Approximation and computation for a photolithography problem

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Photolithography is a key process in the production of integrated circuits.
The mathematical model

**Mask:** $D \subset B_R \subset \mathbb{R}^2$ modeled by

$$m(x) = \chi_D(x)$$

**Light intensity:** $I(x)$

$$I(x) = \int \int m(\xi)K(x - \xi)J(\xi - \eta)K(x - \eta)m(\eta)d\xi d\eta$$

**Coherent point spread function:** $K(x)$

**Mutual intensity function:** $J(x)$ (partial coherence)

**Full coherence:** $J \equiv 1$

$$v(x) = (K \ast m)(x) = \int m(\xi)K(x - \xi)d\xi$$

$$I(x) = v(x)^2 = \int \int m(\xi)K(x - \xi)K(x - \eta)m(\eta)d\xi d\eta$$
The mathematical model: notation

Notation: Jinc function

$$\text{Jinc}(x) = \frac{J_1(\|x\|)}{2\pi\|x\|}, \quad x \in \mathbb{R}^2$$

Note:

$$\widehat{\text{Jinc}}(\xi) = \chi_{B_1}(\xi), \quad \xi \in \mathbb{R}^2$$

Notation: given a function $f$ on $\mathbb{R}^2$, $s > 0$

$$f_s(x) = s^{-2}f(x/s)$$

Note:

$$\|f_s\|_{L^1} = \|f\|_{L^1} \quad \text{and} \quad \hat{f_s}(\xi) = \hat{f}(s\xi)$$
The mathematical model: choice of $K$

The model for $K$

Wavenumber of light: $k > 0$
Numerical aperture: $NA > 0$

$$s = (kNA)^{-1}$$

$$K(x) = \text{Jinc}_s(x) = \frac{kNA}{2\pi} \frac{J_1(kNA\|x\|)}{\|x\|}$$

Remark:

$$\hat{K}(\xi) = \chi_{B_1}(s\xi) = \chi_{B_{1/s}}(\xi) = \chi_{B_{kNA}}(\xi)$$

Remark: if $NA \to +\infty$, that is $s \to 0^+$, then $\hat{K} \to 1$ pointwise, thus $K \to \delta_0$

Remark: $K \in C^{1,\alpha}(\mathbb{R}^2)$ for some $0 < \alpha \leq 1$
The mathematical model: choice of $J$

The model for $J$

Coherency coefficient: $\sigma > 0$

$$J(x) = 4\pi \text{Jinc}((\sigma/s)x) = 2 \frac{J_1((\sigma/s)\|x\|)}{(\sigma/s)\|x\|}$$

Remark:

$$\frac{1}{(2\pi)^2} \hat{J}(\xi) = \frac{1}{\pi(\sigma/s)^2} \chi_B_{\sigma/s}(\xi)$$

Remark: if $\sigma/s \to 0$, then $\hat{J}/(2\pi)^2 \to \delta_0$, thus $J \to 1$ pointwise
From a generalized mask to the light intensity

Notation: \( \text{fix } R > 0 \)

\[
A = \{ u \in L^1(\mathbb{R}^2) : \ 0 \leq u \leq 1 \text{ and } u = 0 \text{ outside } B_R \}
\]

Fixed \( s \) and \( \sigma \), for any \( u \in A \) let \( I = J(u) \) be the light intensity where

\[
J(u)(x) = \int \int u(\xi)K(x - \xi)J(\xi - \eta)K(x - \eta)u(\eta)d\xi d\eta
\]

Properties of the operator \( J \):
\[
J : A \rightarrow C^{1,\alpha}(\mathbb{R}^2)
\]

(i) \( J(u) \geq 0 \)

(ii) for any \( r > 0 \), there exists \( C > 0 \) such that

\[
\| J(u) \|_{C^{1,\alpha}(B_r)} \leq C
\]

(iii) for any \( r > 0 \), \( J \) is uniformly continuous with respect to the \( L^1 \) norm on \( A \) and the \( C^{1,\alpha} \) norm on \( C^{1,\alpha}(B_r) \)

(iv) \( J(u) \rightarrow 0 \) uniformly as \( \| x \| \rightarrow +\infty \), uniformly with respect to \( u \)
From a generalized mask to the circuit

