

Stochastic Truncated Wirtinger Flow Algorithm for Phase Retrieval using Boolean Coded Apertures

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ICASSP 2017



Outline

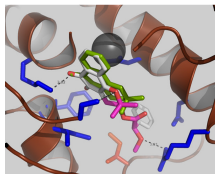
- 1 Crystallography
- 2 Feasible Modulation
- 3 Results
- 4 Conclusions and Future Work

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Crystallography

X-ray crystallography is an experimental technique used in material analysis that allows to measure the atomic positions of the elements present in a crystal.



Drug design



Mineralogy



New materials

Figure: Important applications of X-ray Crystallography

Coded Diffraction Patterns System

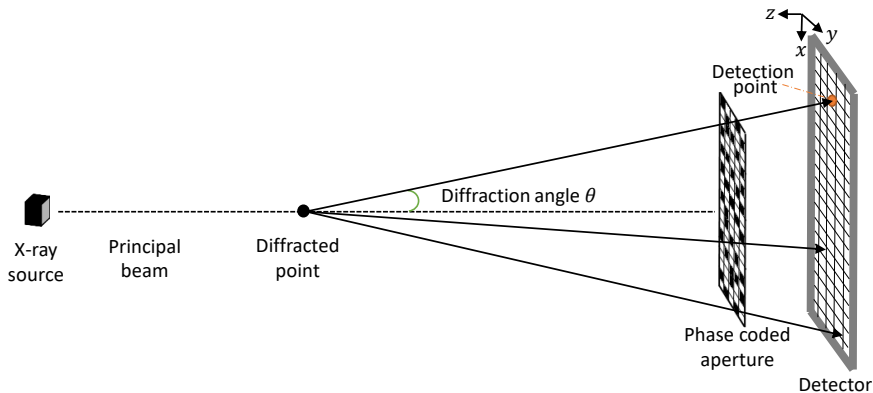


Figure: Coded diffraction pattern system¹.

¹Candes, E. J., Li, X., and Soltanolkotabi, M. (2015). Phase retrieval from coded diffraction patterns. *Applied and Computational Harmonic Analysis*, 39(2), 277-299.

Formulation

Coded Measurements

$$y_k^\ell = |\langle \mathbf{f}_k, \mathbf{G}^\ell \mathbf{x} \rangle|^2, k = 1, \dots, m,$$

where

- $\forall \ell \in \{1, \dots, L\}$, $\mathbf{G}^\ell \in \mathbb{C}^{n \times n}$ is a diagonal matrix.
- $\mathbf{f}_k \in \mathbb{C}^n$ are the rows of the 2D Discrete Fourier Transform matrix.
- $\mathbf{x} \in \mathbb{C}^n$ is unknown.
- $\ell = 1, \dots, L$ is the projection indexing variable.

Inverse Problem

Optimization Problem

$$\begin{aligned} \underset{\mathbf{x} \in \mathbb{C}^n}{\operatorname{argmin}} \quad & \sum_{k=1}^n \mu_k^2 - y_k \log(\mu_k) + \lambda \operatorname{Tr}(\mathbf{X}) \\ \text{subject to} \quad & \mu_k = \mathbf{a}_k^* \mathbf{X} \mathbf{a}_k, \quad k = 1, \dots, m, \\ & \mathbf{X} \succeq 0. \end{aligned}$$

The Truncated Wirtinger Flow Algorithm solves the optimization problem².

²Chen, Y., and Candes, E. (2015). Solving random quadratic systems of equations is nearly as easy as solving linear systems. In *Advances in Neural Information Processing Systems* (pp. 739-747).

TWF Algorithm Characteristics

TWF Reconstruction Algorithm Characteristics:

- It uses $\{i, -i\}$ codes.
- Maximum likelihood estimated is optimized.
- $\forall k \in \{1, \dots, m\}, \mathbf{a}_k \sim \mathcal{CN}(0, \mathbf{I})$.
- It requires truncation parameters, $(\alpha_0, \alpha_1, \alpha_2, \alpha_3)$.

Limitation

The implementation of $\{-i, i\}$ codes are impractical.

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Proposed Modulation

The main idea is to modified the TWF algorithm to adjust block-unblock coded apertures.

Binary Modulation

$$g = \begin{cases} -1 & \text{with probability } 1/2 \\ 1 & \text{with probability } 1/2 \end{cases}$$

where g is a Bernoulli random variable d . Remark that $\mathbb{E}[g] = 0$.

