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.

ϕ Level-set function defined on grid. The zero-crossing of ϕ 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 ϕ 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 ϵ is the smallest positive number available.
2. For all $\hat{\phi}_i$ not adjacent to a boundary point, fix the corresponding ϕ_i as
$$\phi_i = \text{sign}(\hat{\phi}_i) = \begin{cases} -1 & \text{if } \hat{\phi}_i < 0, \\ +1 & \text{if } \hat{\phi}_i > 0. \end{cases} \tag{1}$$
3. To determine the remaining ϕ_i, solve the following:
$$\begin{aligned} \text{minimize} \quad & \|\phi - \text{sign}(\hat{\phi})\|^2 & (2) \\ \text{subject to} \quad & A\phi = 0, & (3) \end{aligned}$$
where A is a matrix which fixes the boundary points by forcing the ratio of the two adjacent values of ϕ_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,

$$p_0 = \mathrm{sign}(\phi_0)((\gamma_1 + \gamma_2) + (\gamma_3 + \gamma_4) - 1), \tag{4}$$

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 γ are determined by

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

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

4 Topology update

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

$$\frac{\partial p}{\partial \phi} = \frac{\partial p}{\partial \gamma}\frac{\partial \gamma}{\partial \phi}, \tag{6}$$

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

$$\frac{\partial p_0}{\partial \gamma_i} = \mathrm{sign}(\phi) \tag{7}$$

and for $i = 1, 3$

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

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

and for $i = 2, 4$

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

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

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

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

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

$p + \Delta p$ 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

$$\lim_{\|\Delta\hat{p}\|\to 0} \|\Delta p - \Delta\hat{p}\| = 0 \tag{14}$$

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,

$$\phi_0 = \frac{\sqrt{\Delta p}}{\sqrt{\Delta p} - 2\sqrt{2}}\phi_i. \tag{15}$$

A Minimum-distance with equality constraints solver

The numerical problems in regularization and topology updates can be cast into the following form,

$$\begin{aligned} \text{minimize} \quad & \|x - x_0\|^2 && (16) \\ \text{subject to} \quad & Ax = b && (17) \end{aligned}$$

whose solution, if A is non-singular, is

$$x = x_0 - A^T(AA^T)^{-1}(Ax_0 - b). \tag{18}$$

Unfortunately, if A is singular, which it often will be for our purposes, one needs to eliminate linearly-dependent rows of A. This can be accomplished using QR-factorization to find the linearly-dependent rows of A and eliminate them, as well as the corresponding entries in b.