Faculty of Engineering, Department of Computer Science

Erasmus+ International PhD Summer School 2025

Mathematics and Machine Learning for Image Analysis

University of Bologna

10 June 2025

UCL

This is joint work with

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Isaac Newton Institute for Mathematical Sciences

Queen Mary University of London
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EPSRC

INδAM

Learning optimal sampling strategies for MRI

- Error estimates in inverse problems
- Computing source condition elements
- Learning variational regularisations with optimal error estimates
- Learning the sampling pattern in MRI
- Conclusions & outlook

Motivation

Magnetic resonance imaging

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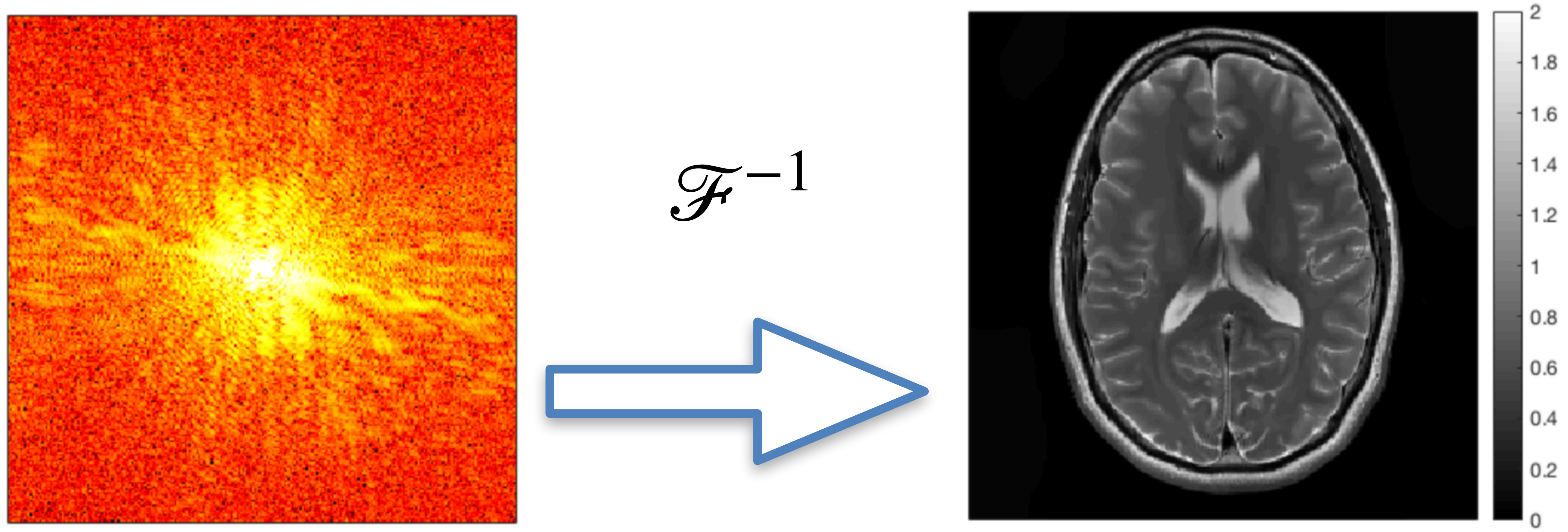
Simplified image reconstruction process



$$(\mathscr{F}u)_{pq} = \frac{1}{\sqrt{n_x n_y}} \sum_{l=0}^{n_y-1} \sum_{j=0}^{n_x-1} u_{lj}\, e^{-i\frac{2\pi pl}{n_y}} e^{-i\frac{2\pi qj}{n_x}}$$

