Bridging High Performance Computing for Experimental Neutron Sciences

Rick Archibald

SIAM UQ – Stochastic Computing and Data Assimilation

April 17th, 2018

OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

UT-BATTELLE

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Motivation: Neutron Facilities

High Flux Isotope Reactor

One of the highest steady-state neutron flux research reactor in the world

Spallation Neutron Source

World's most powerful accelerator-based neutron source

Experimental Facilities

Motivation: Computational Facilities

OLCF
OAK RIDGE LEADERSHIP COMPUTING FACILITY

Some of the most advanced computing resources in the world

CADES

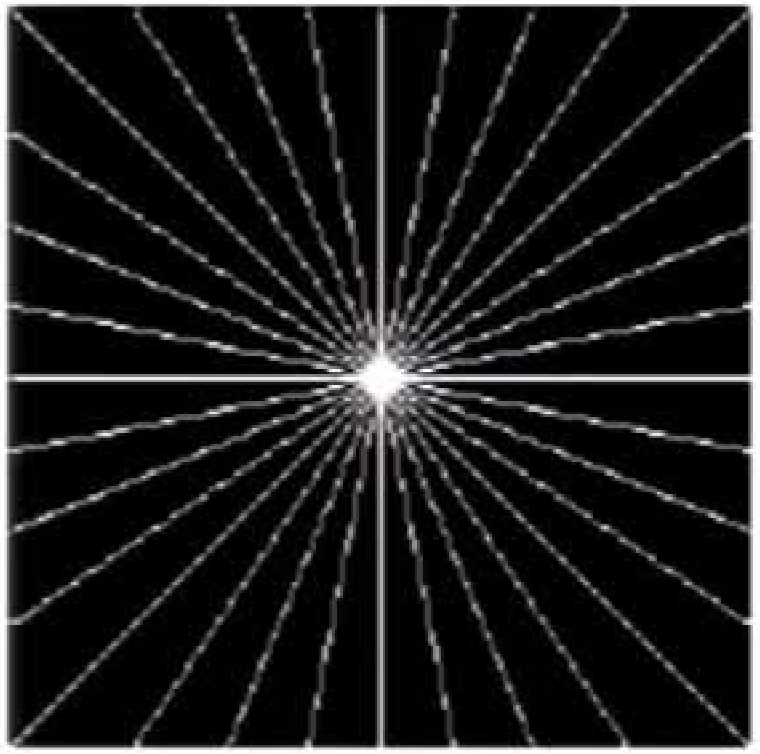
Partially Sampled Fourier Data

Determine $\mathbf{f} = \{f(x_i, y_j) : 0 \leq i, j \leq 2N\}$ that solves the convex optimization problem

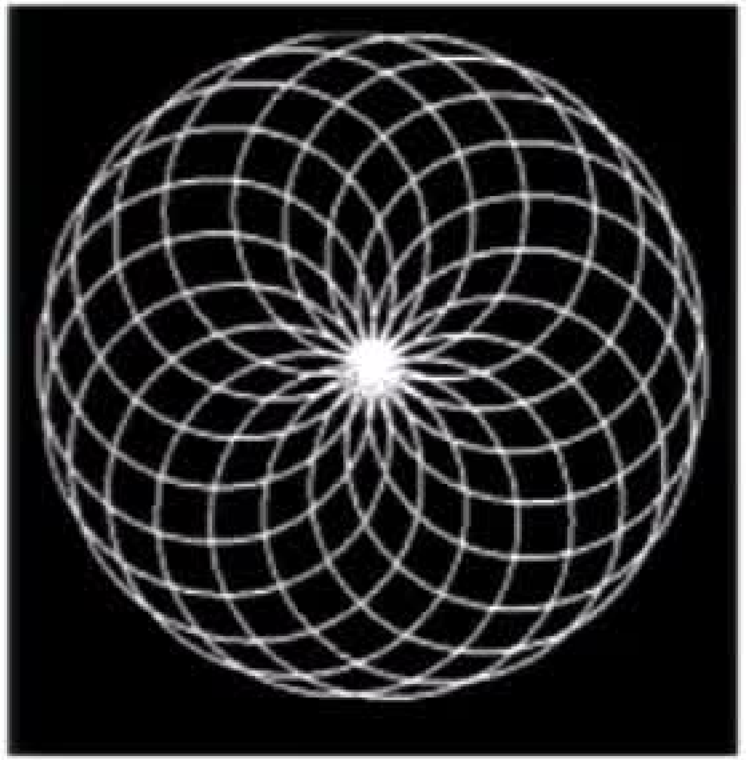
$$\begin{aligned} \text{minimize} \;\; & ||J_x\mathbf{f}||_1 + ||J_y\mathbf{f}||_1, \\ \text{subject to} \;\; & ||MF\mathbf{f} - \hat{\mathbf{f}}||_2 \leq \sigma, \end{aligned}$$

Where the matrix M is a mask that removes unknown Fourier coefficients.

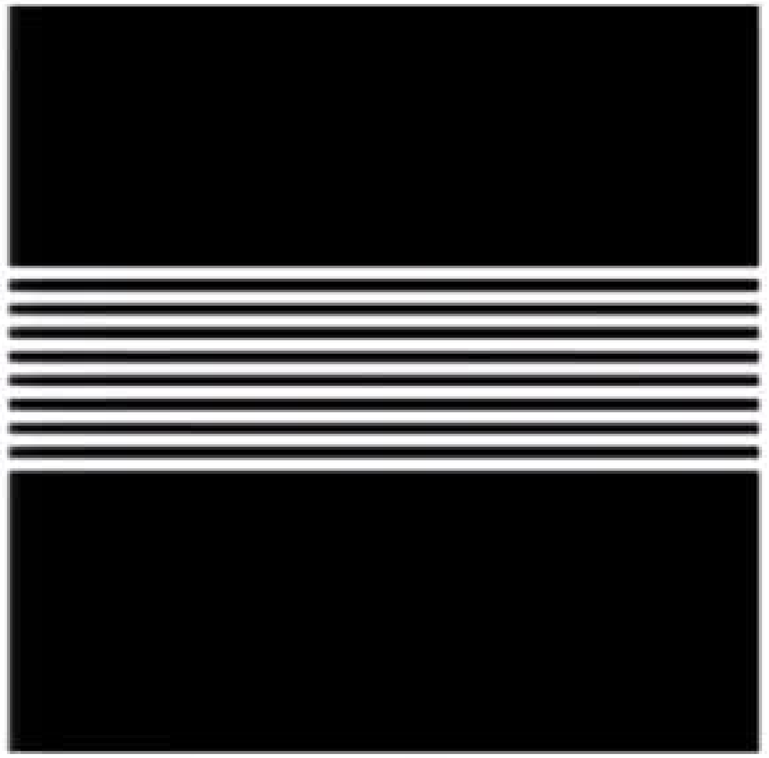
Modalities that fit partial Fourier Data



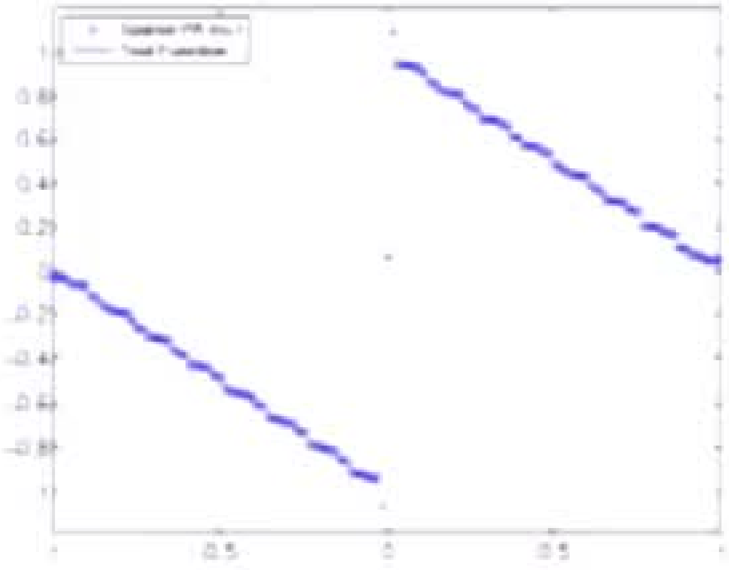
Tomography



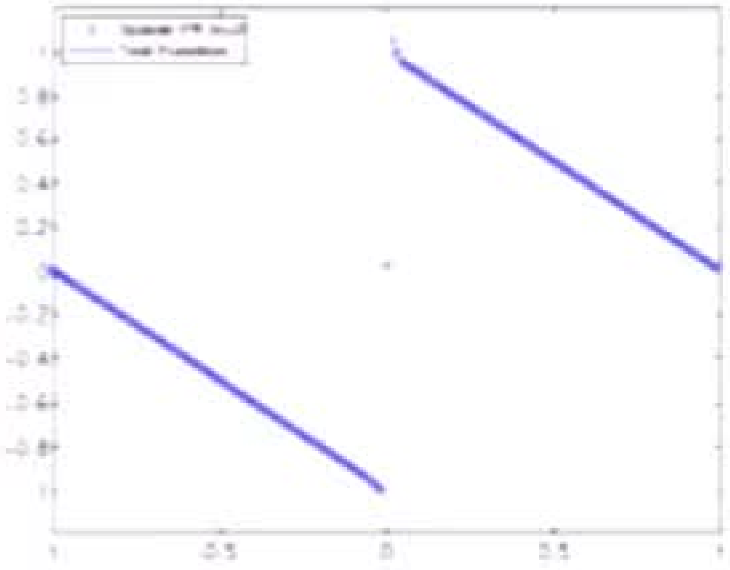
MRI



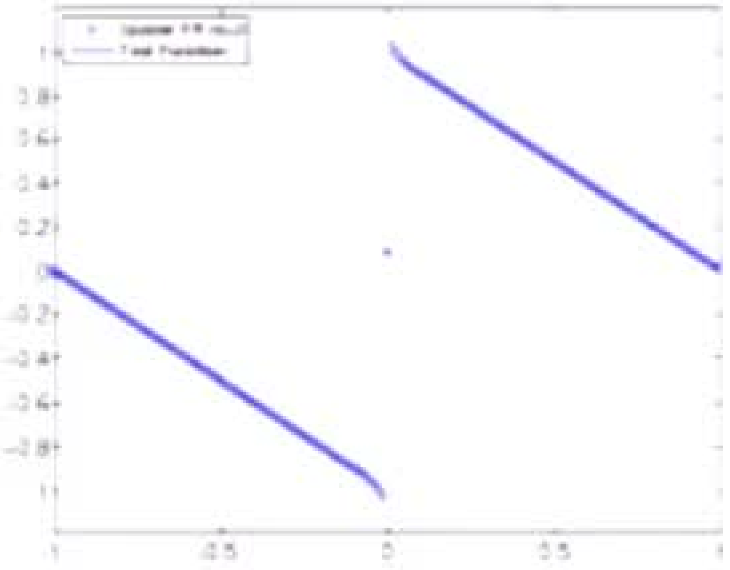
Ultrasound



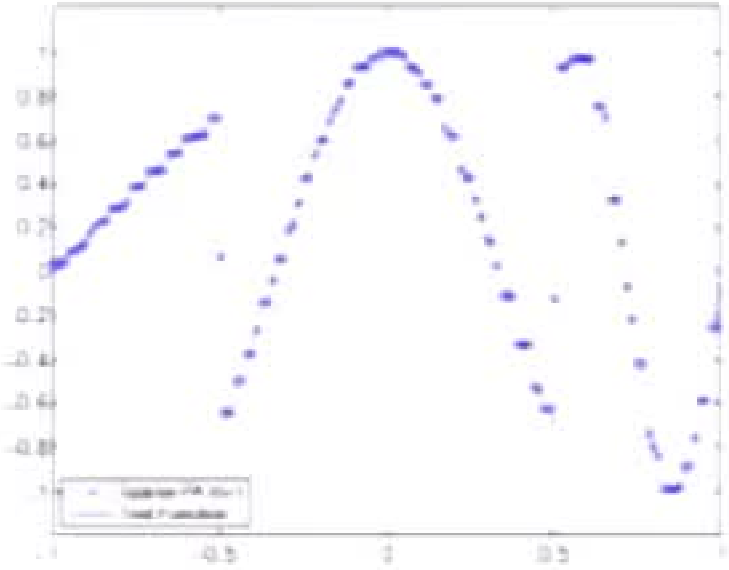
(a) PA l^1 regularization with $m = 1$ for f_a



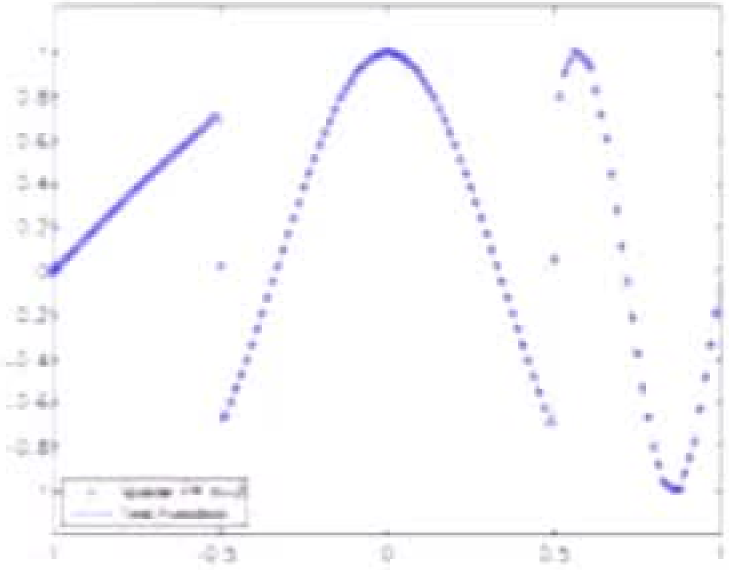
(b) PA l^1 regularization with $m = 2$ for f_a



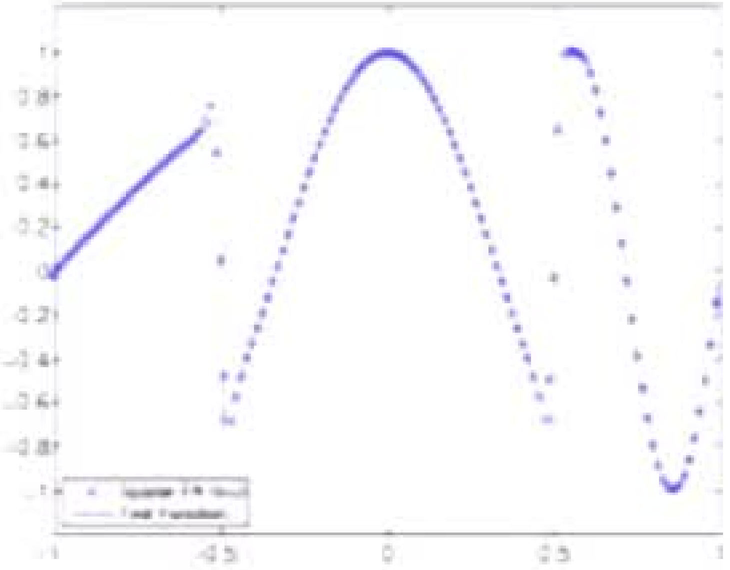
(c) PA l^1 regularization with $m = 3$ for f_a