\( u \in A \) generalized mask; \( I(u) \) corresponding light intensity

Threshold: \( h > 0 \)

Heaviside function: \( \mathcal{H} \)

Superlevel set at level \( h \): for any \( u \in A \)

\[
\Omega(u) = \{ x : I(u)(x) > h \}
\]

\[
\mathcal{W}(u)(x) = \mathcal{H}(I(u)(x) - h) = \chi_{\Omega(u)}(x)
\]

For any mask \( D \subset B_R \) the corresponding constructed circuit \( \Omega \) is

\[
\Omega(D) = \Omega(\chi_D)
\]

- There exists \( R_1 \geq R \) such that \( \Omega(u) \subseteq B_{R_1} \) for any \( u \in A \)
- \( I \) uniformly continuous from \( A \) into \( C^{1,\alpha}(B_{R_1}) \)
Setting of the optimization problem

Desired circuit to be constructed: $\Omega_0$

**Aim**

Find $D \subset B_R$ such that

$$\Omega(D) = \Omega_0$$

**Assumptions on $\Omega_0$:** $\Omega_0 \subset B_R$, regular enough (e.g. with finite perimeter)

**Remark:** there may be no $u \in A$ such that $\Omega(u) = \Omega_0$

**Optimization problem**

$$\min_{D \subset B_R} d(\Omega(D), \Omega_0)$$

**Issues:**

- Class $M$ of admissible masks
- Distance $d$ between two sets
- Instability and computational issues
Literature


This talk:

Admissible masks

\[ \mathcal{M} = \{ \mathcal{D} \subset B_R : \mathcal{D} \text{ is a set of finite perimeter} \} \]

Perimeter functional: define \( \mathcal{P} : A \subset L^1(\mathbb{R}^2) \rightarrow [0, +\infty] \) such that

\[
\mathcal{P}(u) = \begin{cases} 
P(E) \text{ perimeter of } E & \text{if } u = \chi_E, \ E \subset B_R, \\
+\infty & \text{otherwise}
\end{cases}
\]

Remark: if \( E \subset B_R \), set of finite perimeter, the perimeter of \( \mathcal{D} \)

\[
P(E) = \mathcal{P}(\chi_E) = |D\chi_E|(B_{R+1}) = TV(\chi_E, B_{R+1})
\]

Remark: identifying sets with characteristic functions

\[ \mathcal{M} = \{ u \in A : \mathcal{P}(u) < +\infty \} \]
The choice of the distance

Fix $R_1 > 0$ and assume $\Omega_1, \Omega_2 \subseteq B_{R_1}$

We measure the distance between $\Omega_1$ and $\Omega_2$ as follows

- **$L^1$ distance**
  \[
  d_1(\Omega_1, \Omega_2) = |\Omega_1 \Delta \Omega_2| = \int |\chi_{\Omega_1} - \chi_{\Omega_2}|
  \]

Possible variant:

- **strict convergence distance**
  \[
  d_{st}(\Omega_1, \Omega_2) = \int |\chi_{\Omega_1} - \chi_{\Omega_2}| + a |P(\Omega_1) - P(\Omega_2)|
  \]
The choice of the distance

Fix $R_1 > 0$ and assume $\Omega_1, \Omega_2 \in B_{R_1}$

We measure the distance between $\Omega_1$ and $\Omega_2$ as follows

- **$L^1$ distance**

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d_1(\Omega_1, \Omega_2) = |\Omega_1 \Delta \Omega_2| = \int |\chi_{\Omega_1} - \chi_{\Omega_2}|
\]

Possible variant:

- **strict convergence distance**

\[
d_{st}(\Omega_1, \Omega_2) = \int |\chi_{\Omega_1} - \chi_{\Omega_2}| + a|P(\Omega_1) - P(\Omega_2)| = d_{st}(\chi_{\Omega_1}, \chi_{\Omega_2})
\]

Remark: if $\nu_1, \nu_2 \in BV(B_{R_1})$

\[
d_{st}(\nu_1, \nu_2) = \int_{B_{R_1}} |\nu_1 - \nu_2| + a||D\nu_1||B_{R_1}) - |D\nu_2||(B_{R_1})|
\]
Regularized minimization problem

