations defined as

$$\begin{aligned} \mathbf{S}_{\mathbf{u}}(\boldsymbol{\theta}, \mathbf{u})[\mathbf{v}] &= \mathbf{T}\boldsymbol{\Phi}^p(\boldsymbol{\theta}) \mathbf{C}_0 \boldsymbol{\Lambda}'(\mathbf{u})[\mathbf{v}] \mathbf{T}^T = \mathbf{T}\boldsymbol{\Phi}^p(\boldsymbol{\theta}) \mathbf{C}_0 \mathbf{T}^T \mathbf{E}'(\mathbf{u})[\mathbf{v}], \\ \mathbf{E}''[\mathbf{v}, \mathbf{w}] &= \mathbf{E}_B(\mathbf{v}, \mathbf{w}). \end{aligned}$$

By using the same relation we used in Eq. (??), we have

$$- \int_{\Omega_0} (\mathbf{S}_{\mathbf{u}}(\boldsymbol{\theta}, \mathbf{u})[\mathbf{u}'] \cdot \mathbf{E}'(\mathbf{u})[\mathbf{v}_N] + \mathbf{S}(\boldsymbol{\theta}, \mathbf{u}) \cdot \mathbf{E}''[\mathbf{v}_N, \mathbf{u}']) \, dx = - \int_{\Omega_0} \boldsymbol{\Pi}_{\mathbf{u}}^T(\boldsymbol{\theta}, \mathbf{u})[\mathbf{v}_N] \cdot \mathbf{F}'[\mathbf{u}'] \, dx,$$

where

$$\boldsymbol{\Pi}_{\mathbf{u}}(\boldsymbol{\theta}, \mathbf{u})[\mathbf{v}] = \mathbf{S}_{\mathbf{u}}(\boldsymbol{\theta}, \mathbf{u})[\mathbf{v}] \mathbf{F}^T(\mathbf{u}) + \mathbf{S}(\boldsymbol{\theta}, \mathbf{u}) \mathbf{F}'^T[\mathbf{v}].$$

Moreover, since $\mathbf{u}' = \mathbf{0}_{\mathbb{R}^d}$ on Γ_{D0} , using the same relation we used in Eq. (??), we have

$$\begin{aligned} & - \int_{\Omega_0} \mathbf{\Pi}_u^T(\boldsymbol{\theta}, \mathbf{u}) [\mathbf{v}_N] \cdot \mathbf{F}'[\mathbf{u}'] \, dx \\ & = \int_{\Omega_0} (\nabla^T \mathbf{\Pi}_u(\boldsymbol{\theta}, \mathbf{u}) [\mathbf{v}_N])^T \cdot \mathbf{u}' \, dx - \int_{\cup_{i \in \mathcal{V}_0} \partial \Omega_{V0i}} (\mathbf{\Pi}_u^T(\boldsymbol{\theta}, \mathbf{u}) [\mathbf{v}_N] \mathbf{u}') \cdot \boldsymbol{\nu} \, d\gamma. \end{aligned}$$

From the relations above, Eq. (??) can be rewritten as

$$\mathcal{L}_{N\mathbf{u}}(\boldsymbol{\theta}, \mathbf{u}, \mathbf{v}_N) [\mathbf{u}'] = \int_{\Omega_0} (\nabla^T \mathbf{\Pi}_u(\boldsymbol{\theta}, \mathbf{u}) [\mathbf{v}_N])^T \cdot \mathbf{u}' \, dx + \int_{\cup_{i \in \mathcal{V}_0} \partial \Omega_{V0i}} \{ \mathbf{\Pi}_u^T(\boldsymbol{\theta}, \mathbf{u}) [\mathbf{v}_N] \boldsymbol{\nu} \} \cdot \mathbf{u}' \, d\gamma = 0$$

for all $\mathbf{u}' \in U$. Then, the second term of the right-hand side in Eq. (??) becomes 0, if \mathbf{v}_N is the solution of the following adjoint problem.