(d) PA l^1 regularization with $m = 1$ for f_b



(e) PA l^1 regularization with $m = 2$ for f_b



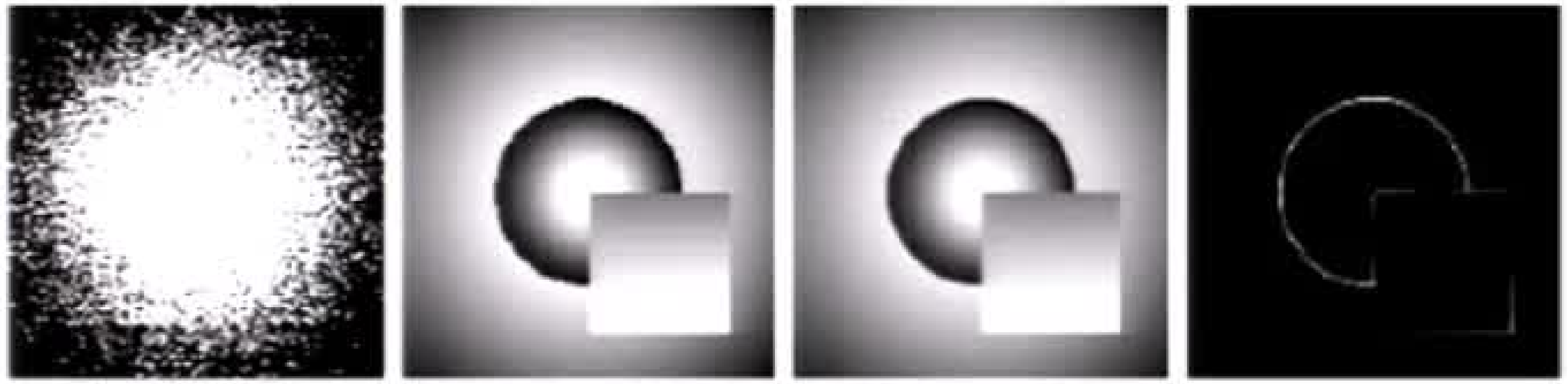
(f) PA l^1 regularization with $m = 3$ for f_b

$$\min_{\mathbf{f}} \quad ||\mathcal{F}\mathbf{f} - \hat{\mathbf{f}}||_2 + \lambda||L^m\mathbf{f}||_1$$

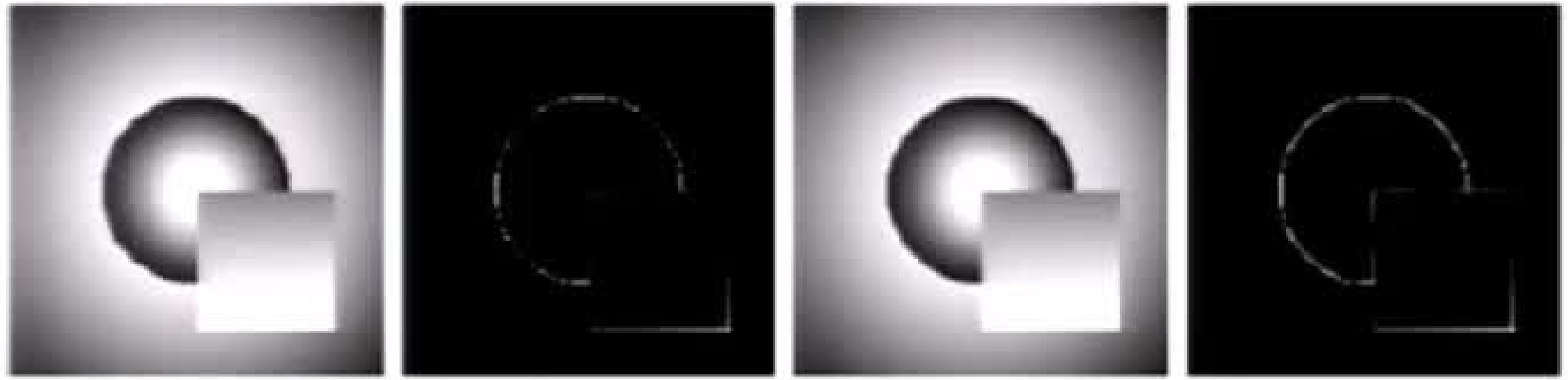
$$L^2 = \frac{1}{2}\begin{bmatrix} 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & & \vdots & & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -2 & 1 \end{bmatrix}$$

$$L^3 = \frac{1}{6}\begin{bmatrix} 1 & -3 & 3 & -1 & & \\ & 1 & -3 & 3 & -1 & \\ & & & \vdots & & \\ & & -1 & 3 & -3 & 1 \\ & & & 1 & 3 & -3 & 1 \end{bmatrix}$$

$$f_a(x) = \begin{cases} -1 - x & \text{if } -1 \le x < 0 \\ 1 - x & \text{otherwise} \end{cases} ; \quad f_b(x) = \begin{cases} \cos\frac{\pi x}{2} & \text{if } 1 \le x < -\frac{1}{2} \\ \cos\frac{3\pi x}{2} & \text{if } -\frac{1}{2} \le x < \frac{1}{2} \\ \cos\frac{7\pi x}{2} & \text{if } \frac{1}{2} \le x \le 1 \end{cases}$$



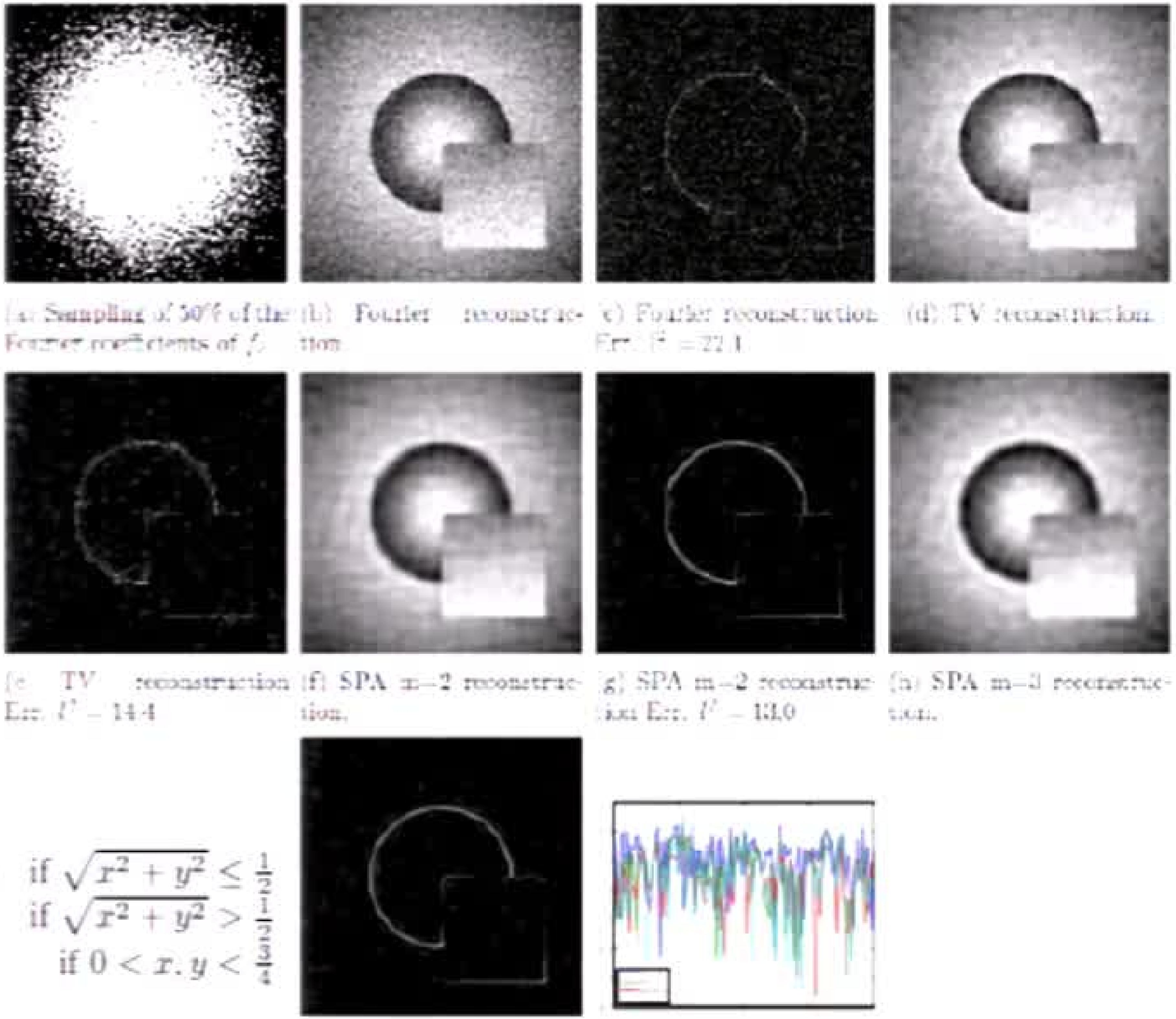
(a) Sampling of 50% of the Fourier coefficients of f_c. (b) f_c on $2N = 128$ (c) Fourier reconstruction. (d) Fourier reconstruction Err. $l^2 = 7.6$



(e) TV reconstruction. (f) TV reconstruction Err. $l^2 = 6.7$ (g) SPA m=2 reconstruction. (h) SPA m=2 reconstruction Err. $l^2 = 6.8$

$$f_c(x,y) = \begin{cases} \cos(3\pi\sqrt{x^2+y^2}/2) & \text{if } \sqrt{x^2+y^2} \le \frac{1}{2} \\ \cos(\pi\sqrt{x^2+y^2}/2) & \text{if } \sqrt{x^2+y^2} > \frac{1}{2} \\ \sin(\pi\sqrt{x^2+y^2}/2) & \text{if } 0 < x, y < \frac{1}{2} \end{cases}$$

(i) SPA m=3 reconstruction. (j) SPA m=3 reconstruction Err. $l^2 = 6.9$ (k) Cross-Section Err. $x = $ [illegible]



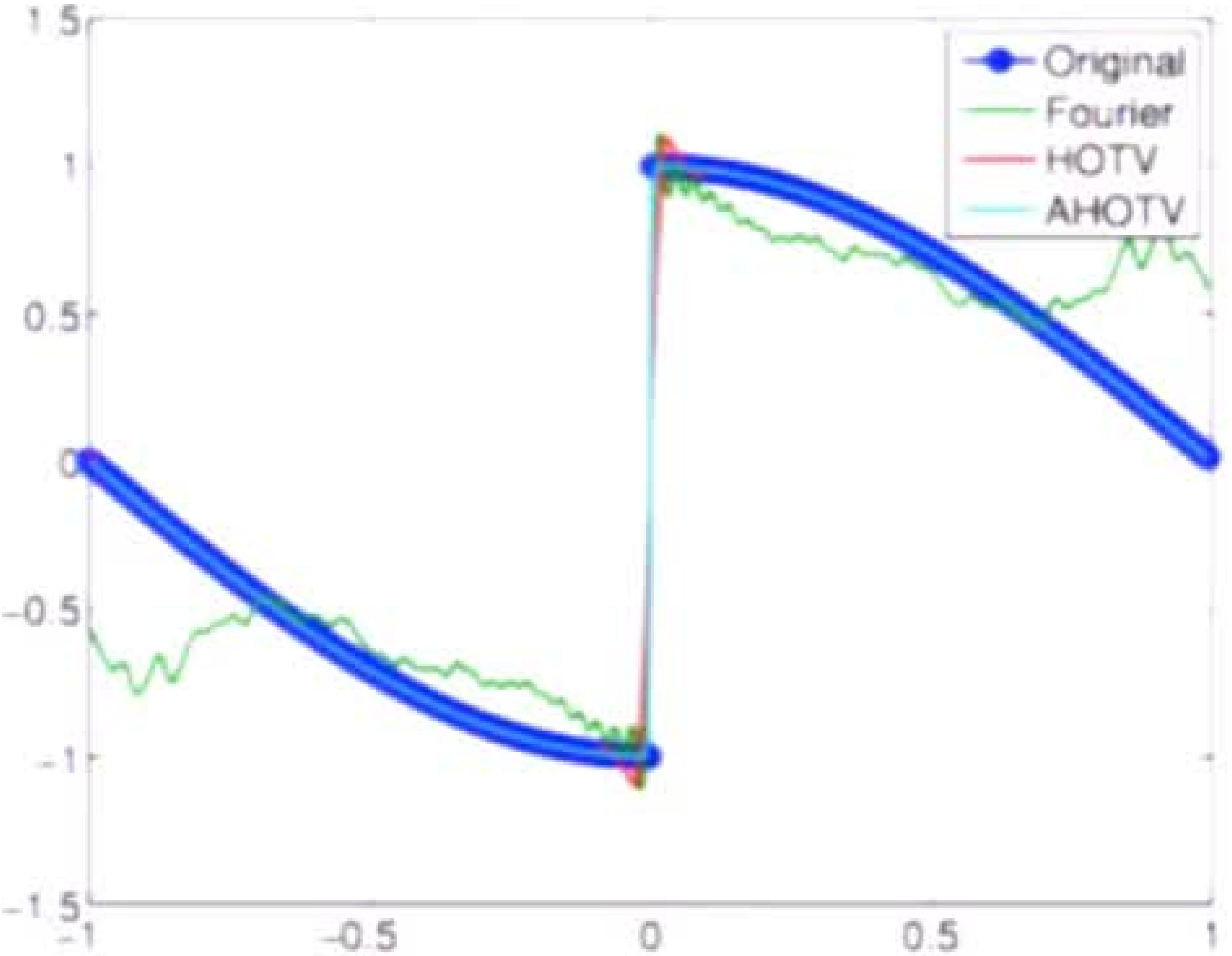
(a) Sampling of 50% of the Fourier coefficients of f_c (b) Fourier reconstruction. (c) Fourier reconstruction Err. $l^2 = 22.1$ (d) TV reconstruction.

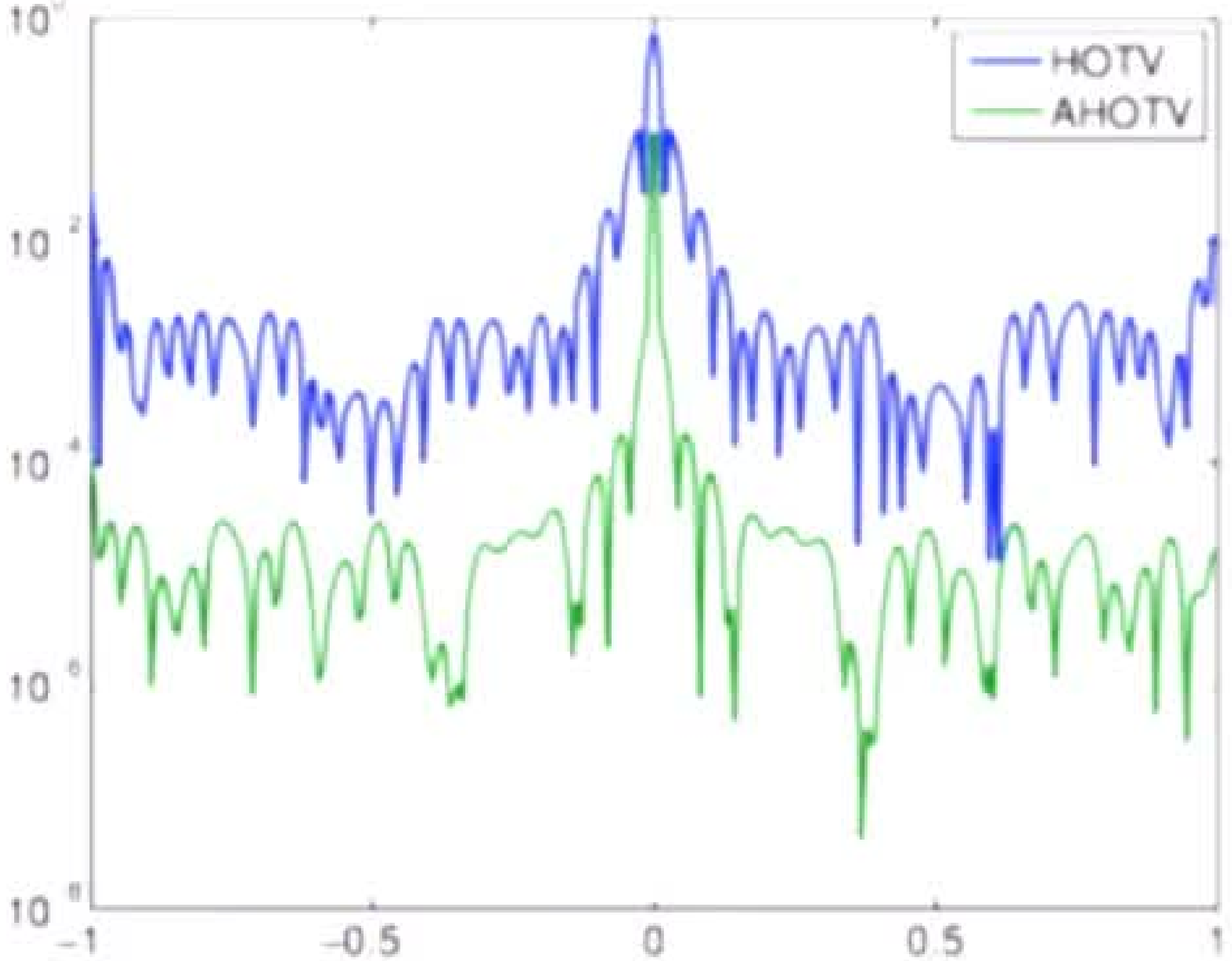
(e) TV reconstruction Err. $l^2 = 14.4$ (f) SPA m=2 reconstruction. (g) SPA m=2 reconstruction Err. $l^2 = 13.0$ (h) SPA m=3 reconstruction.