Our variational approach
Abstract framework

\[ J : \mathcal{A} \rightarrow C^{1,\alpha}(\mathbb{R}^2) \]

Fix a threshold \( h > 0 \) and a desired circuit \( \Omega_0 \subset \mathbb{R}^2 \)

Suplevel set at level \( h \): for any \( u \in \mathcal{A} \)

\[ \Omega(u) = \{ x : J(u)(x) > h \} \]

\[ \mathcal{W}(u)(x) = \mathcal{H}(J(u)(x) - h) = \chi_{\Omega(u)}(x) \]

Optimization problem

\[ \min \{ d(\Omega(D), \Omega_0) : D \in \mathcal{M} \} \]
Abstract framework

\[ J : \mathcal{A} \rightarrow C^{1,\alpha}(\mathbb{R}^2) \]

Fix a threshold \( h > 0 \) and a desired circuit \( \Omega_0 \subset \mathbb{R}^2 \)

Suplevel set at level \( h \): for any \( u \in \mathcal{A} \)

\[ \Omega(u) = \{ x : J(u)(x) > h \} \]

\[ W(u)(x) = H(J(u)(x) - h) = \chi_{\Omega(u)}(x) \]

Optimization problem

\[ \min \{ d(\Omega(u), \Omega_0) : u \in \mathcal{M} \text{ i.e. } u \in \mathcal{A} \text{ and } P(u) < +\infty \} \]
Abstract framework

\[ J : A \rightarrow C^{1,\alpha}(\mathbb{R}^2) \]

Fix a threshold \( h > 0 \) and a desired circuit \( \Omega_0 \subset \mathbb{R}^2 \)
Suplevel set at level \( h \): for any \( u \in A \)

\[ \Omega(u) = \{ x : J(u)(x) > h \} \]
\[ W(u)(x) = \mathcal{H}(J(u)(x) - h) = \chi_{\Omega(u)}(x) \]

Optimization problem

\[ \min \{ d(\Omega(u), \Omega_0) : u \in M \text{ i.e. } u \in A \text{ and } \mathcal{P}(u) < +\infty \} \]

Properties of \( J \):

- There exists \( R_1 \geq R \) such that \( \Omega(u) \subset B_{R_1} \) for any \( u \in A \)
- \( J \) uniformly continuous from \( A \) into \( C^{1,\alpha}(B_{R_1}) \)

Assumptions on \( \Omega_0 \): \( \Omega_0 \subset B_R \), regular enough (e.g. with finite perimeter)
Difficulties

Instability:

- small perturbations of \( u \) may lead to large perturbations of \( \Omega(u) \)
- changes in the topology of \( \Omega(u) \), e.g. in the number of connected components

Crucial remark: such issues happen only if \( h \) is a critical value of \( I(u) \)

Computational issues:

- difficult to minimize on an admissible class of sets
- nonlinearity and noncontinuity of the thresholding operation
- difficult to compute quantities related to \( \Omega(u) \), such as its perimeter
Regularization on the independent variable

Perimeter penalization

\[ \min \{ d(\Omega(D), \Omega_0) : D \in \mathcal{M} \} \]

\[ \sim \]

\[ \min \{ d(\Omega(D), \Omega_0) + bP(D) : D \in \mathcal{M} \} \]
Regularization on the independent variable

Perimeter penalization

\[ \min \left\{ d(\Omega(D), \Omega_0) : D \in \mathcal{M} \right\} \]

\[ \mapsto \]

\[ \min \left\{ d(\Omega(D), \Omega_0) + bP(D) : D \in \mathcal{M} \right\} \]

that is, if \( d = d_1 \),

\[ \min_{u \in A} \left( \int |W(u) - \chi_{\Omega_0}| + bP(u) \right) \]

where

\[ W(u)(x) = \mathcal{H}(J(u)(x) - h) = \chi_{\Omega(u)}(x) \]

and

\[ \Omega(D) = \Omega(\chi_D) \text{ if } u = \chi_D \in \mathcal{M} \]
Regularization on the dependent variable: auxiliary functions