Problem 4 (Adjoint problem with respect to f_N) Let \mathbf{u} be the solution of Problem ???. Find \mathbf{v}_N such that

$$\begin{aligned} & - \nabla^T \mathbf{\Pi}_u(\boldsymbol{\theta}, \mathbf{u}) [\mathbf{v}_N] = \mathbf{0}_{\mathbb{R}^3} \quad \text{in } \Omega_0, \\ & \mathbf{\Pi}_u^T(\boldsymbol{\theta}, \mathbf{u}) [\mathbf{v}_N] \boldsymbol{\nu} = \alpha \{ 2(\mathbf{u} - \mathbf{u}_{0i}) - \mathbf{v} \} \quad \text{on } \cup_{i \in \mathcal{V}_0} \partial \Omega_{V0i}, \\ & \mathbf{\Pi}_u^T(\boldsymbol{\theta}, \mathbf{u}) [\mathbf{v}_N] \boldsymbol{\nu} = \mathbf{0}_{\mathbb{R}^3} \quad \text{on } \bar{\Omega}_0 \setminus (\cup_{i \in \mathcal{V}_0} \partial \Omega_{V0i}) \\ & \mathbf{v}_N = \mathbf{0}_{\mathbb{R}^d} \quad \text{on } \Gamma_D(\phi). \end{aligned}$$

Then, when \mathbf{u} and \mathbf{v}_N are the solutions of Problem ??? and Problem ??? respectively, denoting $f_N(\mathbf{u}(\boldsymbol{\theta}))$ as $\tilde{f}_N(\boldsymbol{\theta})$, Eq. (??) becomes

$$\mathcal{L}_{N\boldsymbol{\theta}}(\boldsymbol{\theta}, \mathbf{u}, \mathbf{v}_N) [\boldsymbol{\vartheta}] = \tilde{f}'_N(\boldsymbol{\theta}) [\boldsymbol{\vartheta}] = \int_{\Omega_0} \mathbf{S}_{\boldsymbol{\theta}}(\boldsymbol{\theta}, \mathbf{u}) [\boldsymbol{\vartheta}] \cdot \mathbf{E}'(\mathbf{u}) [\mathbf{v}_N] \, dx = \int_{\Omega_0} \mathbf{g}_N \cdot \boldsymbol{\vartheta} \, dx = \langle \mathbf{g}_N, \boldsymbol{\vartheta} \rangle. \quad (23)$$

Here,

$$\mathbf{g}_N = \{ \mathbf{T}(\boldsymbol{\Phi}^p(\boldsymbol{\theta}))' \mathbf{C}_0 \boldsymbol{\Lambda}(\mathbf{u}) \mathbf{T}^T \} \cdot \mathbf{E}'(\mathbf{u}) [\mathbf{v}_N], \quad (24)$$

is the $\boldsymbol{\theta}$ gradient of f_N , where

$$(\boldsymbol{\Phi}^p(\boldsymbol{\theta}))' = - \begin{pmatrix} p\phi^{p-1}(\theta_1)/2 \cosh^2 \theta_1 & 0 & 0 \\ 0 & p\phi^{p-1}(\theta_2)/2 \cosh^2 \theta_2 & 0 \\ 0 & 0 & p\phi^{p-1}(\theta_3)/2 \cosh^2 \theta_3 \end{pmatrix}. \quad (25)$$

Using \mathbf{g}_N , the variation of $\boldsymbol{\theta} \in X$ that minimizes f_N can be obtained by the H^1 gradient method [?]. In this study, we use

$$a_X(\boldsymbol{\vartheta}, \boldsymbol{\psi}) = \int_{\Omega_0} (\nabla \boldsymbol{\vartheta}^T \cdot \nabla \boldsymbol{\psi}^T + c_\Omega \boldsymbol{\vartheta} \cdot \boldsymbol{\psi}) \, dx \quad (26)$$