(i) SPA m=3 reconstruction Err. $l^2 = 12.8$ (j) Cross-Section Err. $x = \frac{1}{2}$

$$f_c(x,y) = \begin{cases} \cos(3\pi\sqrt{x^2+y^2}/2) & \text{if } \sqrt{x^2+y^2} \le \frac{1}{2} \\ \cos(\pi\sqrt{x^2+y^2}/2) & \text{if } \sqrt{x^2+y^2} > \frac{1}{2} \\ \sin(\pi\sqrt{x^2+y^2}/2) & \text{if } 0 < x, y < \frac{3}{4} \end{cases}$$

Non-Uniform Fourier Reconstruction





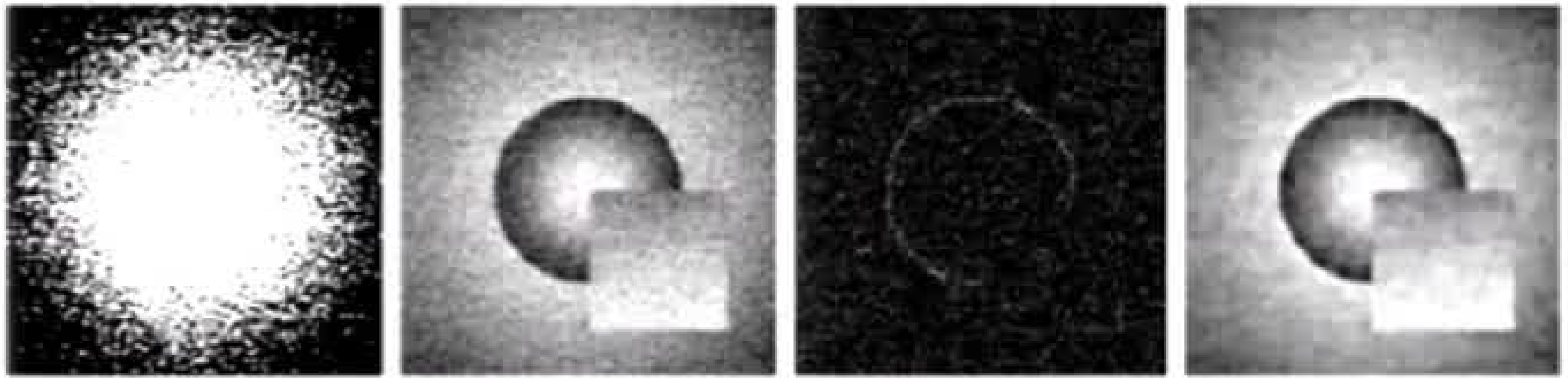
Reconstruction of $n_k = 128$ jittered Fourier coefficients for HOTV and AHOTV of $f(x) = \text{sign}(x)\cos(\pi x)$.

$$\mathbf{f}_{HOTV} = \min_{\mathbf{f}} \lambda ||L^m \mathbf{f}||_1 + \frac{\mu}{2}||\mathcal{F}_{NUFFT}\mathbf{f} - \hat{\mathbf{f}}||_2$$

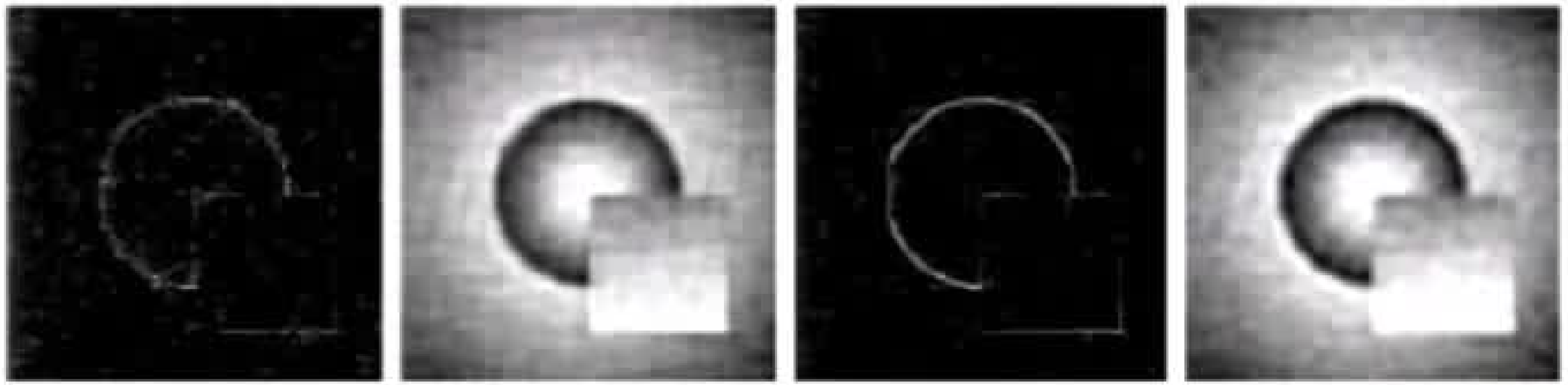
$$\mathbf{f}_{AHOTV} = \min_{\mathbf{f}} \lambda ||M L^m \mathbf{f}||_1 + \frac{\mu}{2}||\mathcal{F}_{NUFFT}\mathbf{f} - \hat{\mathbf{f}}||_2$$

Jittered- $k_i = i - \lfloor \frac{n_k}{2} \rfloor - 1 + \frac{1-2\xi_i}{4}$, such that $\xi_i \sim U([0,1])$

$$\hat{f}_j = \frac{1}{n_x}\sum_{l=1}^{n_x} f(x_l) e^{-\pi i k_j x_l} \quad \& \quad f_{n_x}(x_l) = \sum_{j=1}^{n_k} \hat{f}_j e^{\pi i k_j x_l}$$

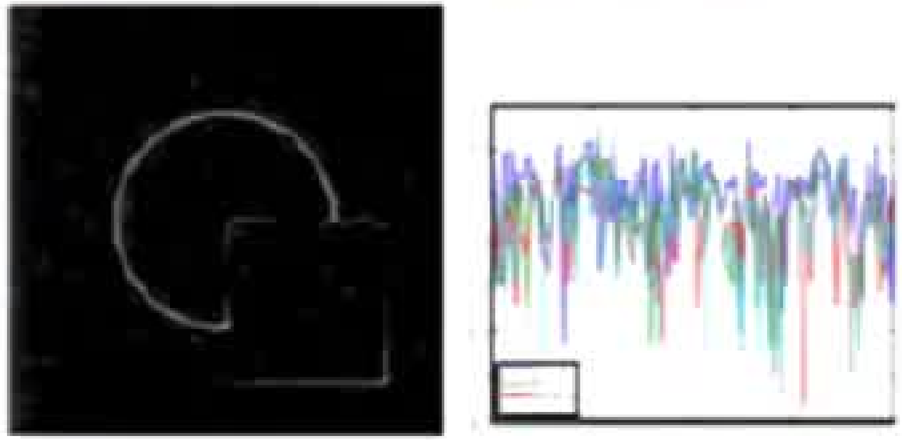


(a) Sampling of 50% of the Fourier coefficients of f_c (b) Fourier reconstruction. (c) Fourier reconstruction Err. $l^2 = 22.4$ (d) TV reconstruction.

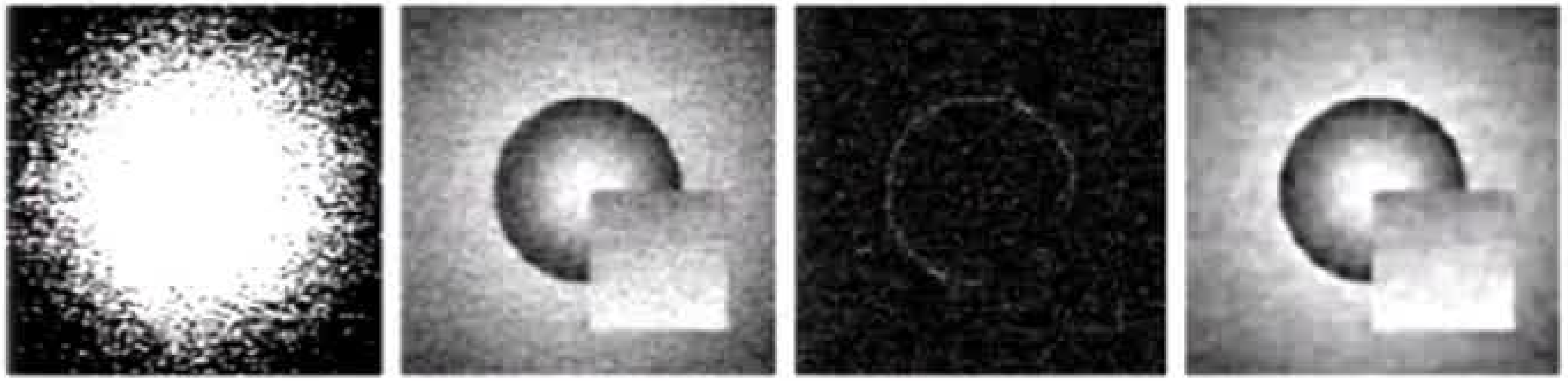


(e) TV reconstruction Err. $l^2 = 14.4$ (f) SPA m=2 reconstruction. (g) SPA m=2 reconstruction Err. $l^2 = 13.0$ (h) SPA m=3 reconstruction.

$$f_c(x,y) = \begin{cases} \cos(3\pi\sqrt{x^2+y^2}/2) & \text{if } \sqrt{x^2+y^2} \le \frac{1}{2} \\ \cos(\pi\sqrt{x^2+y^2}/2) & \text{if } \sqrt{x^2+y^2} > \frac{1}{2} \\ \sin(\pi\sqrt{x^2+y^2}/2) & \text{if } 0 < x, y < \frac{3}{4} \end{cases}$$



(i) SPA m=3 reconstruction Err. $l^2 = 12.8$ (j) Cross-Section Err. $x = \frac{1}{2}$

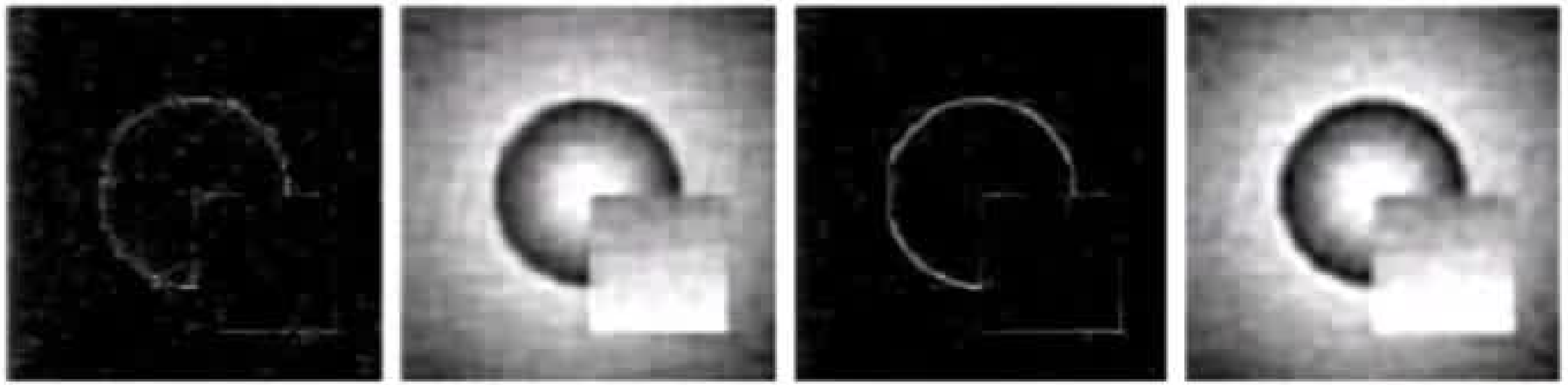


(a) Sampling of 50% of the Fourier coefficients of f_c.

(b) Fourier reconstruction.

(c) Fourier reconstruction Err. $l^2 = 22.1$

(d) TV reconstruction.



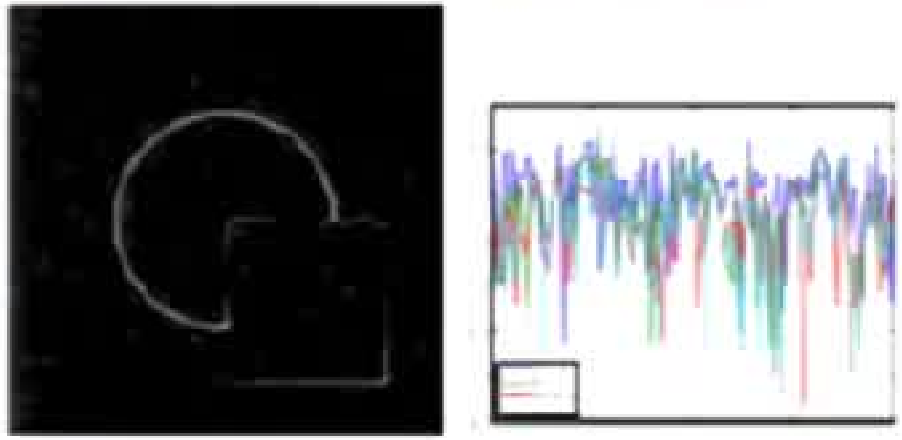
(e) TV reconstruction Err. $l^2 = 14.4$

(f) SPA m=2 reconstruction.