Motivation

Magnetic resonance imaging

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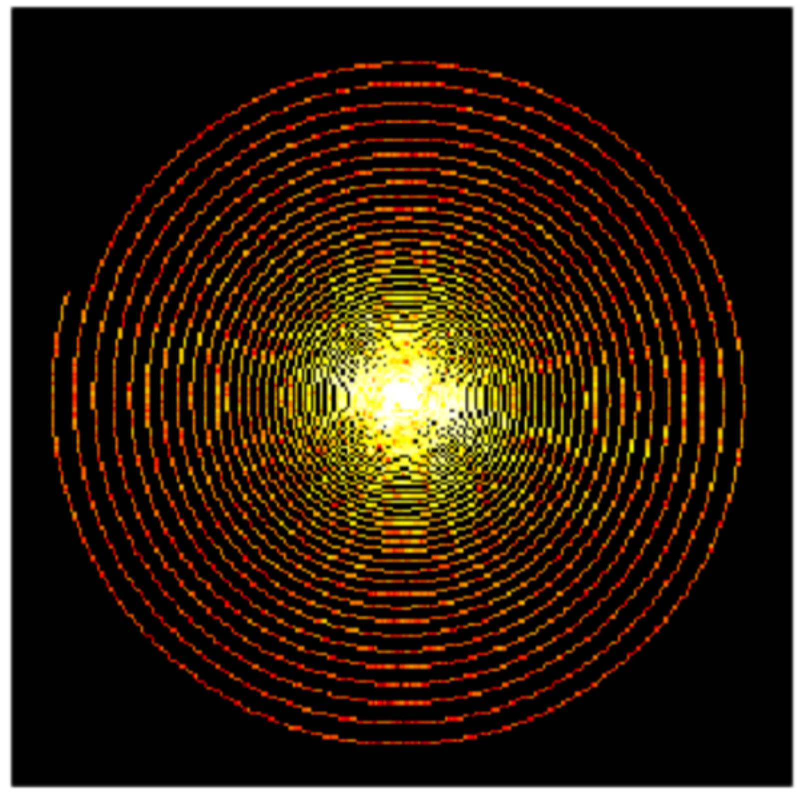
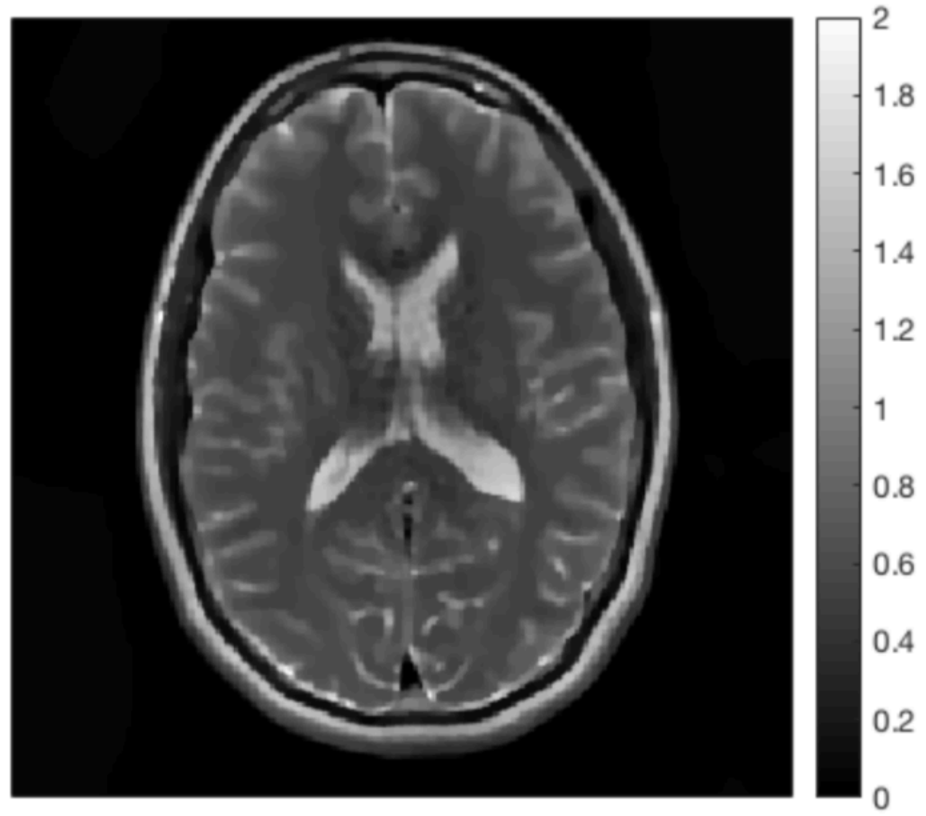
Simplified image reconstruction process





