A Fixed Point Formulation of the k-Means Algorithm and a Connection to Mumford-Shah *

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Abstract

In this note, we present a fixed point formulation of the k-means segmentation algorithm and show that the iteration's fixed points are solutions of the Euler-Lagrange equation for the k-phase Mumford-Shah energy functional.

This short note illustrates a connection between the k-means algorithm and Mumford-Shah segmentation via a fixed point formulation of k-means. This connection is explicitly mentioned in [3, 10], but is made theoretically concrete here. However, since k-means itself has been extensively studied, any further analysis of the method would be redundant, hence the shortness of the discussion.

Let $D \subset L^\infty(\Omega)$ be nonnegative, where $\Omega \subset \mathbb{R}^d$ is a closed, bounded set. The k-means algorithm is a well-known method for segmenting D into k regions [5, 6, 7]. Its formulation is simple: let

$$\operatorname*{ess\,sup}_{x\in\Omega} D(x) = \ell_0 > \ell_1 > \ell_2 > \cdots > \ell_{k-1} > \ell_k = \operatorname*{ess\,inf}_{x\in\Omega} D(x), \tag{1}$$

then the k-means segmentation of D is defined by

$$\Omega_i = \{x \in \Omega \mid \ell_{i-1} \geq D > \ell_i\}, \quad 1 \leq i \leq k, \tag{2}$$

with the ℓ_i's satisfying

$$\int_{\Omega_i} (D - \ell_i)\, dx \Big/ \int_{\Omega_i} dx = \int_{\Omega_j} (D - \ell_j)\, dx \Big/ \int_{\Omega_j} dx, \qquad 1 \leq i, j \leq k. \tag{3}$$

To arrive at the fixed point formulation of k-means, let

$$c_i = \int_{\Omega_i} D\, dx \Big/ \int_{\Omega_i} dx, \quad 1 \leq i \leq k, \tag{4}$$

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and

$$\Phi_i = D - \ell_i, \quad 1 \le i \le k-1. \tag{5}$$

Then, setting $\vec{\Phi} = (\Phi_1, \ldots, \Phi_{k-1})^T$, after some straightforward calculations, one can show that (3) is satisfied provided

$$\vec{\Phi} = S(\vec{\Phi}), \quad \text{where} \quad S(\vec{\Phi}) = \begin{pmatrix} D - \frac{1}{2}(c_1 + c_2) \\ D - \frac{1}{2}(c_2 + c_3) \\ \vdots \\ D - \frac{1}{2}(c_{k-1} + c_k) \end{pmatrix}. \tag{6}$$

Equations (5) and (6) suggest the fixed point iteration:

$$\vec{\Phi}^k = S(\vec{\Phi}^{k-1}), \qquad \vec{\Phi}^0 = D - \begin{pmatrix} D - \ell_1^0 \\ D - \ell_2^0 \\ \vdots \\ D - \ell_{k-1}^0 \end{pmatrix}, \tag{7}$$

where the ℓ_i^0's satisfy the inequality in (1) and are chosen so that Ω_i^0's are nonempty for all $1 \le i \le k$. Iteratioin (7) is exactly the k-means algorithm.

We will now show that the fixed points of S are solutions of the Euler-Lagrange equation for the Mumford-Shah energy functional.

Assume $\Phi_i \in L^2(\Omega)$ for $1 \le i \le k-1$. Then we can define a k-phase segmentation of D via a minimizer of the Mumford-Shah energy functional [9]

$$\begin{aligned} J(\vec{\Phi}) \quad = \quad & \frac{1}{2}\left\{ \int_\Omega (D - c_1)^2 H(\Phi_1)\, dx + \frac{1}{2}\int_\Omega (D - c_2)^2 (H(-\Phi_1) + H(\Phi_2))\, dx \right. \\ & + \ldots + \frac{1}{2}\int_\Omega (D - c_{k-1})^2 (H(-\Phi_{k-2}) + H(\Phi_{k-1}))\, dx \\ & \left. + \int_\Omega (D - c_k)^2 H(-\Phi_{k-1})\, dx \right\}, \end{aligned} \tag{8}$$

where H is the Heaviside function and the c_i's are defined in (4). If $\vec{\Phi}^*$ is such a minimizer, the corresponding segmentation is given by

$$\Omega_i = \begin{cases} \chi(\{x \mid \Phi_i^*(x) \ge 0\}) & i = 1 \\ \chi(\{x \mid \Phi_i^*(x) \le 0\}) & i = k-1 \\ \chi(\{x \mid \Phi_i^*(x) \ge 0 \,\&\, \Phi_{i-1}^*(x) \le 0\}) & 1 < i < k-1, \end{cases}$$

where χ is the indicator function defined on subsects of Ω.

By computing the gradient (or first variation) of J defined in (8), we obtain the Euler-Lagrange equation

$$\begin{pmatrix} (c_2 - c_1)\left(D - \frac{1}{2}(c_1 + c_2)\right)\delta(\Phi_1) \\ (c_3 - c_2)\left(D - \frac{1}{2}(c_2 + c_3)\right)\delta(\Phi_2) \\ \vdots \\ (c_k - c_{k-1})\left(D - \frac{1}{2}(c_{k-1} + c_k)\right)\delta(\Phi_{k-1}) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \tag{9}$$

of the variational problem $\min_{\vec{\Phi}} J(\vec{\Phi})$, which is immediately seen to be satisfied if (6) holds. Thus the fixed points of S are solutions of the Euler-Lagrange equation for the Mumford-Shah segmentation functional. Given the fact that they also correspond to solutions of the k-means problem, we see that the k-means algorithm (7) can be viewed as a fixed point iteration for minimizing the Mumford-Shah energy functional (8).

Convergence of (7) is discussed in [1, 2, 4, 8]. For an extensive bibliography on k-means, see [11].

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