(g) SPA m=2 reconstruction Err. $l^2 = 13.0$

(h) SPA m=3 reconstruction.

$$f_c(x,y) = \begin{cases} \cos(3\pi\sqrt{x^2+y^2}/2) & \text{if } \sqrt{x^2+y^2} \le \frac{1}{2} \\ \cos(\pi\sqrt{x^2+y^2}/2) & \text{if } \sqrt{x^2+y^2} > \frac{1}{2} \\ \sin(\pi\sqrt{x^2+y^2}/2) & \text{if } 0 < x, y < \frac{3}{4} \end{cases}$$



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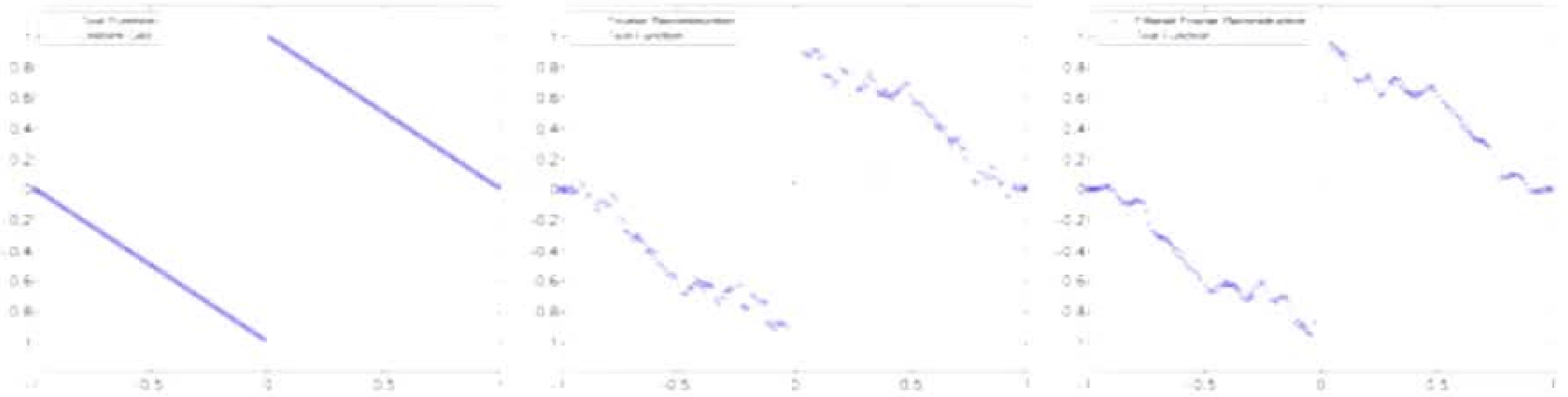
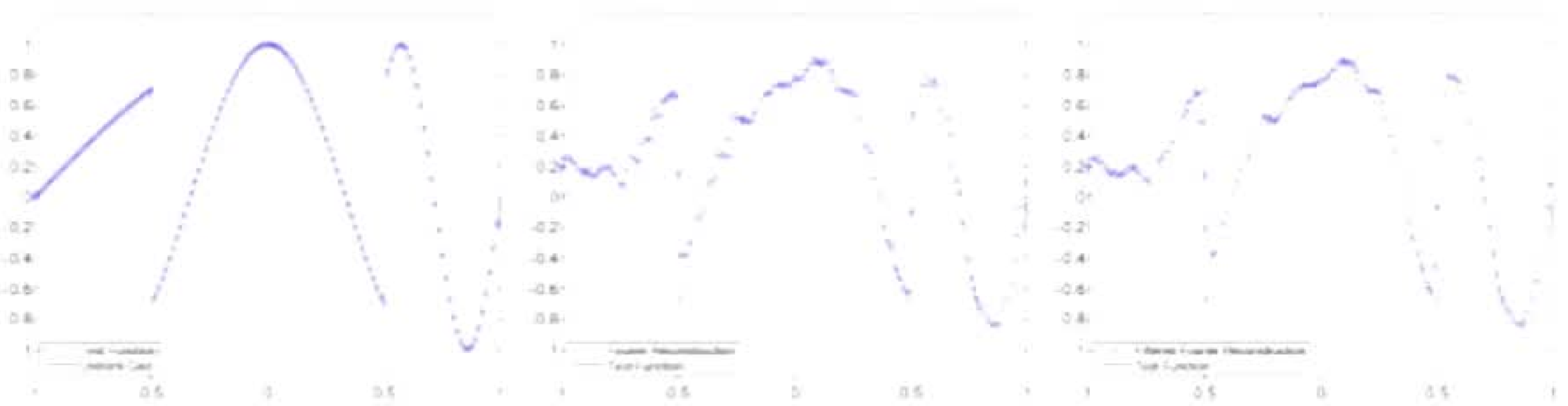
(j) Cross-Section Err. $x = \frac{1}{2}$



(a) $f_a(x)$ (b) $S_N f_a(x)$ (c) $S_N^\sigma f_a(x)$

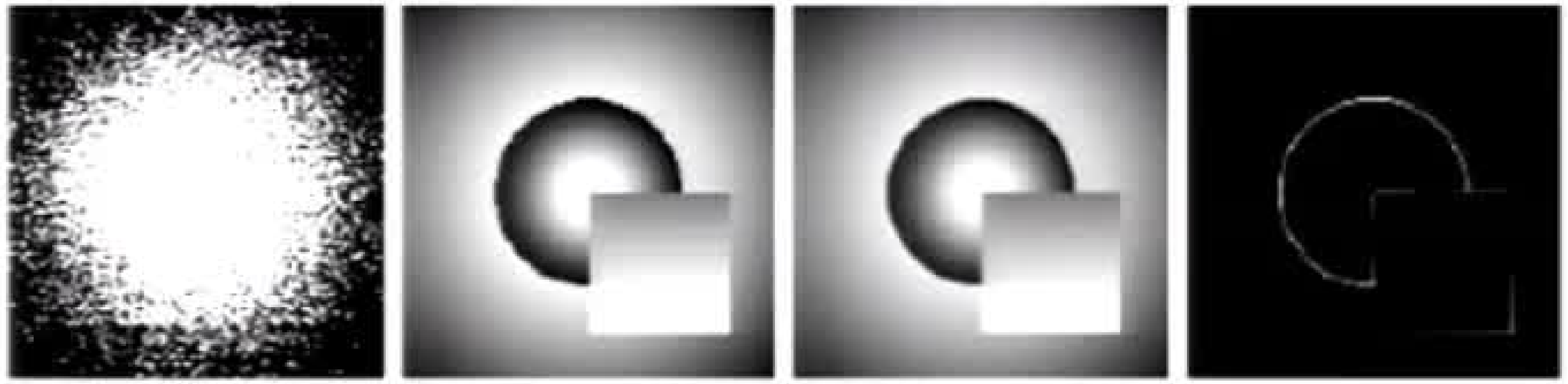


(d) $f_b(x)$ (e) $S_N f_b(x)$ (f) $S_N^\sigma f_b(x)$

$$S_N f(x) = \sum_{k=-N}^{N} \hat{f}_k e^{ik\pi x}$$

$$S_N^\sigma f(x) = \sum_{k=-N}^{N} \sigma_k \hat{f}_k e^{ik\pi x}$$

$$f_a(x) = \begin{cases} -1 - x & \text{if } -1 \le x < 0 \\ 1 - x & \text{otherwise} \end{cases} ; \quad f_b(x) = \begin{cases} \cos \frac{\pi x}{2} & \text{if } 1 \le x < -\frac{1}{2} \\ \cos \frac{3\pi x}{2} & \text{if } -\frac{1}{2} \le x < \frac{1}{2} \\ \cos \frac{7\pi x}{2} & \text{if } \frac{1}{2} \le x \le 1 \end{cases}$$



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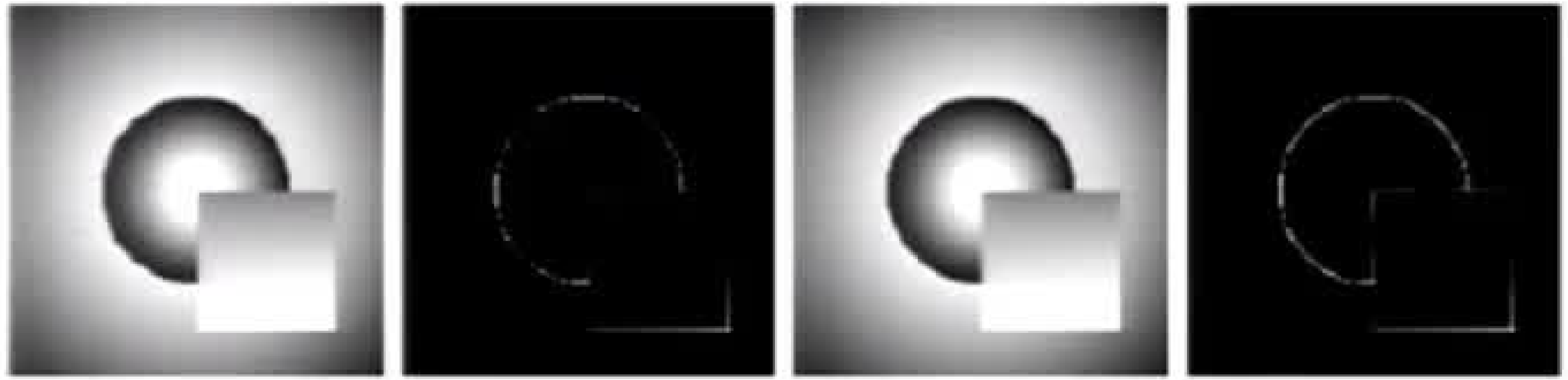
(c) Fourier reconstruction.

(d) Fourier reconstruction Err. $l^2 = 7.6$



(e) TV reconstruction.

(f) TV reconstruction Err. $l^2 = 6.7$

(g) SPA m=2 reconstruction.

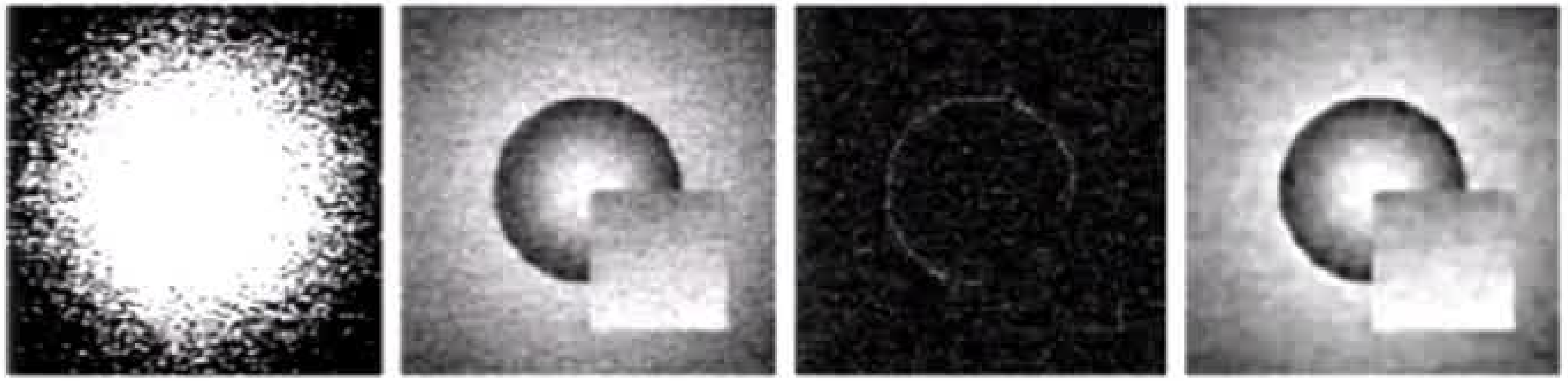
(h) SPA m=2 reconstruction Err. $l^2 = 6.8$

$$f_c(x,y) = \begin{cases} \cos(3\pi\sqrt{x^2+y^2}/2) & \text{if } \sqrt{x^2+y^2} \le \text{[illegible]} \\ \cos(\pi\sqrt{x^2+y^2}/2) & \text{if } \sqrt{x^2+y^2} > \text{[illegible]} \\ \sin(\pi\sqrt{x^2+y^2}/2) & \text{if } 0 < x, y < \text{[illegible]} \end{cases}$$

(i) SPA m=3 reconstruction.

(j) SPA m=3 reconstruction Err. $l^2 = 6.9$

(k) Cross-Section Err. $x =$ [illegible]



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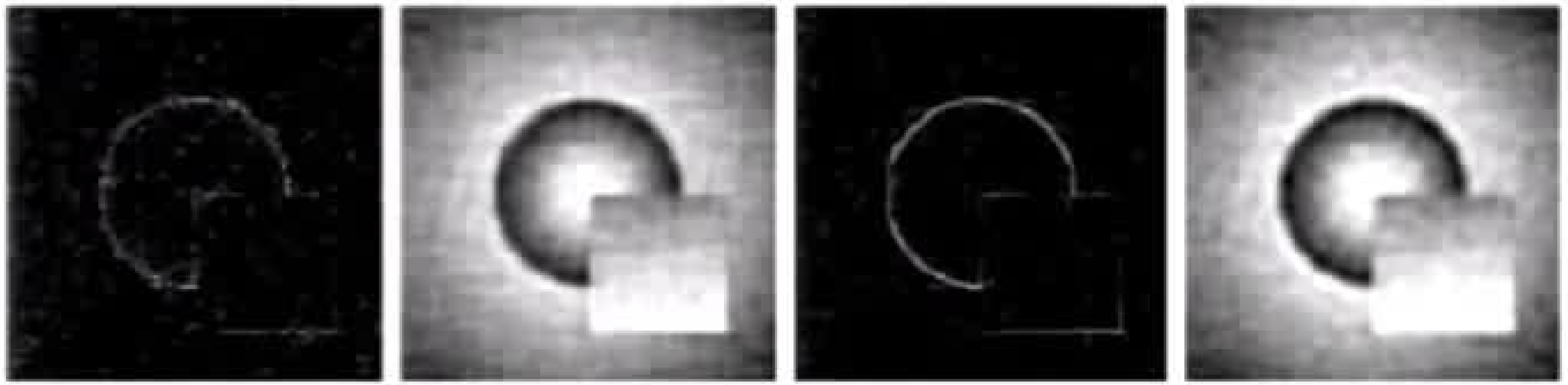