Coded Observation Model:

$$y_k^\ell = |\langle \mathbf{f}_k, \mathbf{G}^\ell \mathbf{x} \rangle|^2 = \overbrace{\left| \sum_{j=1}^n (\mathbf{f}_k)_j \mathbf{G}_{j,j}^\ell (\mathbf{x})_j \right|^2}^{v_k}, k = 1, \dots, m.$$

where $v_k \sim \mathcal{CN}(0, \sigma^2)$ inasmuch $n \rightarrow \infty$, by the Central Limit Theorem³.

³Arguello, H., and Arce, G. R. (2014). Colored coded aperture design by concentration of measure in compressive spectral imaging. *IEEE Transactions on Image Processing*, 23(4), 1896-1908.

Boolean Formulation

Definitions

- $\mathbf{D}^\ell = (\mathbf{G}^\ell + \mathbf{I})/2$

- $\mathbf{E}^\ell = \mathbf{I} - \mathbf{D}^\ell$

where $\mathbf{D}^\ell, \mathbf{E}^\ell \in \{0, 1\}^{n \times n}$ and \mathbf{I} is the identity matrix.

Feasible Implementation

$$\begin{aligned} y_k^\ell &= |\langle \mathbf{f}_k, \mathbf{G}^\ell \mathbf{x} \rangle|^2 \\ &= |\langle \mathbf{f}_k, (\mathbf{D}^\ell - \mathbf{E}^\ell) \mathbf{x} \rangle|^2 \\ &= 2(|\langle \mathbf{f}_k, \mathbf{D}^\ell \mathbf{x} \rangle|^2 + |\langle \mathbf{f}_k, \mathbf{E}^\ell \mathbf{x} \rangle|^2) - |\langle \mathbf{f}_k, \mathbf{x} \rangle|^2. \end{aligned}$$

Remark: The three terms can be implemented by using boolean coded apertures.

Truncated Parameters Estimation

MCMC Scheme

The truncation parameters satisfy that $\alpha_j \geq 0, j = 0, \dots, 3$.

- Independent Priors

$$\alpha_j \sim \frac{1}{\alpha_j \sqrt{2\pi}} \exp \left[\frac{-(\ln(x) - \mu_j)^2}{2\sigma_j^2} \right], \forall j = 0, \dots, 3.$$

- Decision Rule

$$p_r = \min \left\{ 1, \frac{\mathcal{P}(\mathbf{p}^{new} | \mu_0, \dots, \mu_3) q(\mathbf{p}^{old} | \mathbf{p}^{new})}{\mathcal{P}(\mathbf{p}^{old} | \mu_0, \dots, \mu_3) q(\mathbf{p}^{new} | \mathbf{p}^{old})} \right\}.$$

where $q(\mathbf{p}^{new} | \mathbf{p}^{old}) = \prod_{j=0}^3 \frac{1}{\alpha_j \sqrt{2\pi}} \exp \left[\frac{-(\ln(\mathbf{p}_j^{old}) - \mu_j)^2}{2\sigma_j^2} \right]$ and

$\mathbf{p} = [\alpha_0, \dots, \alpha_3]$.

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Stochastic Truncated Wirtinger Flow Algorithm

Algorithm 1 STWF-Algorithm¹

function STWF-ALGORITHM (\mathbf{y}, T)

$\{\tilde{\mathbf{a}}_k = \mathbf{G}\mathbf{f}_k \in \mathbb{C}^n \mid 1 \leq k \leq n\}$

$\{\alpha_0, \alpha_1, \alpha_2, \alpha_3\}$ (truncation parameters)

$$\lambda_0 \leftarrow \sqrt{\frac{1}{n} \sum_{k=1}^n y_k}$$

$$\mathbf{H} \leftarrow \frac{1}{n} \sum_{k=1}^n y_k \tilde{\mathbf{a}}_k \tilde{\mathbf{a}}_k^* \mathbf{1}_{\{|y_k| \leq \alpha_3 \lambda_0^2\}}$$

$$\mathbf{x}^{(0)} \leftarrow \sqrt{\frac{n^2}{\sum_{k=1}^n \|\tilde{\mathbf{a}}_k\|^2}} \lambda_0 \tilde{\mathbf{x}} \quad (\tilde{\mathbf{x}} \text{ is the leading eigenvector of } \mathbf{H})$$

for $t = 1$ to T **do**

$$\mathbf{x}^{(t+1)} \leftarrow \mathbf{x}^{(t)} + \frac{2\mu_t}{n} \sum_{k=1}^n \frac{(y_k - |\tilde{\mathbf{a}}_k^* \mathbf{x}^{(t)}|^2)}{\mathbf{x}^{(t)H} \tilde{\mathbf{a}}_k} \tilde{\mathbf{a}}_k \mathbf{1}_{\epsilon_1^k} \cap \epsilon_2^k$$

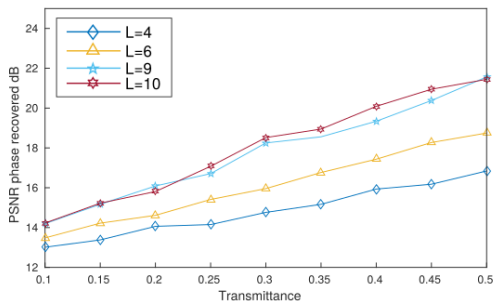
end for

return $\mathbf{x}^{(T)}$

end function

¹Candes, E. J., Li, X., and Soltanolkotabi, M. (2015). Phase retrieval from coded diffraction patterns. *Applied and Computational Harmonic Analysis*, 39(2), 277-299.