Goal: speed up acquisition process

$$(\mathscr{F}u)_{pq} = \frac{1}{\sqrt{n_x n_y}} \sum_{l=0}^{n_y-1} \sum_{j=0}^{n_x-1} u_{lj}\, e^{-i\frac{2\pi pl}{n_y}} e^{-i\frac{2\pi qj}{n_x}}$$

Motivation

Magnetic resonance imaging

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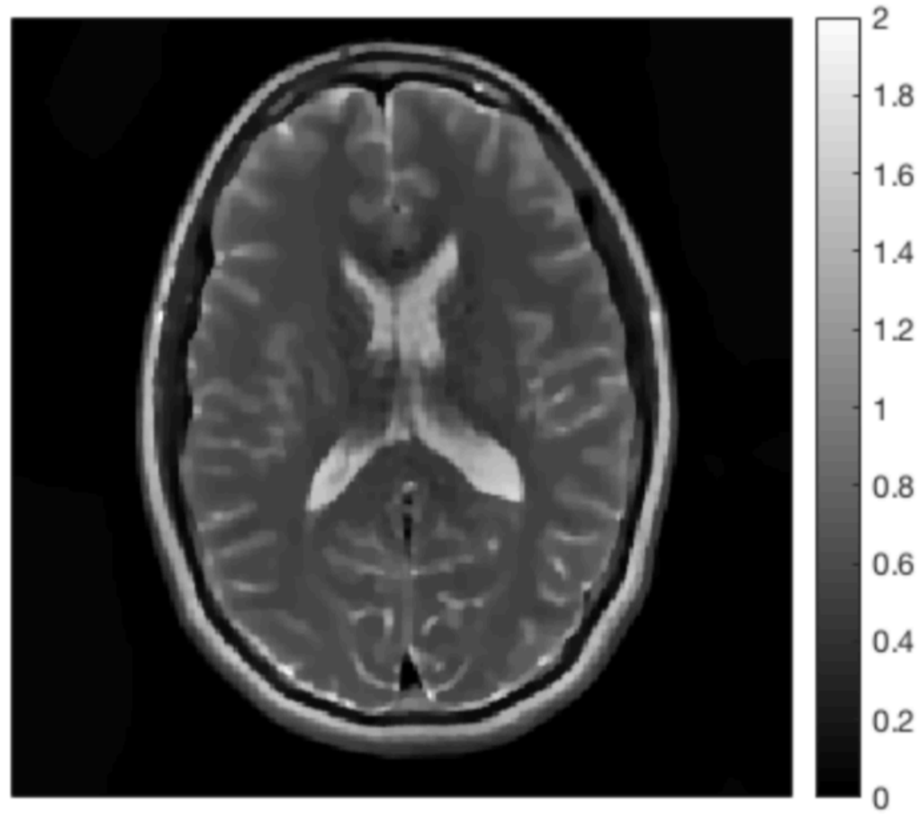
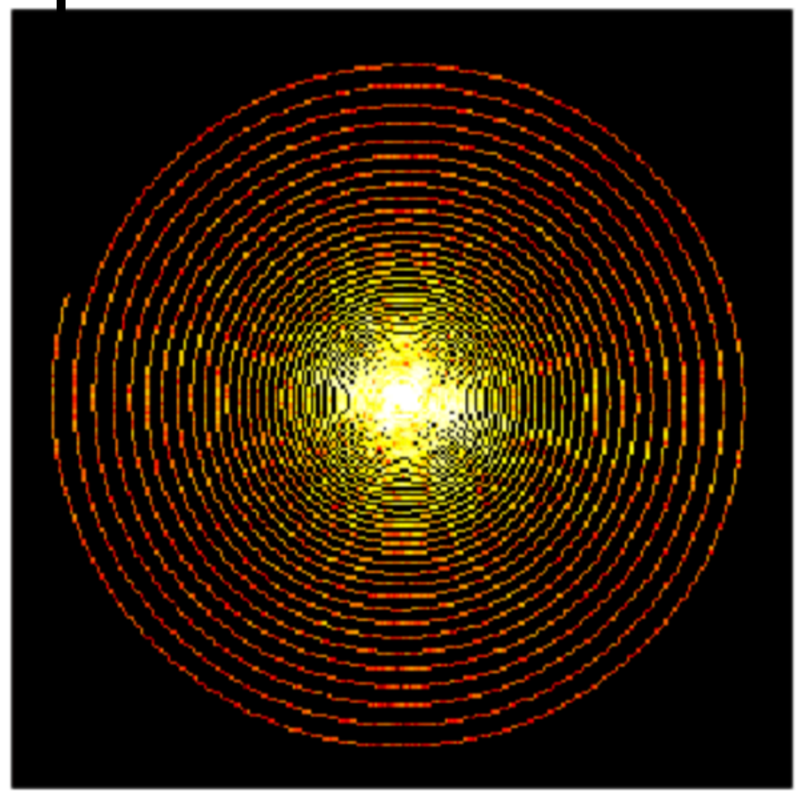
Simplified image formation process