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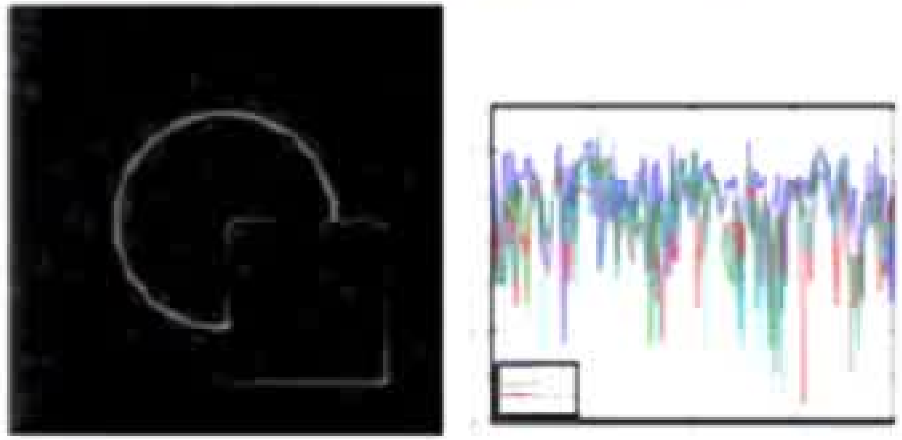
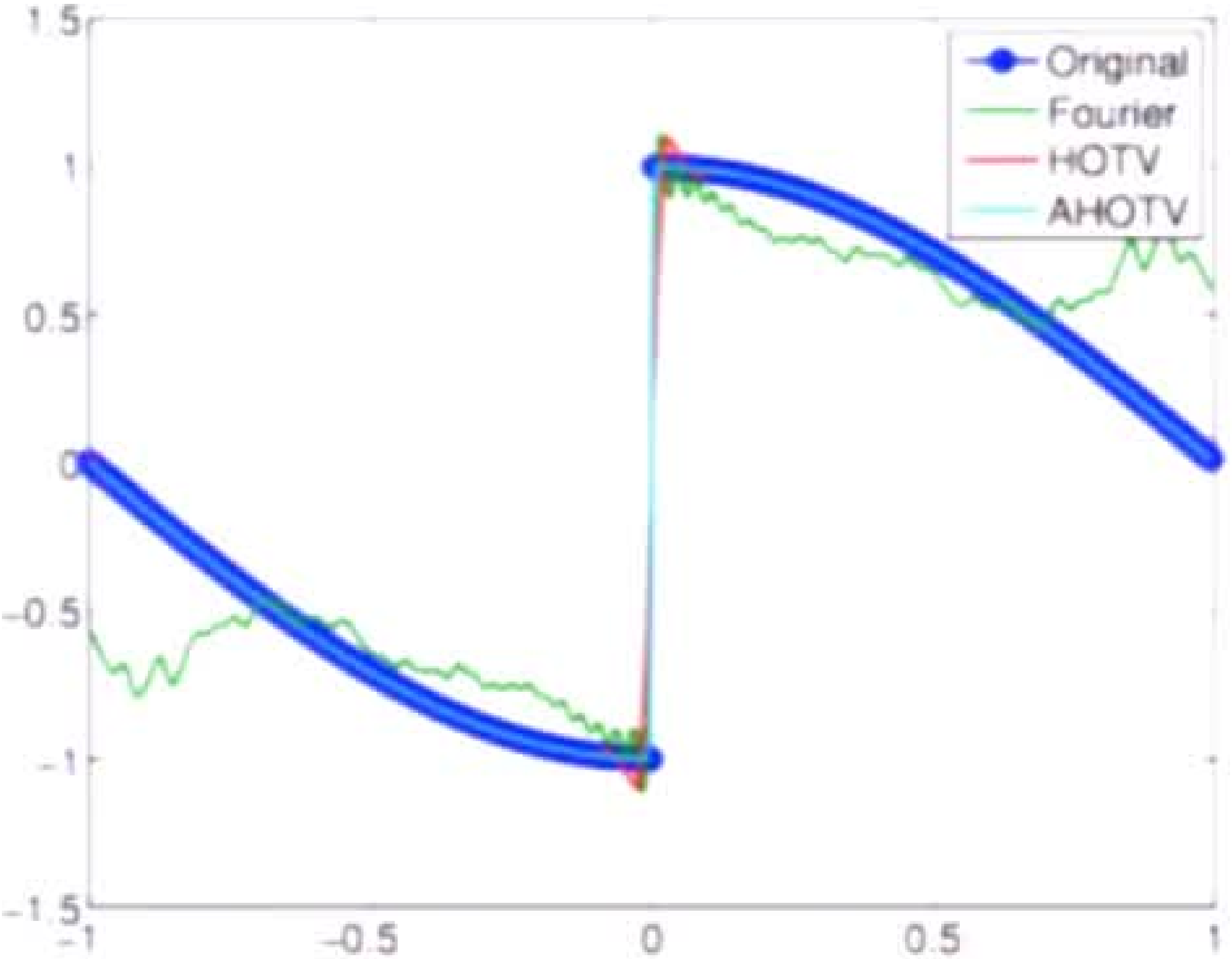
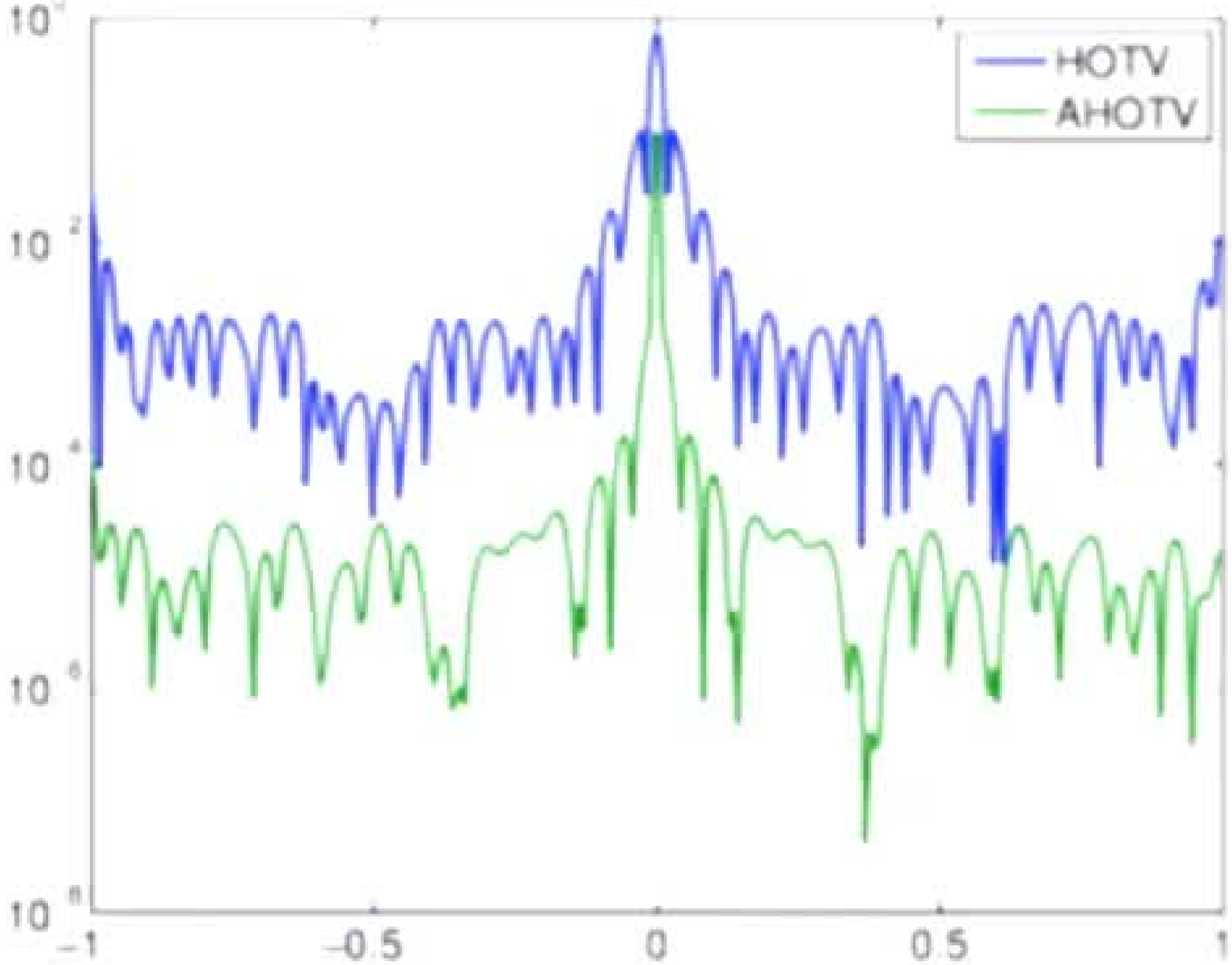


(i) SPA m=3 reconstruction Err. $l^2 = 12.8$ (j) Cross-Section Err. $x = \frac{1}{2}$

Non-Uniform Fourier Reconstruction





Reconstruction of $n_k = 128$ jittered Fourier coefficients for HOTV and AHOTV of $f(x) = \text{sign}(x)\cos(\pi x)$.

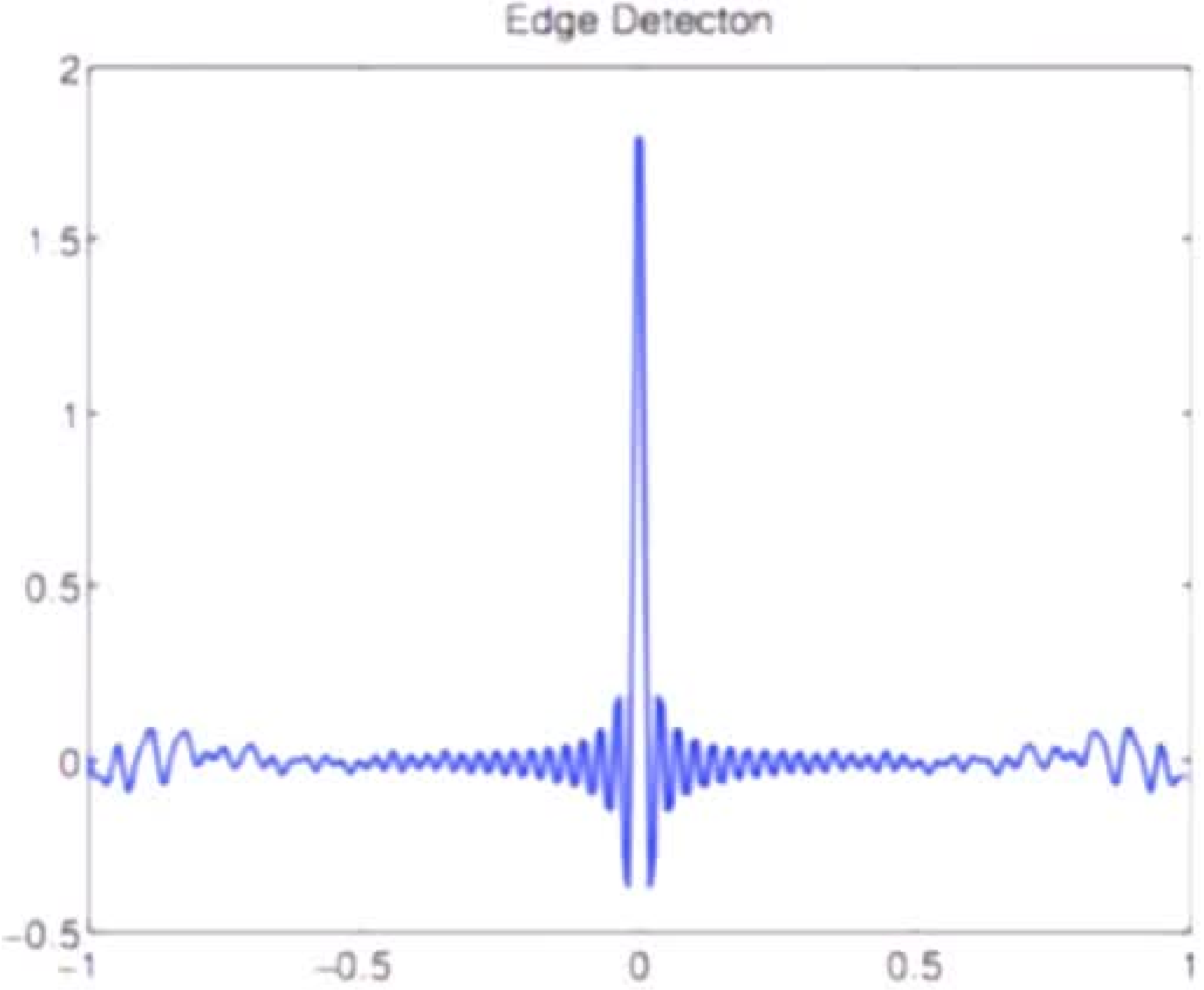
$$\mathbf{f}_{HOTV} = \min_{\mathbf{f}} \lambda ||L^m \mathbf{f}||_1 + \frac{\mu}{2}||\mathcal{F}_{NUFFT}\mathbf{f} - \hat{\mathbf{f}}||_2$$

$$\mathbf{f}_{AHOTV} = \min_{\mathbf{f}} \lambda ||M L^m \mathbf{f}||_1 + \frac{\mu}{2}||\mathcal{F}_{NUFFT}\mathbf{f} - \hat{\mathbf{f}}||_2$$

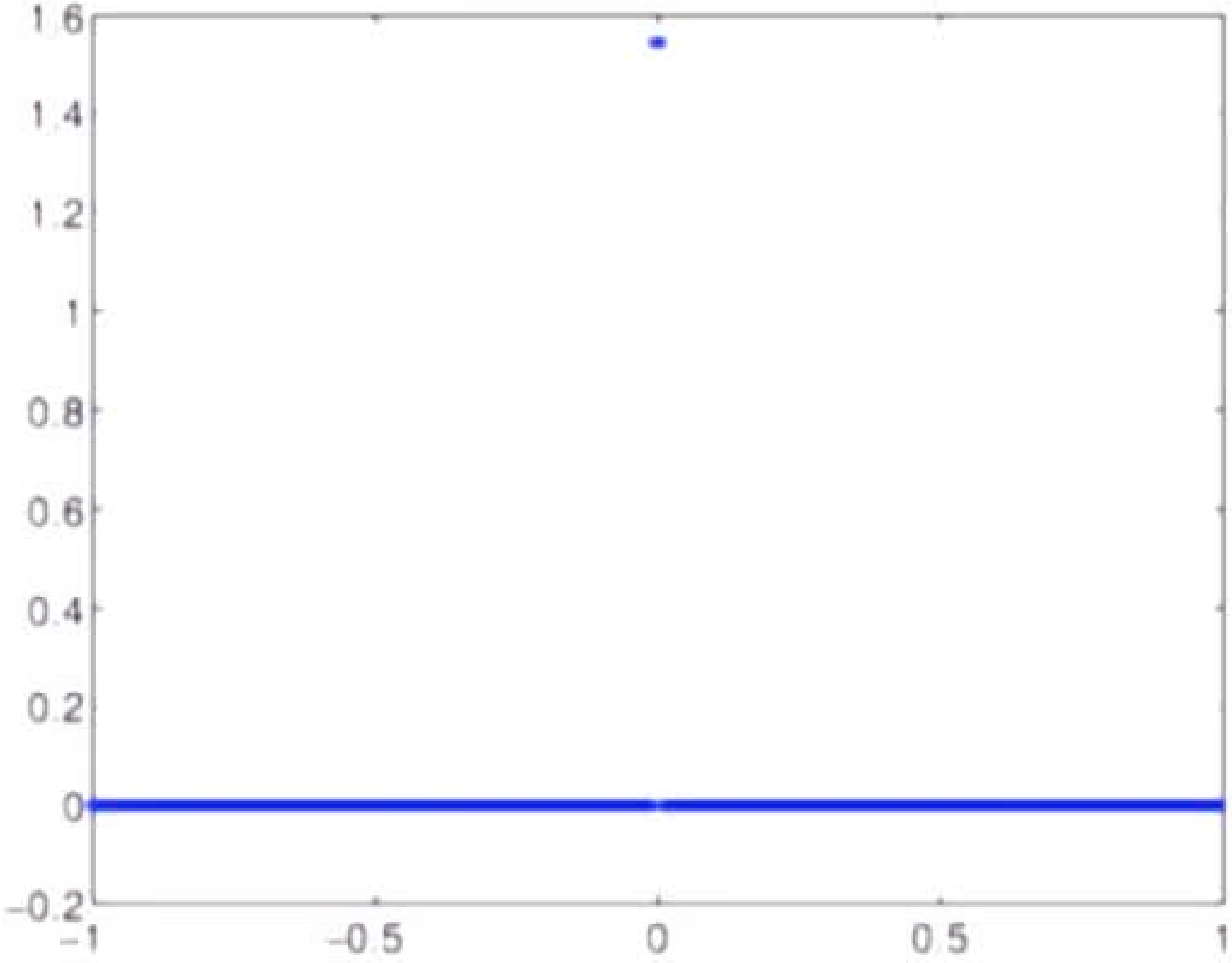
Jittered- $k_i = i - \lfloor \frac{n_k}{2} \rfloor - 1 + \frac{1-2\xi_i}{4}$, such that $\xi_i \sim U([0,1])$

$\hat{f}_j = \frac{1}{n_x}\sum_{l=1}^{n_x} f(x_l) e^{-\pi i k_j x_l}$ & $f_{n_x}(x_l) = \sum_{j=1}^{n_k} \hat{f}_j e^{\pi i k_j x_l}$