with respect to $\boldsymbol{\vartheta}, \boldsymbol{\psi} \in X$ as a bounded and coercive bilinear form, where c_Ω is a positive constant. In the H^1 gradient method, the variation $\boldsymbol{\vartheta}_g$ of $\boldsymbol{\theta} \in X$ is determined by the weak form as

$$c_a a_X(\boldsymbol{\vartheta}_g, \boldsymbol{\psi}) = - \langle \mathbf{g}_N, \boldsymbol{\psi} \rangle \quad (27)$$

for all $\boldsymbol{\psi} \in X$, where c_a is a positive constant to control the step size $\|\boldsymbol{\vartheta}_g\|_X$. The strong form of Eq. (??) is as follows.

Problem 5 (H^1 gradient method) For \mathbf{g}_N , find $\boldsymbol{\vartheta}_g \in X$ such that

$$\begin{aligned} & - c_a \{ \nabla^T (\nabla \boldsymbol{\vartheta}_g^T) + c_\Omega \boldsymbol{\vartheta}_g^T \} = \mathbf{g}_N^T \quad \text{in } \Omega_0, \\ & c_a (\nabla \boldsymbol{\vartheta}_g^T) \boldsymbol{\nu} = \mathbf{0}_{\mathbb{R}^3} \quad \text{on } \partial \Omega_0. \end{aligned}$$

3. Numerical Example

In this study, CT image was provided by Meijo Hospital, Nagoya City. Normal spine finite element model was constructed by Azegami laboratory using commercial data (Viewpoint Premier, catalog numbers of VP2886 and VP3611, Viewpoint Corporation, 498 7th Ave. Suite 1810, New York, NY 10018, USA). For the calculation of the main problems (Eq.(4)) and adjoint problems (Eq.(7)) in nonparametric fitting problem, commercial finite element program (Abaqus 6.12, Abaqus, Inc.) was employed. For boundary Γ_D , the bottom surface of L5 and the top surface of C2 were constrained in every position. Besides, $\mathcal{V}_0 = \{\text{T11, T12, L1}\}$ were selected as the patient model and material properties of normal finite element model are shown in Table 1.

Table 1. Material Properties

	Longitudinal elastic modulus(MPa)	Poisson's ratio
Cortical bone	17000	0.3
Cortical bone(intermediate)	1000	0.3
Epiphysis	1000	0.3
Cancellous bone	200	0.3
Hyaline bone	100	0.3
Intervertebral disk (nucleus pulposus)	0.1	0.3
Intervertebral disk (annulus fibrosus)	2.5	0.3
Intervertebral joint (cervical vertebrae)	7.5	0.3
Intervertebral joint (thoracic vertebrae)	7.5	0.3
Intervertebral joint (lumbar vertebrae)	0.6	0.3