Sampling operator



$S\mathcal{F}$



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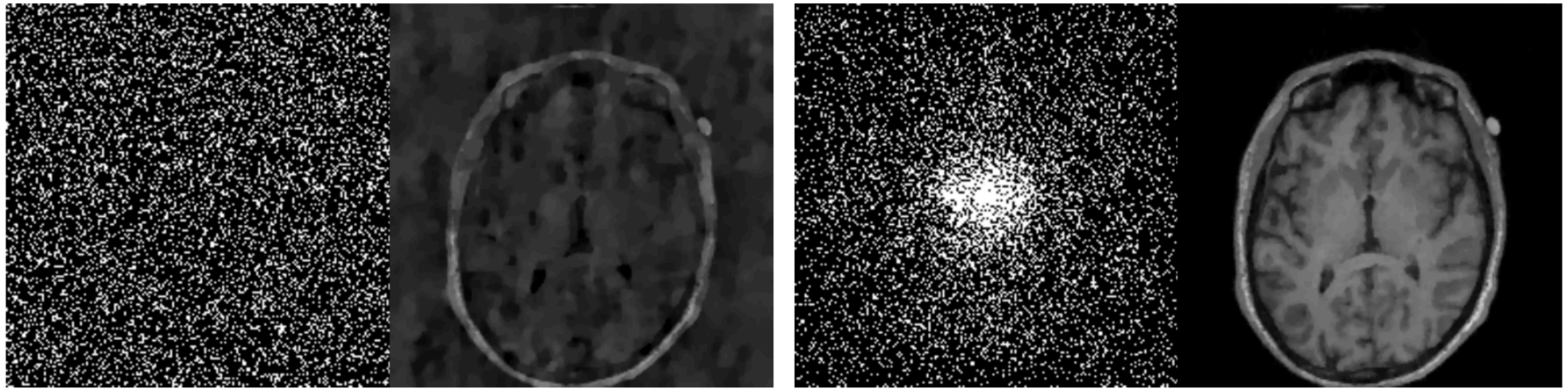
Motivation