Simulations - Hadamard Structure



Hadamard Structure

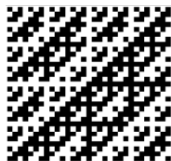
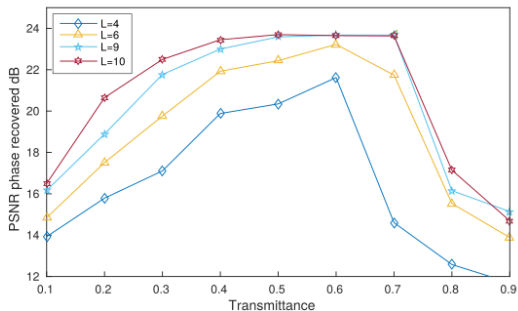


Figure: Performance in recovering the phase by Hadamard structure

Remark

- Optimal transmittance: 50%
- Optimal projections: $m = 9n$

Simulations - Random



Random

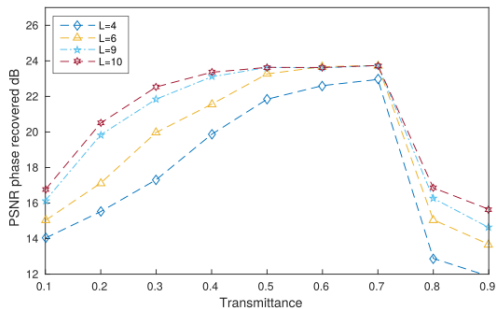


Figure: Performance in recovering the phase by random coded apertures

Remark

- Optimal transmittance: 50%
- Optimal projections: $m = 9n$

Simulations - DFT Pattern



DFT Pattern

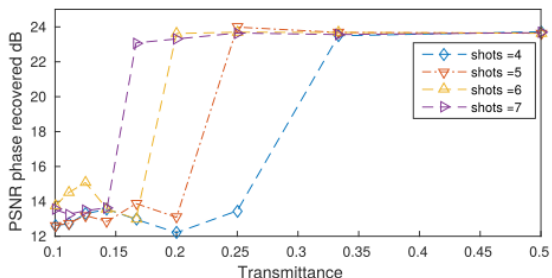


Figure: Performance in recovering the phase by DFT patterns

Remark

- Optimal transmittance: 50%
- Optimal projections: $m = 6n$

Simulations - Blue Noise Pattern



Blue Noise Pattern

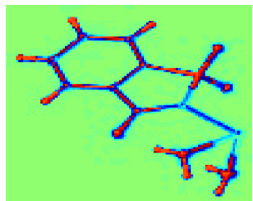


Figure: Performance in recovering the phase by Blue Noise Pattern

Remark

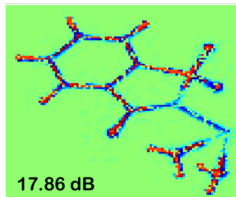
- Optimal transmittance: 50%
- Optimal projections: $m = 4n$

Reconstructions



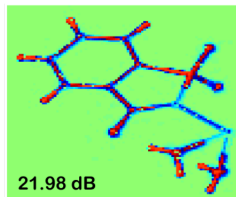
Original

Hadamard



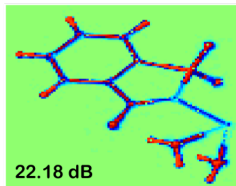
17.86 dB

Random



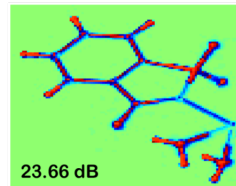
21.98 dB

DFT Pattern



22.18 dB

Blue Noise Pattern



23.66 dB

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Conclusion and Future Work

Conclusions

- The STWF algorithm is presented.
- Boolean modulation can be implemented for a coded crystallography system.
- MCMC scheme calculates the optimal truncated parameters.
- Blue noise pattern provides the highest reconstruction quality.

Prospects

- Optimize the coded apertures.
- Implement a real architecture for coded diffraction patterns.

Thanks!



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