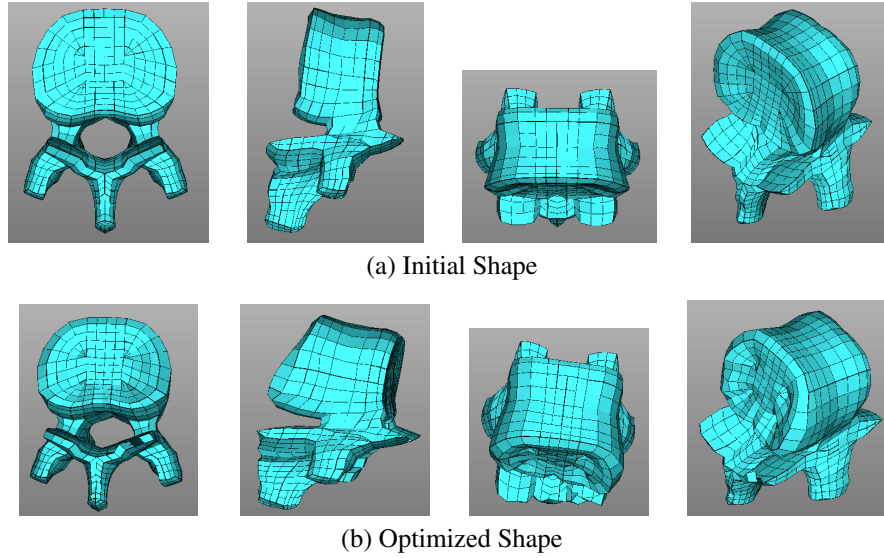


Figure 6. Parametric shape fitting of T11

4. Results and Discussion

Comparison between initial shapes and after optimization shapes of T11, T12 and L1 for parametric shape fitting problem are shown in Figure 6 to Figure 11. The shape of the vertebrae deformed based on design variables (translation, rotation and scaling) that set in the fitting process.

Comparison between CT voxel data, initial shape and optimized shape of spine model for density type nonparametric shape fitting problem are shown in Figure 12. Similarity between CT image and optimized shape of spine model can be observed whereby the spine model curved at T11, T12 and L1.

Figure 13 shows the iteration history of the objective function in optimum density distribution for density type nonparametric shape fitting problem. From initial shape, the value of objective function rapidly decreases until iteration number 5 that indicates normal spine model deforms toward patient model (T11, T12 and L1) from iteration number 0 to 5. Then, objective function slightly decreases from iteration number 5 to 10 before become static from iteration number 10 to 20. Although similar deformation and curve between CT image and optimized spine model can be observed in Figure 12, the objective function only decrease to about 67% from initial shape. This result specifies the normal spine model is not fully deformed to fit the patient model. Therefore adjustment should be made to enhance the result of fitting problem and one of the easiest way is to increase the external force apply at $\partial\Omega_i$. As shown in second equation in Eq.(3), external force is directly proportional to the value of α . Therefore, in this study, analysis is conducted by manipulating the value of α and its effect to the objective function. Figure 14 shows the iteration history of the objective function in optimum density distribution for different value of α where the initial value of α is 2.68. When $\alpha = 3.0$, the value of objective function is rapidly decrease until iteration number 11 before it become static until iteration number 20 at 54%. Besides, when $\alpha = 3.2$, the value of objective function is also rapidly decrease until iteration number 9 before become static until iteration number 20 at 44% while on the other hand, when $\alpha = 3.4$, the value of objective function is slowly decrease until iteration number 7 before become static until iteration number 20 at 73%. From these analyses, we can conclude that the manipulation of α can enhance the fitting result up to 23% of decrement of objective function. However, there is limitation where the

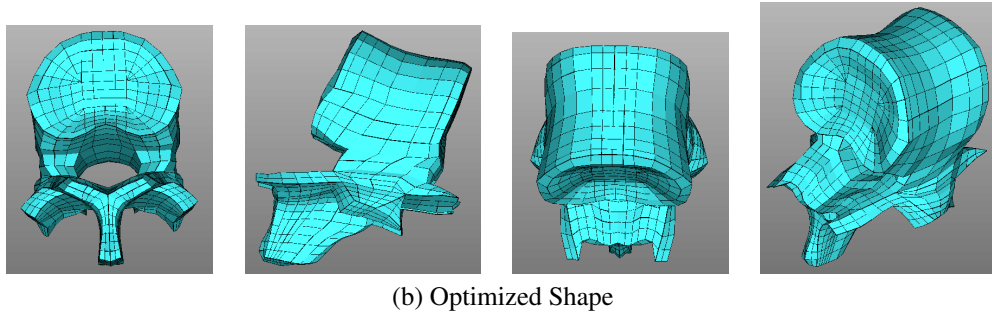
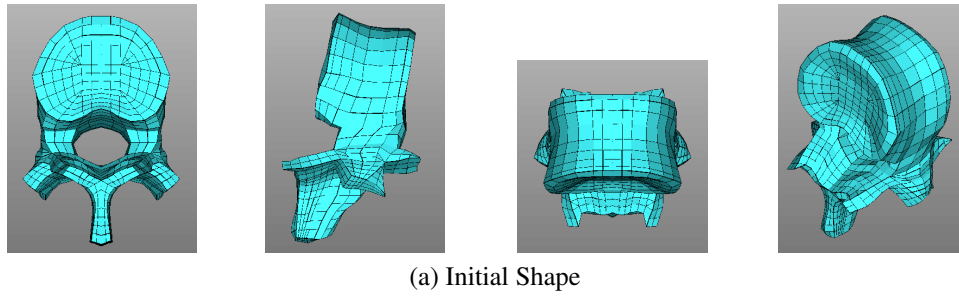