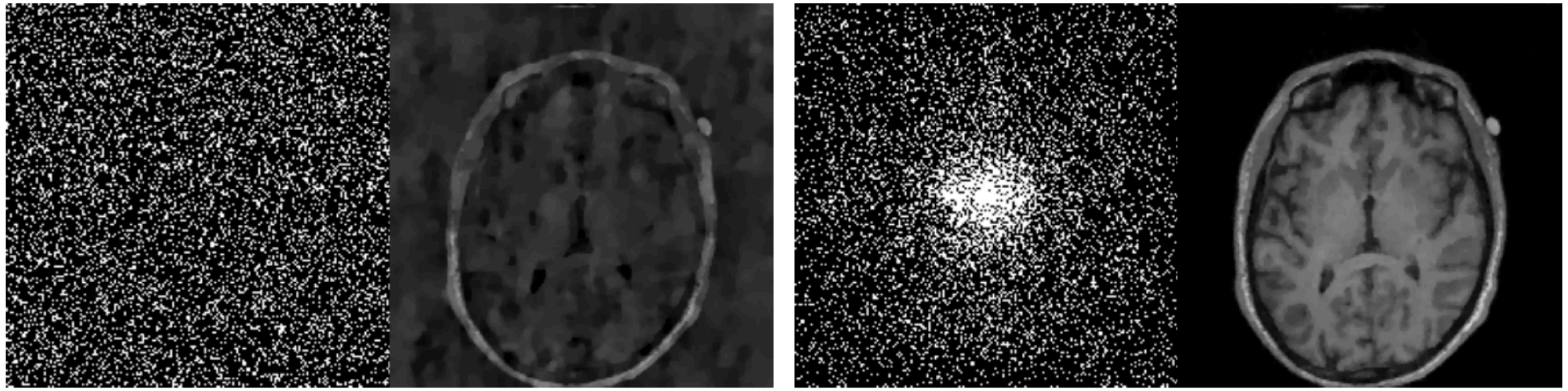


Uniform random   Reconstruction   Learned   Reconstruction

from*

*Sherry, F., MB, De los Reyes, J. C., Graves, M. J., Maierhofer, G., Williams, G., Schönlieb, C.-B. & Ehrhardt, M. J. (2020). Learning the sampling pattern for MRI. *IEEE Transactions on Medical Imaging*, *39*(12), 4310-4321.

Motivation



Uniform random | Reconstruction | Learned | Reconstruction

from*

Our approach back then:

$$\min_{S,\alpha} \|R_{S,\alpha}(f^\delta) - u^\dagger\|^2 + \mathscr{R}(S)$$

subject to

$$R_{S,\alpha}(f^\delta) \in \arg\min_u \left\{ \frac{1}{2}\|S\mathscr{F}u - f^\delta\|^2 + \alpha J(u) \right\}$$

Complex bilevel optimisation approach

Today's talk:
simple convex minimisation problem(s)

*Sherry, F., MB, De los Reyes, J. C., Graves, M. J., Maierhofer, G., Williams, G., Schönlieb, C.-B. & Ehrhardt, M. J. (2020). Learning the sampling pattern for MRI. *IEEE Transactions on Medical Imaging*, *39*(12), 4310-4321.

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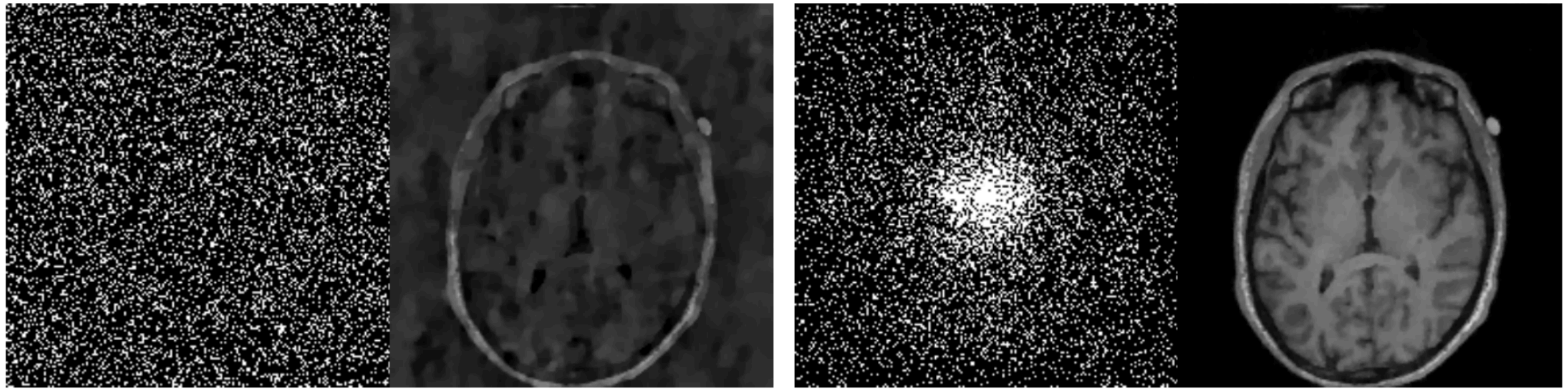