Let $f : \mathbb{R} \to [0, +\infty]$ continuous decreasing such that

(i) $f \equiv +\infty$ on $(-\infty, 0]$  
(ii) $f \equiv 0$ on $[\delta, +\infty)$, for some $\delta > 0$  
(iii) \[ \lim_{s \to 0^+} f(s)s^{2/\alpha} \geq C > 0 \]

Let $\varphi : \mathbb{R} \to \mathbb{R} C^1$ such that

(i) $\varphi(h) > 0$  
(ii) $\varphi$ is increasing before $h$ and decreasing after $h$  
(iii) $\varphi(h \pm \delta_0) < -\delta$, for some $\delta_0$, $0 < \delta_0 \leq h/2$
Auxiliary functions

function $f$

function $\varphi$
Define $\mathcal{R} : \Lambda \to [0, +\infty]$ such that

$$\mathcal{R}(u) = \int_{B_{R_1}} f \left( \|\nabla (I(u))\|^2 - \varphi(I(u)) \right)$$

for suitable auxiliary functions $f$ and $\varphi$

**Remark:** by the uniform decay at infinity, for any $u \in \Lambda$ we have

$$\mathcal{R}(u) = \int_{B_{R_1}} f \left( \|\nabla (I(u))\|^2 - \varphi(I(u)) \right)$$

$$\int |\mathcal{W}(u) - \chi_{\Omega_0}| = \int_{B_{R_1}} |\mathcal{W}(u) - \chi_{\Omega_0}|$$

$$P(\Omega(u)) = TV(\mathcal{W}(u)) = |D(\mathcal{W}(u))|(B_{R_1})$$
Consequences of the regularization

How it works:
- let $I(u) = h$; if $\|\nabla(I(u))\|^2$ is not greater than $\varphi(h) > 0$ then
  $$\|\nabla(I(u))\|^2 - \varphi(I(u)) < 0 \quad \text{and} \quad f(\|\nabla(I(u))\|^2 - \varphi(I(u))) = +\infty$$
- if $|I(u) - h| \geq \delta_0$ then
  $$\|\nabla(I(u))\|^2 - \varphi(I(u)) \geq \delta \quad \text{and} \quad f(\|\nabla(I(u))\|^2 - \varphi(I(u))) = 0$$

What it means:
- only $u \in A$ such that $h$ is not a critical value of $I(u)$ are competitors for the minimization problem
- no effect on the behavior of $I(u)$ at values away from $h$

Advantages:
- **Stability:** stability of $\Omega(u)$ under small perturbations of $u$ and $h$
- **Computations:** allows to approximate the Heaviside function, thus the binary function $\mathcal{W}(u)$, with a smooth function

Drawback:
- we cannot recover $\Omega_0$ exactly if $\Omega_0$ is not smooth (e.g. it has corners)
Let $1 \leq p < +\infty$, $a \geq 0$, $b > 0$, $c > 0$.

Define $F_0 : A \to [0, +\infty]$ such that

$$F_0(u) = \int_{B_{R_1}} |\mathcal{W}(u) - \chi_{\Omega_0}|^p + a |\text{D}(\mathcal{W}(u))| (B_{R_1}) - \mathcal{P}(\Omega_0)| + b \mathcal{P}(u) + c \mathcal{R}(u)$$

where $\mathcal{W}(u)(x) = \mathcal{H}(J(u)(x) - h)$
Existence of minimizers

Regularized minimization problem

\((MP_0)\) \hspace{2cm} \min_{u \in A} F_0(u)

A priori assumptions on minimizers of \(F_0\): there exists \(\tilde{u} \in A\) such that \(F_0(\tilde{u})\) is finite and such that \(F_0(\tilde{u}) < |\Omega_0| + aP(\Omega_0)\).