Figure 7. Parametric shape fitting of T12

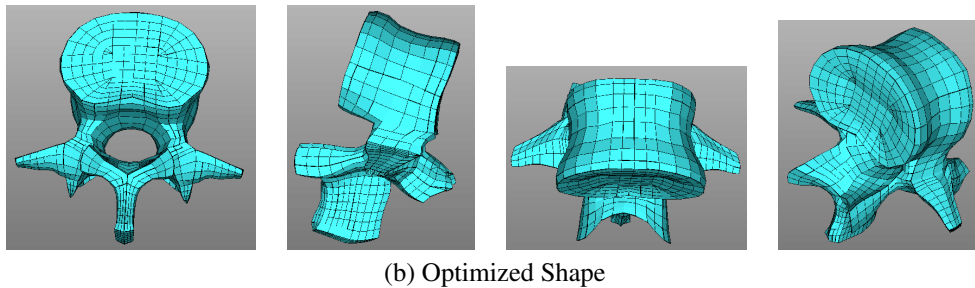
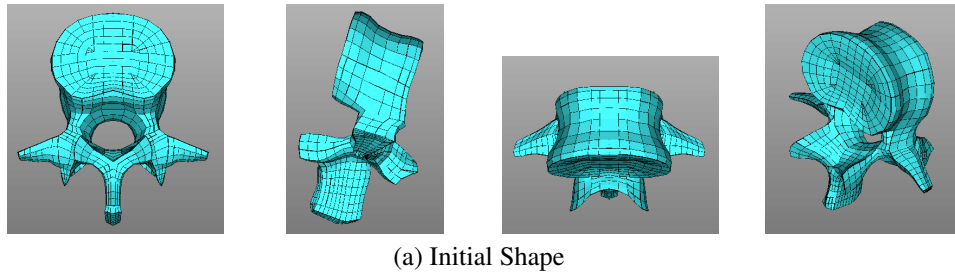


Figure 8. Parametric shape fitting of L1

minimum value of objective function is 44%.

5. Conclusion

In this study, 2 type of shape fitting approaches were introduced. Construction of finite element spine model from patient's CT image can be completed by solving the parametric shape fitting problem for each vertebrae using normal finite element vertebrae models. Then, solving the density type nonparametric shape fitting problem of normal finite element spine model fitting to the shapes of vertebrae preliminary obtained in parametric result. Besides, manipulation of force weight, can be used to enhance the results of nonparametric fitting problem.