Uniform random Reconstruction Learned Reconstruction

from*

Many other relevant works:

Gözcü et al. 2018, 2019 , Sanchez et al. 2019, Weiss et al. 2019, Bahadir et al. 2019, Jin, Unser, Yi 2019, Gossard, Gournay, Weiss 2022, Bakker et al. 2022, etc.

*Sherry, F., MB, De los Reyes, J. C., Graves, M. J., Maierhofer, G., Williams, G., Schönlieb, C.-B. & Ehrhardt, M. J. (2020). Learning the sampling pattern for MRI. *IEEE Transactions on Medical Imaging*, *39*(12), 4310-4321.

Error estimates in inverse problems

Error estimates in inverse problems

If we approximate the solution of an inverse problem $Ku^\dagger = f$ with regularisations R_α, we ideally want convergent regularisations

We would like to establish

$$D\left(u^\dagger, R_\alpha(f^\delta)\right) \leq C\,\delta$$

such that

$$\limsup_{\delta \to 0} \left\{ D\left(u^\dagger, R_\alpha(f^\delta)\right) \,\middle|\, \text{ for } f = Ku^\dagger \text{ and } f^\delta \text{ with } \|f - f^\delta\| \leq \delta \right\} = 0$$

for some distance measure D (not necessarily a metric)

Engl, H. W., Hanke, M., & Neubauer, A. (1996). *Regularization of inverse problems* (Vol. 375). Springer Science & Business Media.
Scherzer, O., Grasmair, M., Grossauer, H., Haltmeier, M., & Lenzen, F. (2009). Variational methods in imaging.
MB, & Burger, M. (2018). Modern regularization methods for inverse problems. *Acta Numerica*, *27*, 1-111.

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Making this small subject to constraints is a surrogate to the previous upper level problem

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Error estimates in inverse problems

We would like to establish

$$D\left(u^{\dagger}, R_{\alpha}(f^{\delta})\right) \leq C\,\delta$$

Example: variational regularisation

$$R_{\alpha}: f^{\delta} \mapsto u_{\alpha} \in \arg\min_{u \in X} \left\{ \frac{1}{2}\|Ku - f^{\delta}\|_{Y}^{2} + \alpha J(u) \right\}$$

Assume source (or range) condition:

$$\exists\, v \in Y: \qquad K^{*}v \in \partial J(u^{\dagger}) = \{p \mid J(v) - J(u^{\dagger}) - \langle p, v - u^{\dagger}\rangle \geq 0, \forall v\}$$

Error estimates in inverse problems

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$$\exists\, v \in Y: \qquad K^* v = \nabla J(u^{\dagger})$$

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$$R_\alpha : f^\delta \mapsto u_\alpha \in \arg\min_{u\in X} \left\{ \frac{1}{2}\|Ku - f^\delta\|_Y^2 + \alpha J(u) \right\}$$

Assume source (or range) condition:

$$\exists\, v \in Y: \qquad K^* v \in \partial J(u^\dagger)$$

(equivalent to $u^\dagger \in \arg\min_{u\in X} \left\{ \frac{1}{2}\|Ku - g_\alpha\|_Y^2 + \alpha J(u) \right\}$ with $g_\alpha = \alpha v + K u^\dagger = \alpha v + f$)

Error estimates in inverse problems

We would like to establish

$$D\left(u^\dagger, R_\alpha(f^\delta)\right) \leq C\,\delta$$

Example: variational regularisation

$$R_\alpha : f^\delta \mapsto u_\alpha \in \arg\min_{u\in X} \left\{ \frac{1}{2}\|Ku - f^\delta\|_Y^2 + \alpha J(u) \right\}$$