Proposition

- There exists \(u\) minimizer of \(F_0\)
- For any minimizer \(u\) of \(F_0\) we have that \(\Omega(u)\) is not empty
- The function \(u_0 \equiv 0\) is not a minimizer of \(F_0\)
The regularized minimization problem

Approximation and computational approach
Approximation of $\mathcal{W}(u)$

Notation: $\phi \in C^\infty(\mathbb{R})$, increasing, $\phi \equiv 0$ on $(-\infty, -1]$, $\phi \equiv 1$ on $[1, +\infty)$

Fix the approximation parameter $\varepsilon > 0$

$$\mathcal{W}(u) = \mathcal{H}(I(u) - h)$$

$$\mathcal{W}_\varepsilon(u) = \phi \left( \frac{I(u) - h}{\varepsilon} \right)$$

$$d_p(\mathcal{W}(u), \chi_{\Omega_0}) = \int_{B_{R_1}} |\mathcal{W}(u) - \chi_{\Omega_0}|^p + a \|D\mathcal{W}(u)||_{(B_{R_1})} - P(\Omega_0)|$$

$$d_p(\mathcal{W}_\varepsilon(u), \chi_{\Omega_0}) = \int_{B_{R_1}} |\mathcal{W}_\varepsilon(u) - \chi_{\Omega_0}|^p + a \left| \int_{B_{R_1}} \|
abla(\mathcal{W}_\varepsilon(u))\|_{(B_{R_1})} - P(\Omega_0) \right|$$
Approximation of the perimeter functional $\mathcal{P}$

Let $V$ be a double-well potential centered at 0 and 1.

For instance $V(t) = t^2(t-1)^2$

or $V(t) = |t||t-1|

For any $\varepsilon > 0$ the Modica-Mortola functional $MM_\varepsilon : \Lambda \rightarrow [0, +\infty]$ is

$$MM_\varepsilon(u) = \begin{cases} 
\int_{B_R} \left( \frac{c_2}{2\varepsilon} V(u) + \frac{c_2\varepsilon}{2} \|\nabla u\|^2 \right) & \text{if } u \in H^1_0(B_R, [0, 1]) \\
+\infty & \text{otherwise}
\end{cases}$$

$$\mathcal{P}(u) \sim MM_\varepsilon(u) = \frac{c_2}{2\varepsilon} \int_{B_R} |u||u-1| + \frac{c_2\varepsilon}{2} \int_{B_R} \|\nabla u\|^2$$
Approximation of the regularization functional $\mathcal{R}$

For any $\varepsilon > 0$ define $f_\varepsilon : \mathbb{R} \rightarrow [0, +\infty)$ s.t.

- $f_\varepsilon$ is continuous decreasing
- $f_{\varepsilon_1} \leq f_{\varepsilon_2} \leq f$ for any $0 < \varepsilon_2 \leq \varepsilon_1$
- $\lim_{\varepsilon \to 0^+} f_\varepsilon(s) = f(s)$ for any $s \in \mathbb{R}$

\[
\mathcal{R}(u) = \int_{B_{R_1}} f \left( \|\nabla (I(u))\|^2 - \varphi(I(u)) \right)
\]

$\sim$ \[
\mathcal{R}_\varepsilon(u) = \int_{B_{R_1}} f_\varepsilon \left( \|\nabla (I(u))\|^2 - \varphi(I(u)) \right)
\]
Approximated functional

Define $F_\varepsilon : \mathcal{A} \to [0, +\infty]$ such that for any $u \in \mathcal{A}$

$$F_\varepsilon (u) = d_p (W_\varepsilon (u), \chi_{\Omega_0}) + bM M_\varepsilon (u) + cR_\varepsilon (u)$$

If $u \in H^1_0(B_R, [0, 1])$

$$F_\varepsilon (u) = \int_{B_{R_1}} |W_\varepsilon (u) - \chi_{\Omega_0}|^p + a \left| \int_{B_{R_1}} \|\nabla (W_\varepsilon (u))\| - P(\Omega_0) \right| + b \left( \frac{c_2}{2\varepsilon} \int_{B_R} |u| |u - 1| + \frac{c_2\varepsilon}{2} \int_{B_R} \|\nabla u\|^2 \right)$$

$$+ c \left( \int_{B_{R_1}} f_\varepsilon (\|\nabla (I(u))\|^2 - \varphi (I(u))) \right)$$

and $F_\varepsilon (u) = +\infty$ otherwise
Existence and convergence of minimizers

Approximated minimization problem

\[(\text{MP}_\varepsilon) \quad \min_{u \in H^1_0(B_R, [0,1])} F_\varepsilon(u)\]