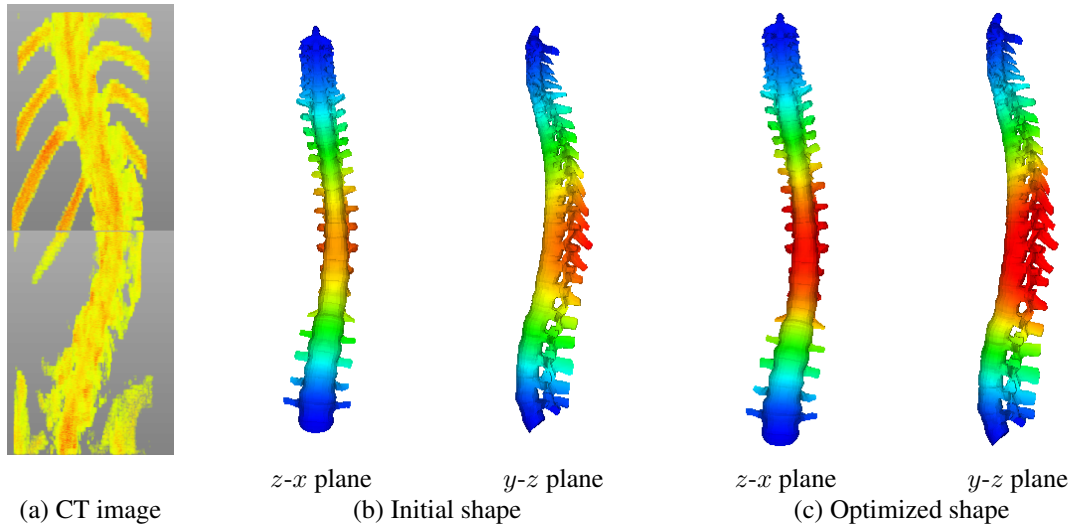


Figure 9. Results of density type shape fitting problem(color denotes displacement)

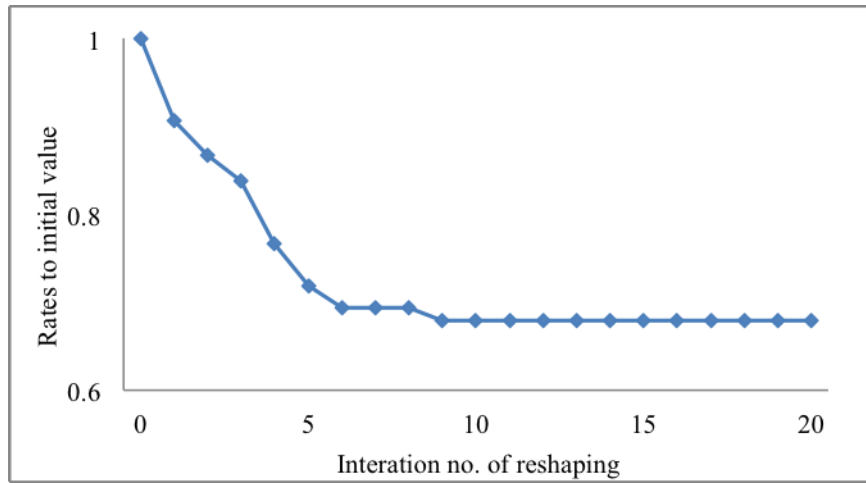


Figure 10. Iteration history

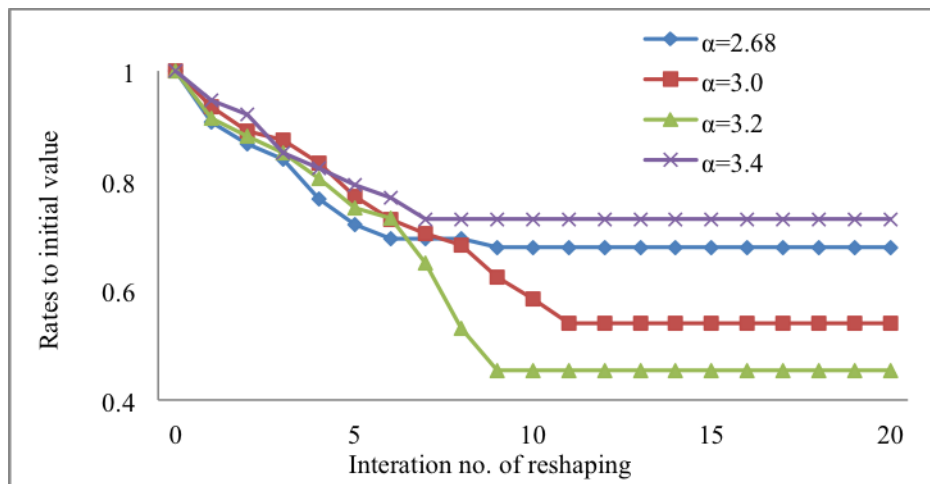


Figure 11. Effect of α to the objective function