Assume source (or range) condition:

$$\exists\, v \in Y: \qquad K^* v \in \partial J(u^\dagger)$$

Then one can prove

$$D\left(R_{\alpha(\delta)}(f^\delta), u^\dagger\right) \leq \|v\|_Y\,\delta \qquad \text{for } \alpha(\delta) = \delta/\|v\|_Y$$

where D is a suitable (symmetrised) Bregman distance/divergence w.r.t J

Motivation

This presentation in a nutshell

Example:

$$D\left(R_{\alpha(\delta)}(f^{\delta}), u^{\dagger}\right) \leq \|v\|_Y \, \delta$$

we want to study this quantity

$u^{\dagger}$

$$K = I$$

$$J(u) = \mathrm{TV}(u) \quad *$$

*To be defined later, if you haven't seen this before

v

Motivation

This presentation in a nutshell

Example:

$$D\left(R_{\alpha(\delta)}(f^\delta), u^\dagger\right) \le \|v\|_Y \, \delta$$

we want to study this quantity

$= \alpha$

$+$

g_α $\qquad v \qquad$ $u^\dagger$

Motivation

This presentation in a nutshell

Example:

$$D\left(R_{\alpha(\delta)}(f^\delta), u^\dagger\right) \leq \|v\|_Y \,\delta$$

R_α () $=$ 

g_α $\qquad$ $u^\dagger$

Ideally, we want

$v =$ 

to have small norm $\|v\|_Y$

How do we compute v in order to estimate (or even control) $\|v\|_Y$?

Computing source condition elements

Computing source condition elements

Approach 1: we can modify the source condition

$$K^*v \in \partial J(u^\dagger)$$

Computing source condition elements

Approach 1: we can modify the source condition to

$$u^\dagger + K^* v \in \partial\left(\frac{1}{2}\|\cdot\|^2 + J\right)(u^\dagger)$$

Now we use the Fenchel-Young equality:

$$p \in \partial F(u) \quad \Longleftrightarrow \quad F(u) + F^\star(p) = \langle u, p\rangle$$

where $F^\star$ denotes the convex conjugate of F, i.e.

$$F^\star(p) := \sup_u \langle u, p\rangle - F(u)$$

Werner Fenchel, *Convex cones, sets, and functions*. Princeton University, 1953
Theorem 23.5, Ralph Tyrell Rockafellar, Convex analysis, Princeton university press, 1970

Computing source condition elements

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$$F^\star(p) := \sup_u \langle u, p \rangle - F(u)$$

Proof: $p \in \partial F(u) \Longleftrightarrow \quad p \in \{q \,|\, F(v) \geq F(u) + \langle q, v-u \rangle, \forall v\}$

$$\Longleftrightarrow \quad \langle p, u \rangle - F(u) \geq \langle p, v \rangle - F(v) \qquad \forall v$$

$$\Longleftrightarrow \quad \langle p, u \rangle - F(u) = F^\star(p)$$

$$\Longleftrightarrow \quad F(u) + F^\star(p) = \langle u, p \rangle$$

Werner Fenchel, *Convex cones, sets, and functions*. Princeton University, 1953
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Computing source condition elements

Approach 1: we can modify the source condition to

$$u^{\dagger} + K^{*}v \in \partial\left(\frac{1}{2}\|\cdot\|^{2} + J\right)(u^{\dagger})$$

Now we use the Fenchel-Young equality:

$$p \in \partial F(u) \qquad \Longleftrightarrow \qquad F(u) + F^{\star}(p) = \langle u, p\rangle$$

This implies

$$\left(\frac{1}{2}\|\cdot\|^{2} + J\right)(u^{\dagger}) + \left(\frac{1}{2}\|\cdot\|^{2} + J\right)^{\star}\left(u^{\dagger} + K^{*}v\right) = \langle u^{\dagger}, u^{\dagger} + K^{*}v\rangle$$

Werner Fenchel, *Convex cones, sets, and functions*. Princeton University, 1953
Theorem 23.5, Ralph Tyrell Rockafellar, Convex analysis, Princeton university press, 1970

Computing source condition elements

Instead of enforcing a strict equality, we can define

$$G_J(v) := \left(\frac{1}{2}\|\cdot\|^2 + J\right)(u^\dagger) + \left(\frac{1}{2}\|\cdot\|^2 + J\right)^\star \left(u^\dagger + K^*v\right) - \langle u^\dagger, u^\dagger + K^*v\rangle$$

MB, Tatiana A. Bubba, Luca Ratti, and Danilo Riccio. "Trust your source: quantifying source condition elements for variational regularisation methods." IMA Journal of Applied Mathematics (2024): hxae008.