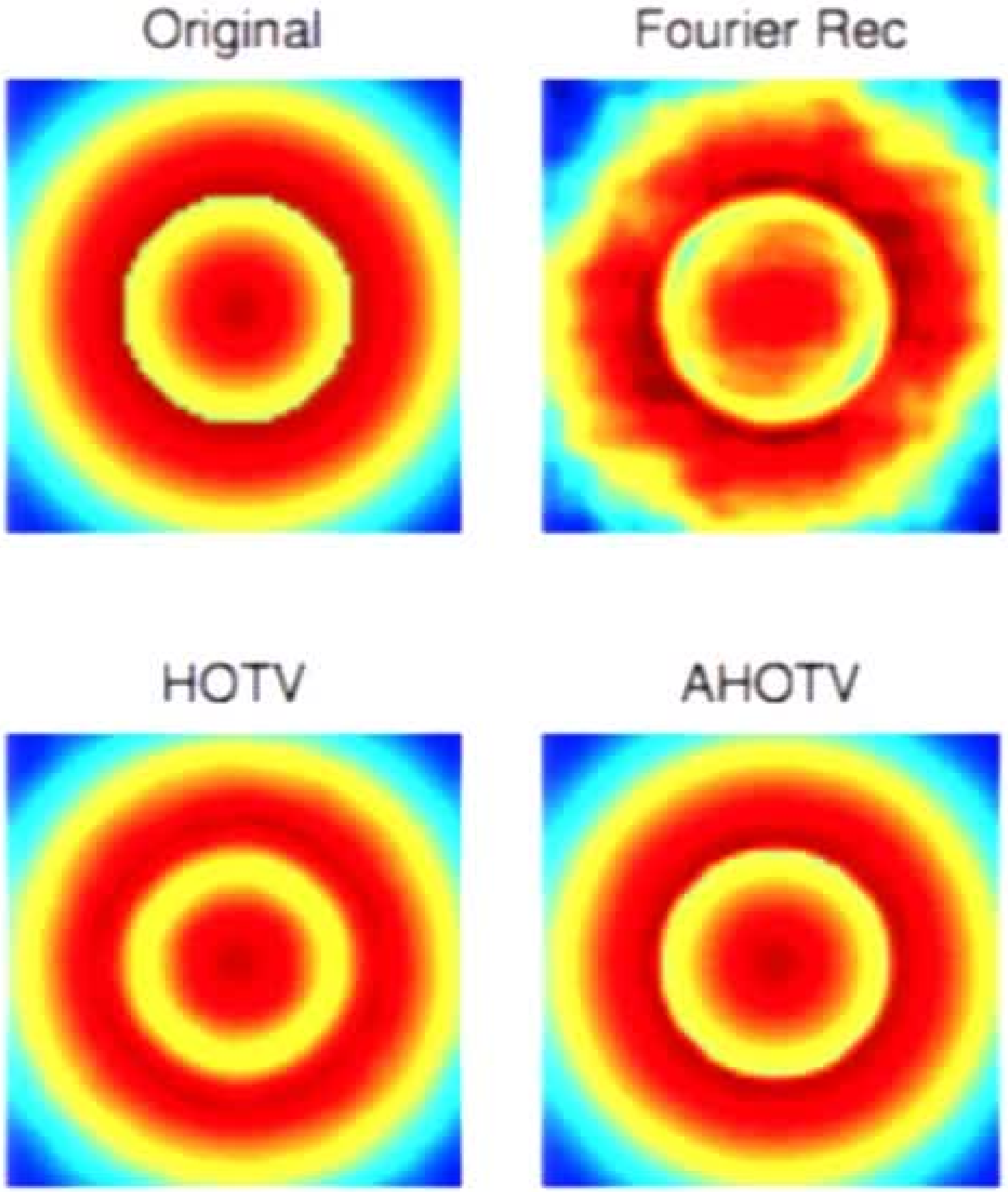
Optimization of Edge Detection

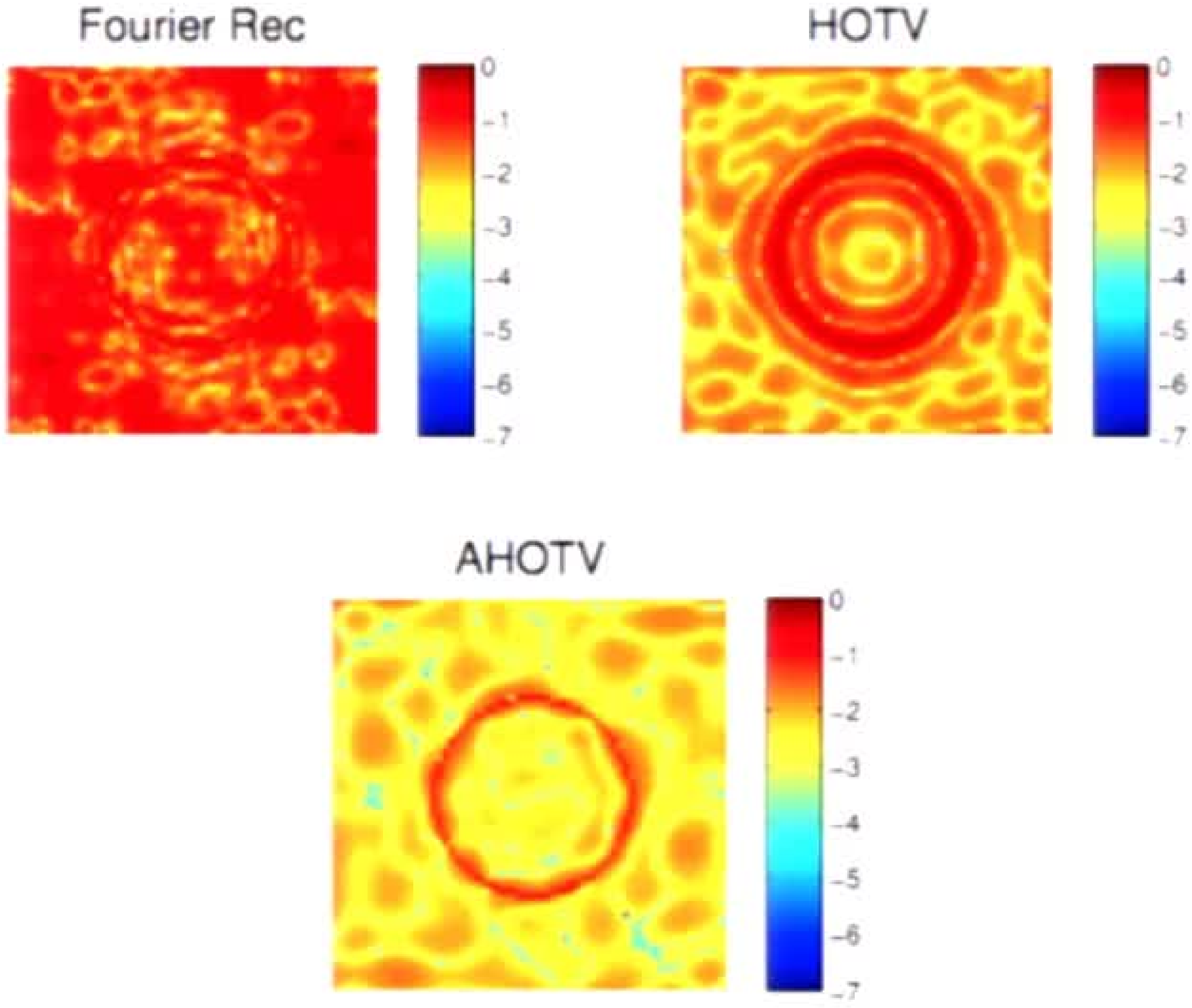


$$\mathcal{F}^{-1}_{NUFFT}(\sigma\hat{\mathbf{f}})$$

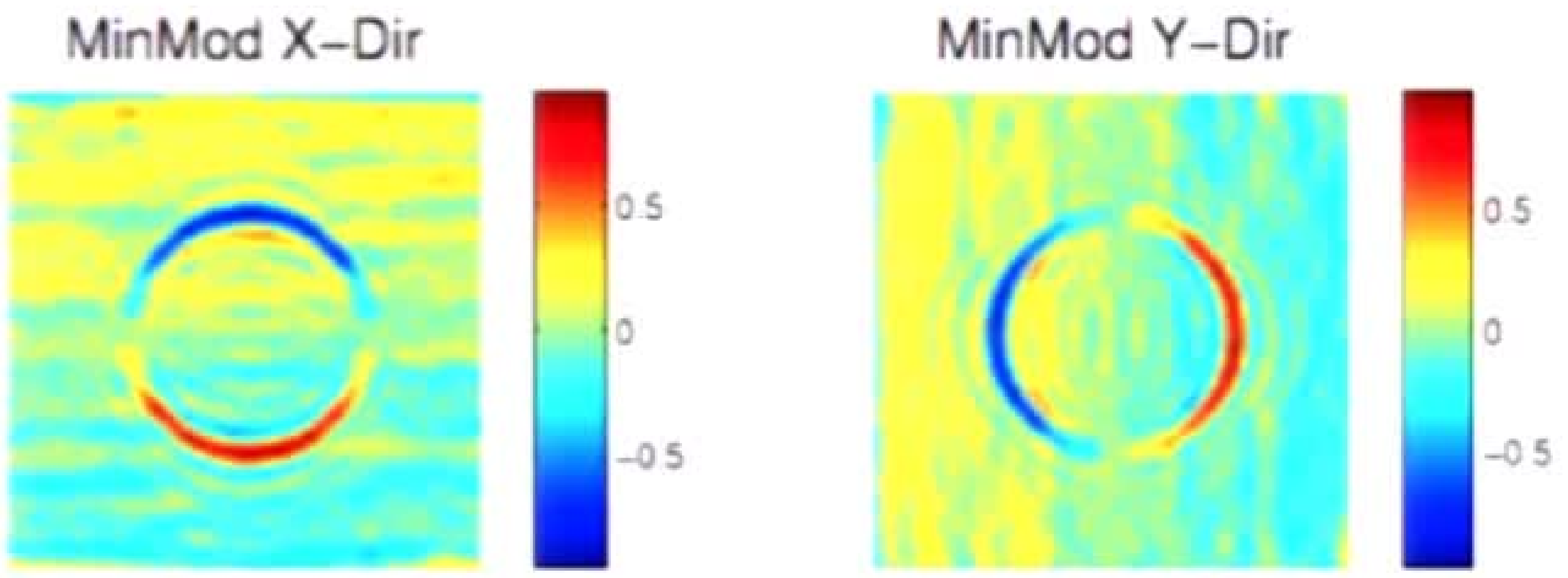


$$\mathbf{f}_{BD} \quad = \quad \min_{\mathbf{f}} \lambda||\mathbf{f}||_1 + \frac{\mu}{2}||\mathbf{Af} - \sigma\hat{\mathbf{f}}||_2$$

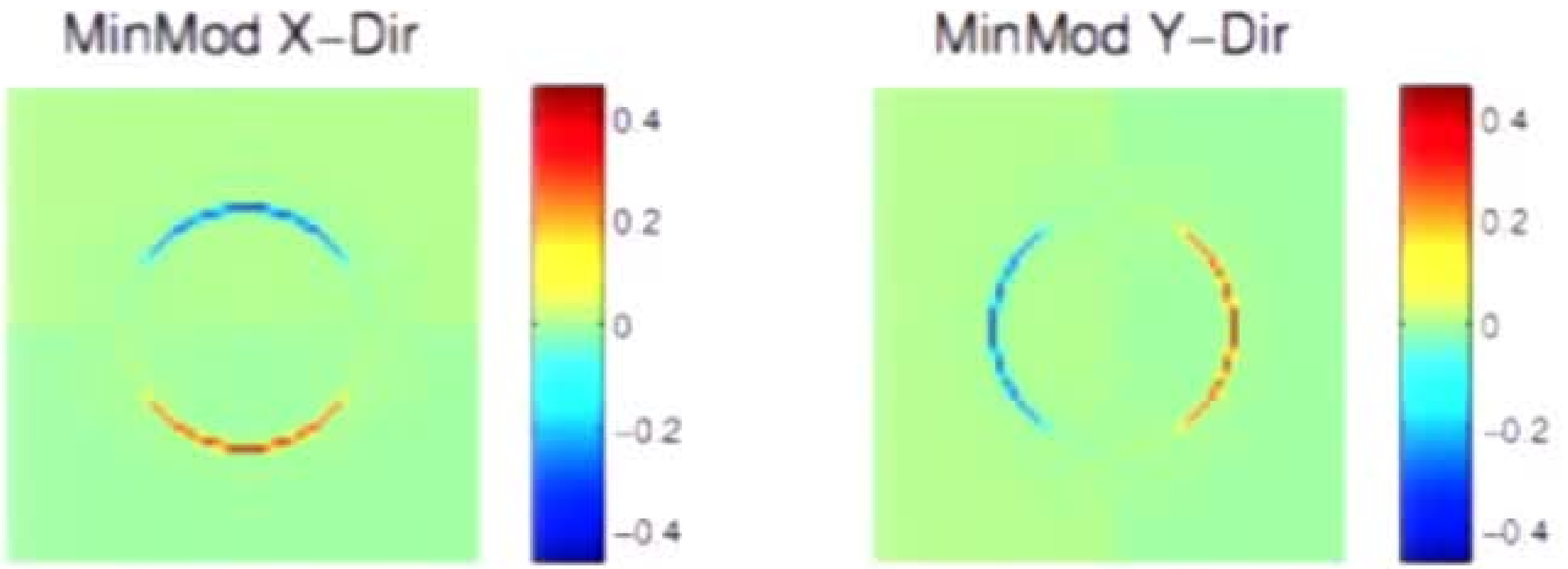




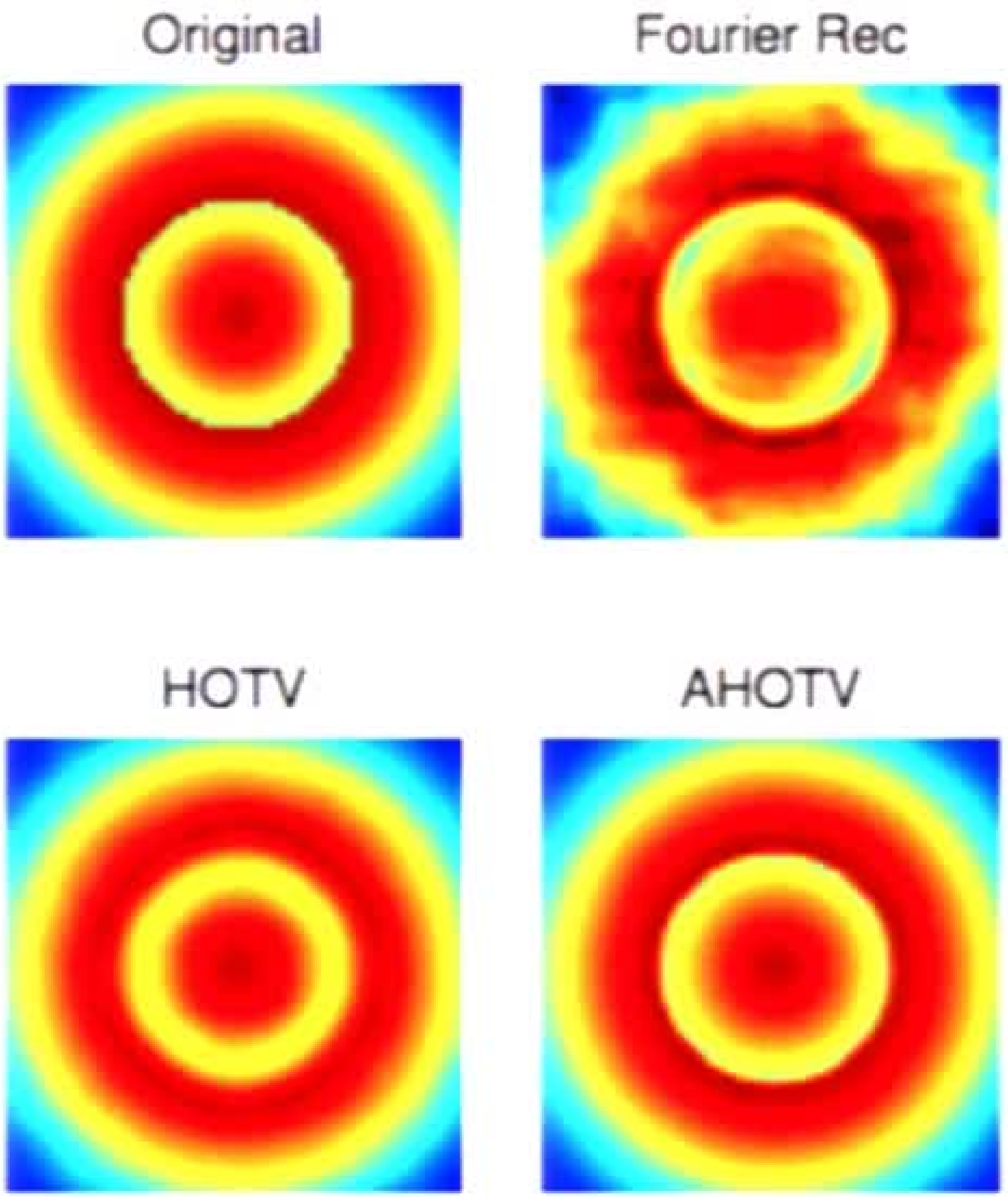
$$f(x,y) = \begin{cases} \cos(\pi\sqrt{x^2+y^2}/2) & \text{if } \sqrt{x^2+y^2} < 1/2 \\ \cos(\pi\sqrt{x^2+y^2}/2 - \pi/2) & \text{otherwise.} \end{cases}$$

