

# Theory for `lset-opt` package

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## 1 Definitions

**grid** A two-dimensional  $m \times n$  regularly-spaced set of points. The grid spacing is 1 in both  $x$  and  $y$  directions.

**cell** A box with length and height equal to 1, centered at a grid point.

$\phi$  Level-set function defined on grid. The zero-crossing of  $\phi$  defines the contour of the shapes on the grid.

$p$  Fractional-filling function. Values of  $p$  range from -1 to 1 depending on the relative volume of each material found in its cell.

## 2 Regularization

Given a candidate level-set function,  $\hat{\phi}$ , a regularized  $\phi$  is computed in the following way:

1. If any element of  $\hat{\phi}$ ,  $\hat{\phi}_i$ , is exactly equal to 0, then let  $\hat{\phi}_i = \epsilon$  where  $\epsilon$  is the smallest positive number available.

2. For all  $\hat{\phi}_i$  not adjacent to a boundary point, fix the corresponding  $\phi_i$  as

$$\phi_i = \text{sign}(\hat{\phi}_i) = \begin{cases} -1 & \text{if } \hat{\phi}_i < 0, \\ +1 & \text{if } \hat{\phi}_i > 0. \end{cases} \quad (1)$$

3. To determine the remaining  $\phi_i$ , solve the following:

$$\text{minimize } \|\phi - \text{sign}(\hat{\phi})\|^2 \quad (2)$$

$$\text{subject to } A\phi = 0, \quad (3)$$

where  $A$  is a matrix which fixes the boundary points by forcing the ratio of the two adjacent values of  $\phi_i$  to remain the same. The motivation behind the minimization objective is simply to keep values of  $\phi$  from being unnecessarily small or large.

### 3 Conversion to fractional-filling

The fractional-filling,  $p$ , of each cell is calculated in the following way,

$$p_0 = \text{sign}(\phi_0)(-1 + 2(\gamma_1 + \gamma_2)(\gamma_3 + \gamma_4)), \quad (4)$$

where the subscript 0 refers to the value at the current grid point, and the subscripts 1, 2, 3, and 4 refer to values to the left, right, up, and down of the current grid point.

The values of  $\gamma$  are determined by

$$\gamma_i = \begin{cases} \frac{\phi_0}{\phi_0 - \phi_i} & \text{if } |\phi_0| < |\phi_i| \text{ and } \text{sign}(\phi_0) \neq \text{sign}(\phi_i), \\ 0.5 & \text{otherwise.} \end{cases} \quad (5)$$

for  $i = 1, 2, 3, 4$ .

### 4 Topology update

The topology defined by  $\phi$  can be dynamically updated by specifying a desired change in  $p$ ,  $\Delta p$ . A realizable change in  $p$ ,  $\Delta p$ , is then computed by first finding the matrix  $\partial p / \partial \phi$ ,

$$\frac{\partial p}{\partial \phi} = \frac{\partial p}{\partial \gamma} \frac{\partial \gamma}{\partial \phi}, \quad (6)$$

where

$$\frac{\partial p_0}{\partial \gamma_i} = \begin{cases} 2\text{sign}(\phi)(\gamma_3 + \gamma_4) & \text{for } i = 1, 2, \\ 2\text{sign}(\phi)(\gamma_1 + \gamma_2) & \text{for } i = 3, 4. \end{cases} \quad (7)$$

and for  $i = 1, 2$

$$\frac{\partial \gamma_i}{\partial \phi_0} = \begin{cases} \frac{-\phi_i}{(\phi_0 - \phi_i)^2} & \text{if } |\phi_0| < |\phi_i| \text{ and } \text{sign}(\phi_0) \neq \text{sign}(\phi_i), \\ 0 & \text{otherwise.} \end{cases} \quad (8)$$

$$\frac{\partial \gamma_i}{\partial \phi_i} = \begin{cases} \frac{-\phi_0}{(\phi_0 - \phi_i)^2} & \text{if } |\phi_0| < |\phi_i| \text{ and } \text{sign}(\phi_0) \neq \text{sign}(\phi_i), \\ 0 & \text{otherwise.} \end{cases} \quad (9)$$

and for  $i = 3, 4$

$$\frac{\partial \gamma_i}{\partial \phi_0} = \begin{cases} \frac{-\phi_i}{(\phi_0 - \phi_i)^2} & \text{if } |\phi_0| \leq |\phi_i| \text{ and } \text{sign}(\phi_0) \neq \text{sign}(\phi_i), \\ 0 & \text{otherwise.} \end{cases} \quad (10)$$

$$\frac{\partial \gamma_i}{\partial \phi_i} = \begin{cases} \frac{-\phi_0}{(\phi_0 - \phi_i)^2} & \text{if } |\phi_0| \leq |\phi_i| \text{ and } \text{sign}(\phi_0) \neq \text{sign}(\phi_i), \\ 0 & \text{otherwise.} \end{cases} \quad (11)$$

Once we have  $\partial p / \partial \phi$  then we solve the following for  $\Delta \phi$ ,

$$\text{minimize } \|\Delta \phi\|^2 \quad (12)$$

$$\text{subject to } \Delta \hat{p} = \frac{\partial p}{\partial \phi} \Delta \phi. \quad (13)$$

$p + \Delta p$  is then given by converting  $\phi + \Delta \phi$  to fractional-filling. In general, there will be a large discrepancy between  $p + \Delta p$  and  $p + \Delta \hat{p}$  because only certain fractional-fillings correspond to valid topologies. However, for

$$\lim_{\|\Delta \hat{p}\| \rightarrow 0} \|\Delta p - \Delta \hat{p}\| = 0 \quad (14)$$

if  $\Delta \hat{p} = 0$  wherever  $p = -1, +1$ .

## 5 Island nucleation

When performing a topological update, the nucleation of islands can be performed. An island can be formed where  $\phi_{0,1,2,3,4}$  all equal either -1 or +1, and where  $\Delta \hat{p}_0$  is of opposite sign. In this case,

$$\phi_0 = \frac{\sqrt{\Delta p}}{\sqrt{\Delta p} - 2\sqrt{2}} \phi_i. \quad (15)$$