Let \(\varepsilon_n > 0\) be such that \(\lim_n \varepsilon_n = 0\). There exists \(u_n\) solution to the approximated minimization problem \((\text{MP}_\varepsilon)\):

Convergence of minimizers

Up to a subsequence

\[u_n \rightarrow u \quad \text{in} \ L^1\]

where \(u\) is a solution to the regularized minimization problem

\[(\text{MP}_0) \quad \min_{u \in \mathcal{A}} F_0(u)\]
The approximated minimization problem

Numerical experiments
Minimization problem

We solve numerically the approximated minimization problem with \( p = 2, \alpha = 0 \), that is

\[
\begin{align*}
\text{(MP}_\varepsilon) & \quad \min_{u \in H^1_0(B_R, [0,1])} F_\varepsilon(u) \\
F_\varepsilon(u) & = \int_{B_{R_1}} |\mathcal{W}_\varepsilon(u) - \chi_{\Omega_0}|^2 \\
& \quad + b \left( \frac{c_2}{2\varepsilon} \int_{B_R} |u - 1| + \frac{c_2\varepsilon}{2} \int_{B_R} \|\nabla u\|^2 \right) \\
& \quad + c \left( \int_{B_{R_1}} f_\varepsilon \left( \|\nabla (I(u))\|^2 - \varphi(I(u)) \right) \right)
\end{align*}
\]
The test target patterns and physical setting

Target 1

Target 2

Computational domain: 1600nm × 1600nm subdivided into 128 × 128 squares, each with sides of length 12.5nm

Physical and model parameters:

\[ \lambda = \frac{2\pi}{k} = 193\text{nm} \quad \text{NA} = 1 \quad \sigma = 0.067 \]
Target 1: initial guess

Initial guess

Mask

Output
Assist features

Without cut option

Mask – Initial guess n.1

Output – Initial guess n.1

With cut option

Mask – Initial guess n.1 – cut option

Output – Initial guess n.1 – cut option
Target 2: initial guess

Initial guess

Target 2 – Initial guess n.1

Mask

Mask – Initial guess n.1

Output

Output – Initial guess n.1

Target 2 – Initial guess n.2

Mask – Initial guess n.2

Output – Initial guess n.2
The role of the regularization $\mathcal{R}$

Remark: in the previous tests: $c = 0$ that is no regularization term $\mathcal{R}!$

Test 1: no change if we add the regularization term $\mathcal{R}$, the threshold $h$ is not close to a critical value of $I(u)$

Test 2: the threshold $h$ is close to a critical value of $I(u)$!

In order to show the role of the regularization term $\mathcal{R}$ we shall alter the value of the threshold $h$ by a percentage value of $h_{\text{var}}$ that is

$$\text{threshold} = h(100 + h_{\text{var}})/100$$
The role of the regularization $R$: first test (1)

**hvar = 0**

Top: $c = 0$. Bottom: $c = 5 \times 10^{-4}$. 

**hvar = 0.5**

**hvar = 2.5**
The role of the regularization $R$: first test (2)

$hvar = 0$

Output $- c=5e^{-4}, hvar=0$

$hvar = 0.5$

Output $- c=5e^{-4}, hvar=0.5$

$hvar = 2.5$

Output $- c=5e^{-4}, hvar=2.5$

Output $- c=2e^{-3}, hvar=0$

Output $- c=2e^{-3}, hvar=0.5$

Output $- c=2e^{-3}, hvar=2.5$

Top: $c = 5 \times 10^{-4}$. Bottom: $c = 2 \times 10^{-3}$. 
The role of the regularization $\mathcal{R}$: second test (1)

**hvar = $-0.5$**

Top: $c = 0$. Bottom: $c = 5 \times 10^{-4}$. 

**hvar = 0**

**hvar = 3.5**
The role of the regularization $R$: second test (2)

**$hvar = -0.5$**

- Top: $c = 5 \times 10^{-4}$. Bottom: $c = 2 \times 10^{-3}$.
The complete model

We add the term

\[ a \left| \int_{B_{R1}} \| \nabla (W_\varepsilon(u)) \| - P(\Omega_0) \right| \]

Parameters value: \( c = 5 \times 10^{-4}, \ a = 0.5 \)

Mask

Output