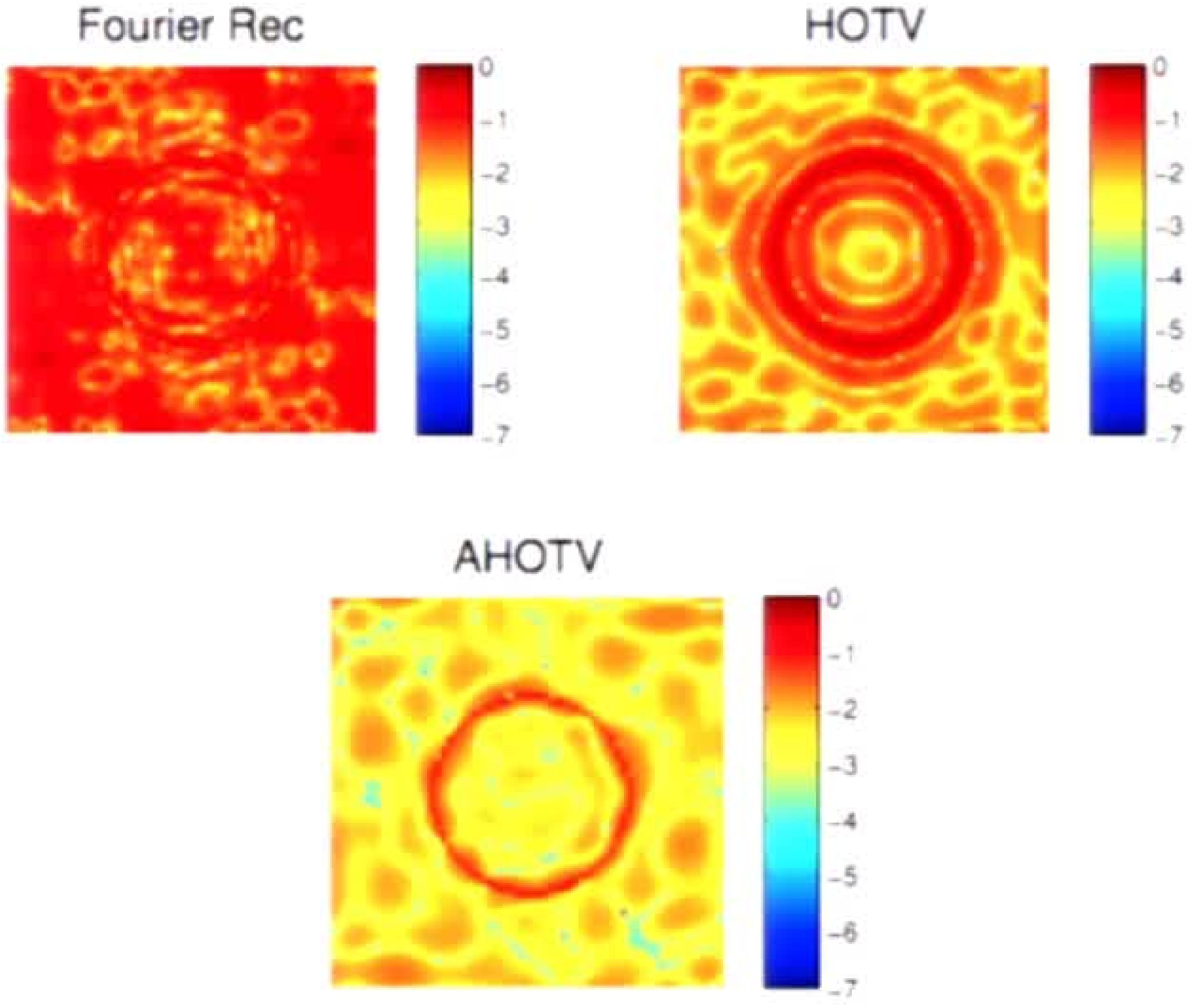


$\mathcal{F}^{-1}_{NUFFT}(\sigma_{\mathbf{x}}\hat{\mathbf{f}})$ $\mathcal{F}^{-1}_{NUFFT}(\sigma_{\mathbf{y}}\hat{\mathbf{f}})$

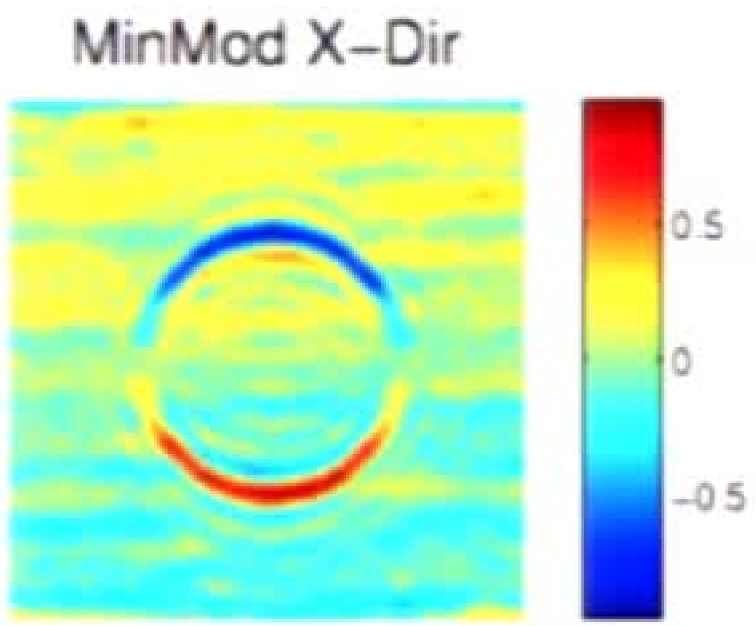


$\mathbf{f}_{BDx} = \min_{\mathbf{f}} ||\mathbf{f}||_1 + \frac{\mu}{2}||\mathbf{A}\mathbf{f} - \sigma_{\mathbf{x}}\hat{\mathbf{f}}||_2$ $\mathbf{f}_{BDy} = \min_{\mathbf{f}} ||\mathbf{f}||_1 + \frac{\mu}{2}||\mathbf{f}\mathbf{A}^{\mathbf{T}} - \sigma_{\mathbf{y}}\hat{\mathbf{f}}||_2$

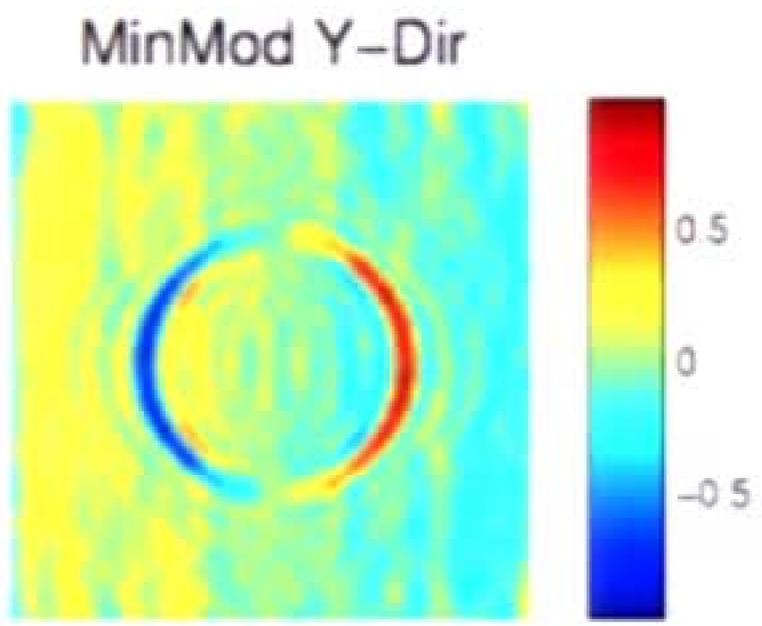




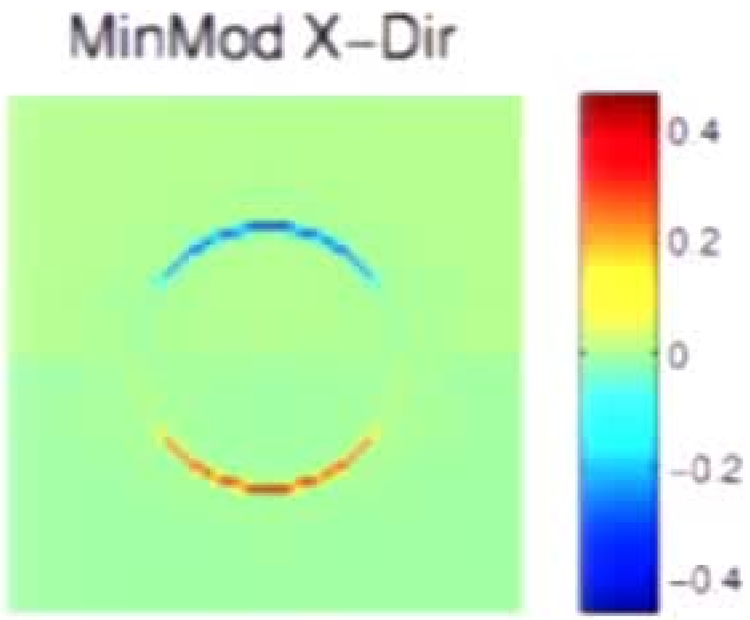
$$f(x,y) = \begin{cases} \cos(\pi\sqrt{x^2+y^2}/2) & \text{if } \sqrt{x^2+y^2} < 1/2 \\ \cos(\pi\sqrt{x^2+y^2}/2 - \pi/2) & \text{otherwise.} \end{cases}$$



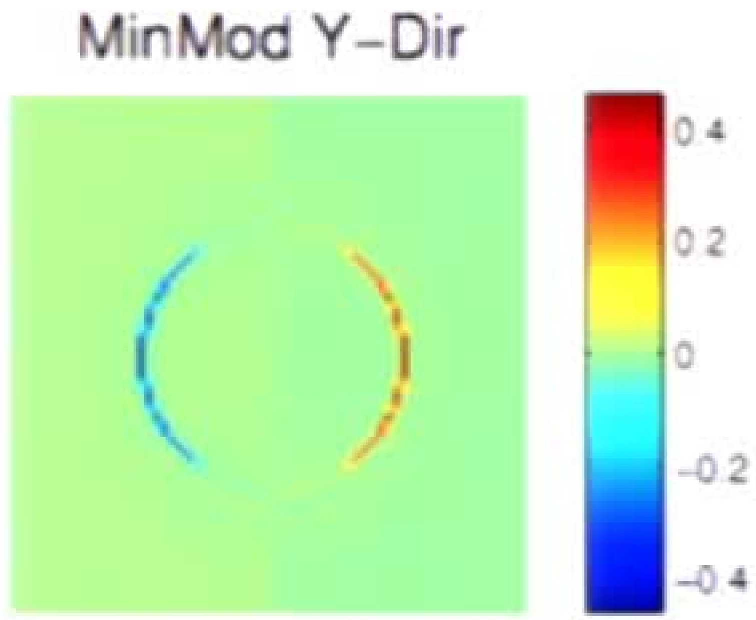
$$\mathcal{F}^{-1}_{NUFFT}(\sigma_{\mathbf{x}}\hat{\mathbf{f}})$$



$$\mathcal{F}^{-1}_{NUFFT}(\sigma_{\mathbf{y}}\hat{\mathbf{f}})$$



$$\mathbf{f}_{BDx} = \min_{\mathbf{f}} ||\mathbf{f}||_1 + \frac{\mu}{2}||\mathbf{A}\mathbf{f} - \sigma_{\mathbf{x}}\hat{\mathbf{f}}||_2$$



$$\mathbf{f}_{BDy} = \min_{\mathbf{f}} ||\mathbf{f}||_1 + \frac{\mu}{2}||\mathbf{f}\mathbf{A}^{\mathrm{T}} - \sigma_{\mathbf{y}}\hat{\mathbf{f}}||_2$$

Thank You.

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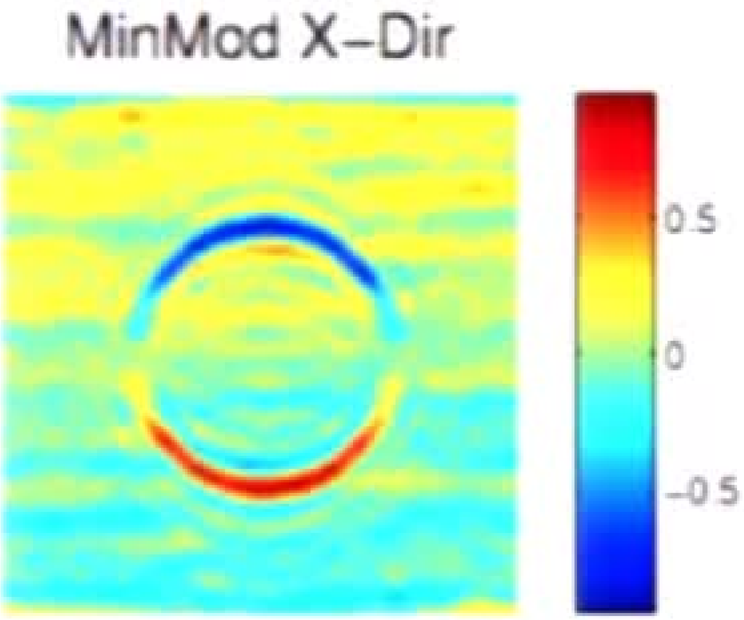
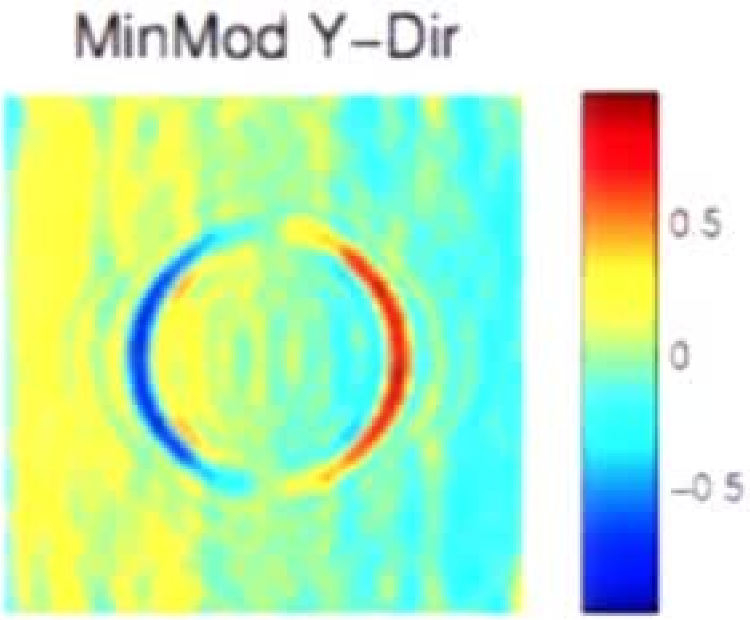
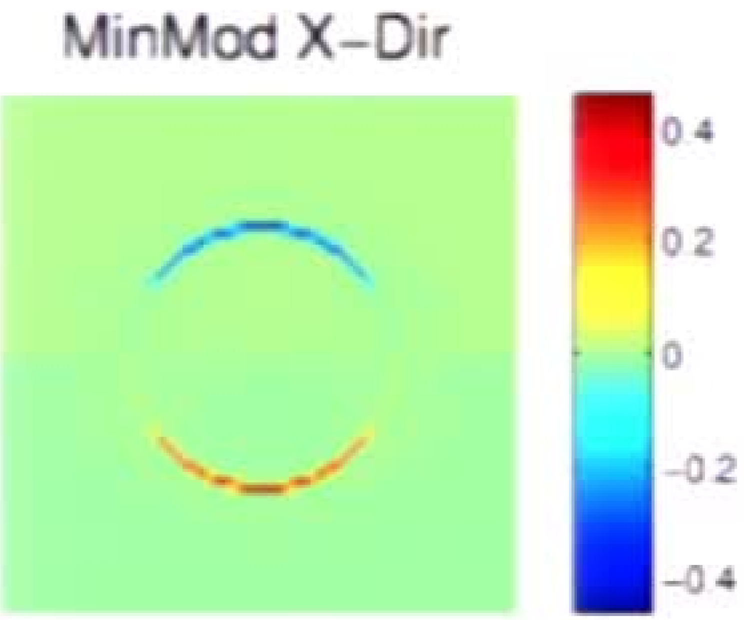
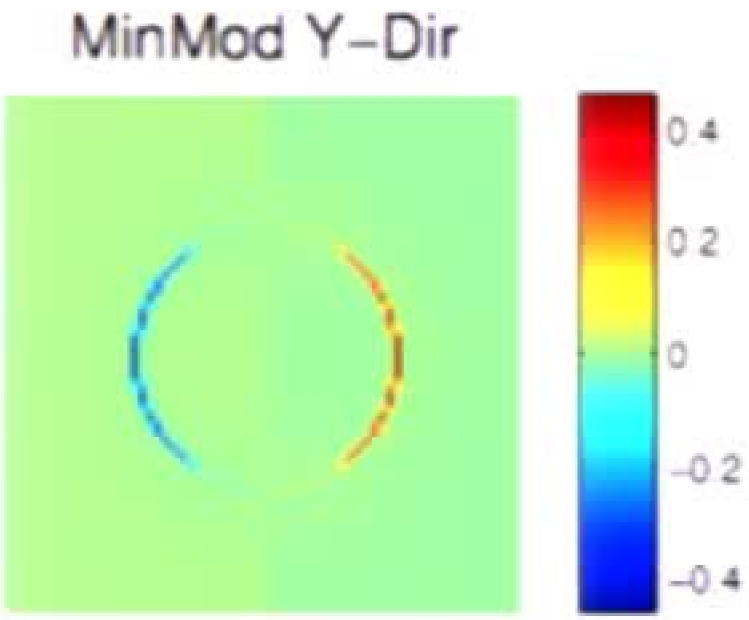


$$\mathcal{F}^{-1}_{NUFFT}(\sigma_{\mathbf{x}}\hat{\mathbf{f}})$$



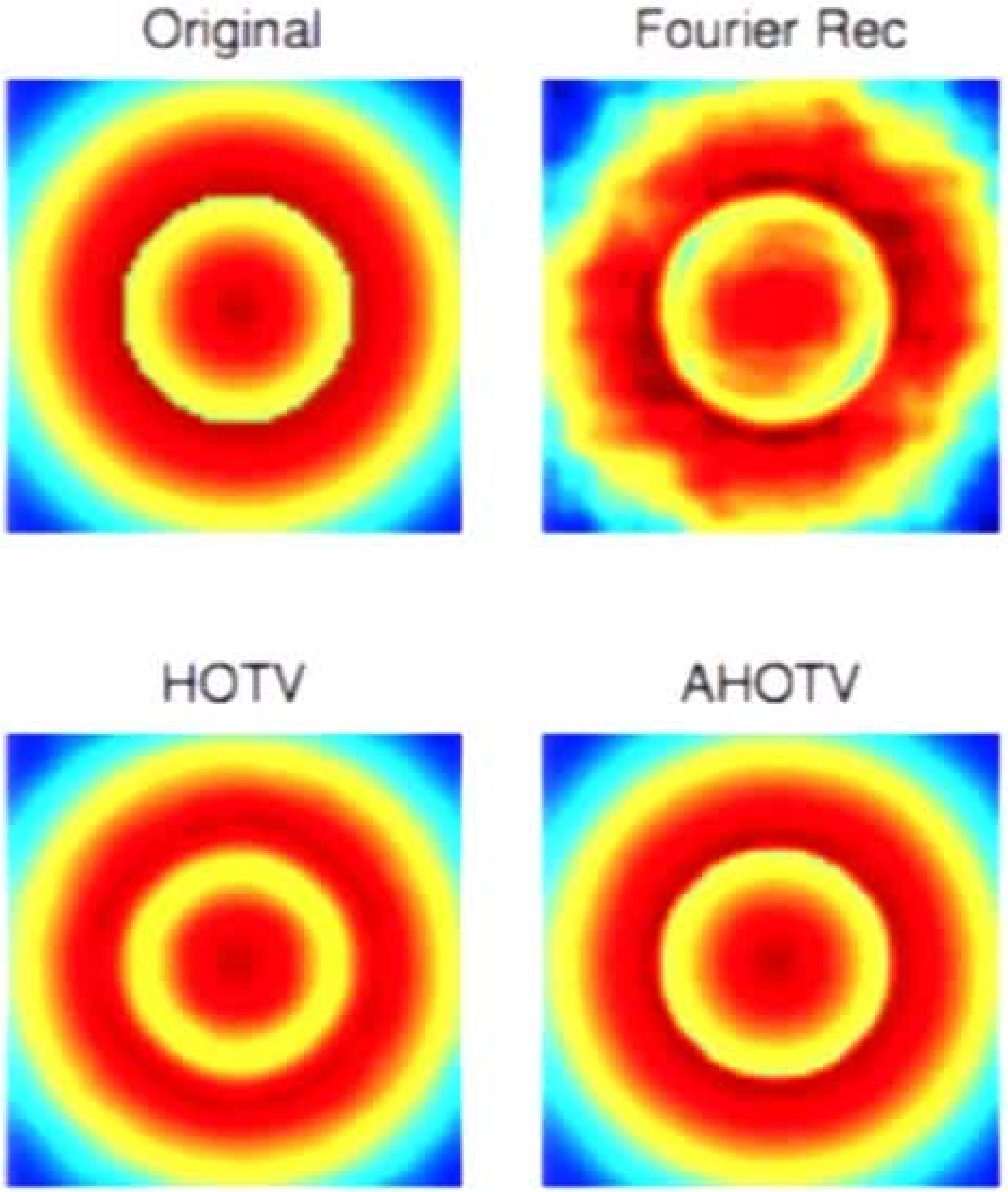
$$\mathcal{F}^{-1}_{NUFFT}(\sigma_{\mathbf{y}}\hat{\mathbf{f}})$$

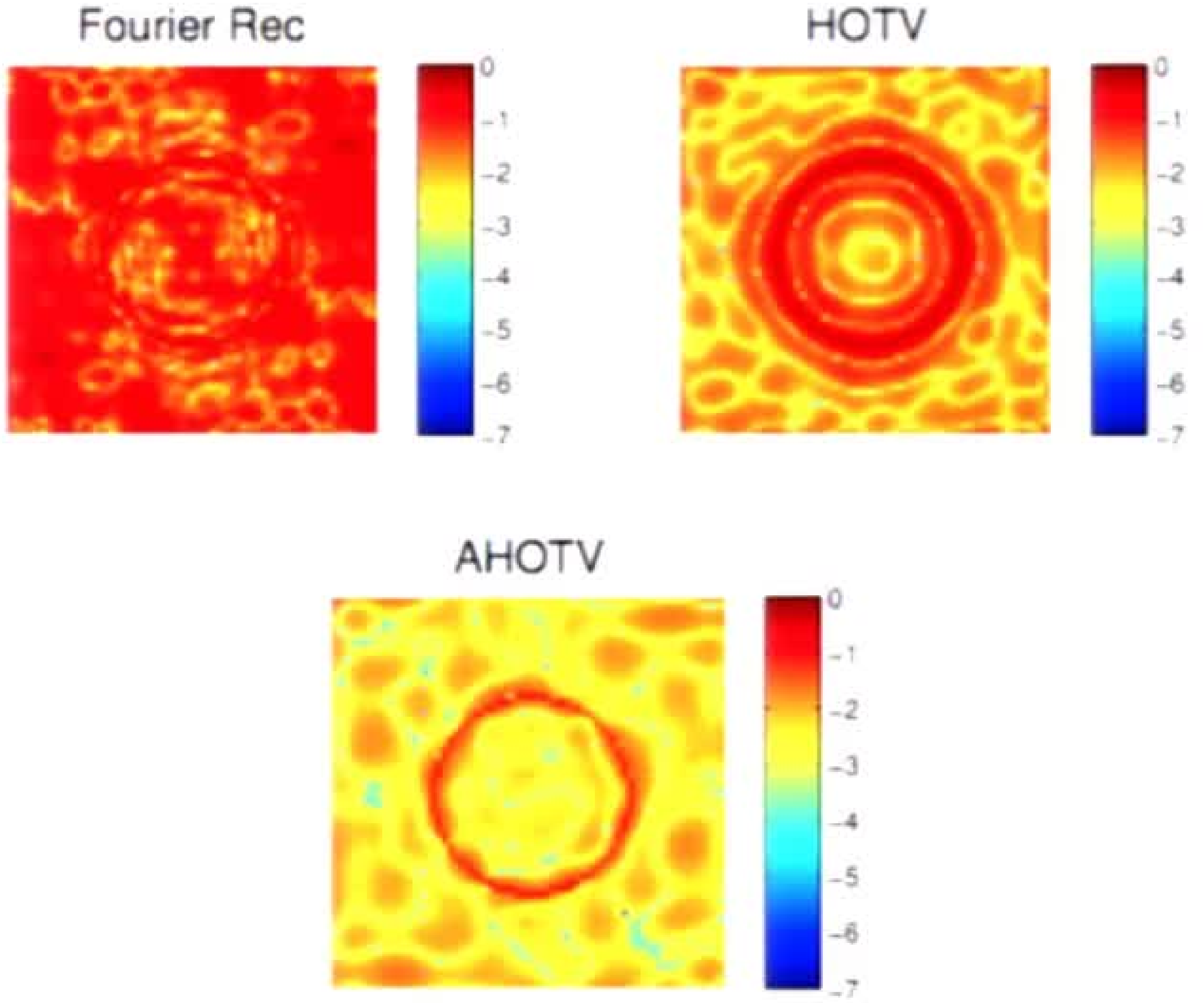




$$\mathbf{f}_{BDx} = \min_{\mathbf{f}} ||\mathbf{f}||_1 + \frac{\mu}{2}||\mathbf{A}\mathbf{f} - \sigma_{\mathbf{x}}\hat{\mathbf{f}}||_2$$

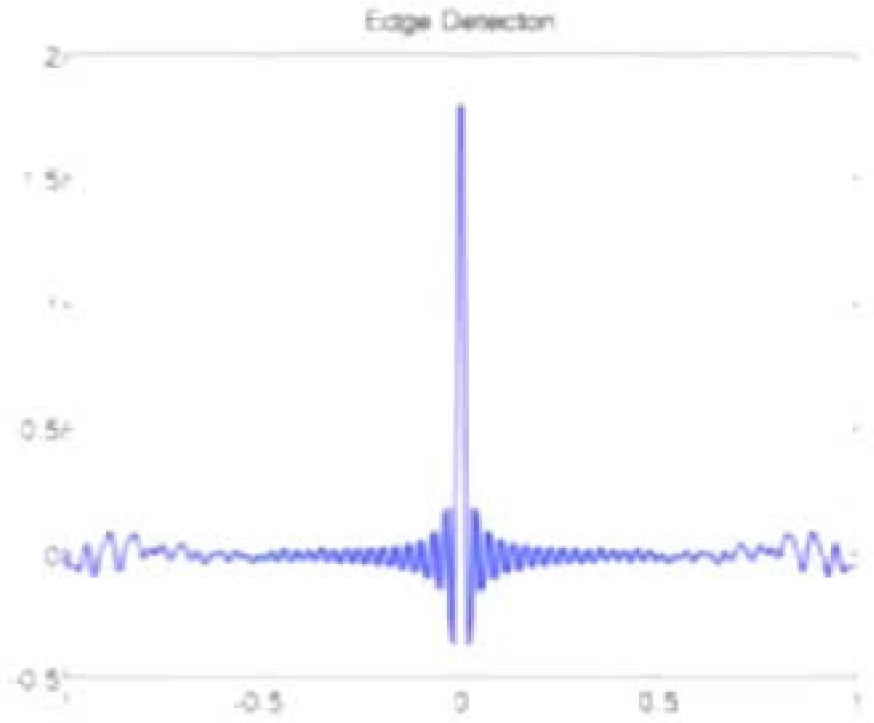
$$\mathbf{f}_{BDy} = \min_{\mathbf{f}} ||\mathbf{f}||_1 + \frac{\mu}{2}||\mathbf{f}\mathbf{A}^{\mathbf{T}} - \sigma_{\mathbf{y}}\hat{\mathbf{f}}||_2$$



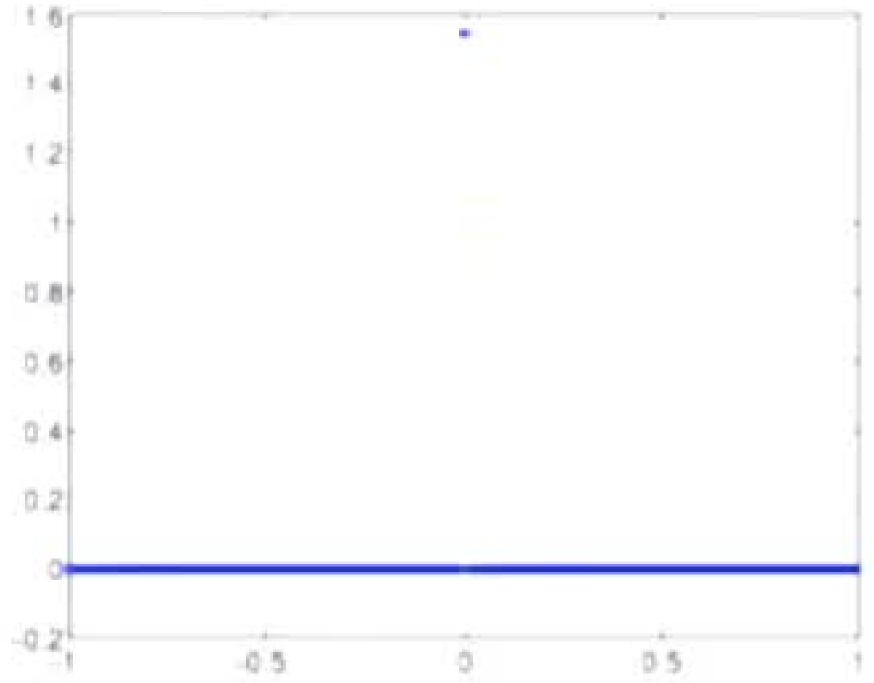


$$f(x,y) = \begin{cases} \cos(\pi\sqrt{x^2+y^2}/2) & \text{if } \sqrt{x^2+y^2} < 1/2 \\ \cos(\pi\sqrt{x^2+y^2}/2 - \pi/2) & \text{otherwise.} \end{cases}$$

Optimization of Edge Detection



$$\mathcal{F}^{-1}_{NUFFT}(\sigma \hat{\mathbf{f}})$$



$$\mathbf{f}_{BD} \quad = \quad \min_{\mathbf{f}} \lambda ||\mathbf{f}||_1 + \frac{\mu}{2} ||\mathbf{A}\mathbf{f} - \sigma \hat{\mathbf{f}}||_2$$

Here, $\sigma = \frac{2i\pi\mathbf{k}}{n_k}$ and the j^{th} row of $\mathbf{A}$ is $e^{-i\pi\mathbf{k}*x_l}\hat{\mathbf{f}}_{ramp}$

$$f_{ramp}(x) = \begin{cases} -\frac{x+1}{2} & \text{if } x \in [-1, 0] \\ -\frac{x-1}{2} & \text{if } x \in (0, -1] \\ 0 & \text{for all other } x. \end{cases}$$