Computing source condition elements

Instead of enforcing a strict equality, we can define

$$G_J(v) := \left(\frac{1}{2}\|\cdot\|^2 + J\right)(u^\dagger) + \left(\frac{1}{2}\|\cdot\|^2 + J\right)^{\star}(u^\dagger + K^*v) \;-\; \langle u^\dagger, u^\dagger + K^*v\rangle$$

Proposition: the gradient ∇G_J of G_J exists and reads

$$\boxed{\nabla G_J(v) = K\,\mathrm{prox}_J(u^\dagger + K^*v) - Ku^\dagger.}$$

Here prox denotes the proximal map, i.e.

$$\mathrm{prox}_F : Z \to Z, \qquad \mathrm{prox}_F(z) := \arg\min_{u \in Z} \left\{ \frac{1}{2}\|u - z\|_Z^2 + F(u) \right\}$$

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Computing source condition elements

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$$G_J(v) := \left(\frac{1}{2}\|\cdot\|^2 + J\right)(u^\dagger) + \left(\frac{1}{2}\|\cdot\|^2 + J\right)^\star \left(u^\dagger + K^*v\right) \; - \; \langle u^\dagger, u^\dagger + K^*v\rangle$$

Because of the Fréchet-differentiability of G_J, we can solve

$$\hat{v} = \arg\min_v G_J(v)$$

for instance via gradient descent, i.e

$$v^{k+1} = v^k - \tau K\left(\mathrm{prox}_J\left(u^\dagger + K^*v^k\right) - u^\dagger\right)$$

which is globally convergent for $\tau \leq 1/\|K\|^2$

MB, Tatiana A. Bubba, Luca Ratti, and Danilo Riccio. "Trust your source: quantifying source condition elements for variational regularisation methods." IMA Journal of Applied Mathematics (2024): hxae008.

Extension to more general functions and range conditions

We can also consider composite functionals

$$J(u) = H(Au + b)$$

Example: $J = \mathrm{TV}\colon \mathbb{R}^{n_y \times n_x} \to \mathbb{R}$ with

$$\mathrm{TV}(u) = \sum_{i=1}^{n_y-1} \sum_{j=1}^{n_x-1} \sqrt{\left|u_{(i+1)j} - u_{ij}\right|^2 + \left|u_{i(j+1)} - u_{ij}\right|^2}$$

We obtain this for $b = 0,\ A\colon \mathbb{R}^{n_y \times n_x} \to \mathbb{R}^{(n_y-1)\times(n_x-1)\times 2}$ with

$$(Au)_{ijp} = \begin{cases} u_{(i+1)j} - u_{ij} & p = 1 \\ u_{i(j+1)} - u_{ij} & p = 2 \end{cases},$$

and $H\colon \mathbb{R}^{(n_y-1)\times(n_x-1)\times 2} \to \mathbb{R}$ with $H(q) = \sum_{i=1}^{n_y-1} \sum_{j=1}^{n_x-1} \sqrt{\left|q_{ij1}\right|^2 + \left|q_{ij2}\right|^2}$.

MB, Tatiana A. Bubba, Luca Ratti, and Danilo Riccio. "Trust your source: quantifying source condition elements for variational regularisation methods." IMA Journal of Applied Mathematics (2024): hxae008.

Extension to more general functions and range conditions

We can also consider composite functionals

$$J(u) = H(Au + b)$$

Consider the range condition

$$u^\dagger \in \arg\min_{u \in X} \left\{ \frac{1}{2}\|Ku - g_\alpha\|^2 + \alpha J(u) \right\} ,$$

respectively it's optimality condition

$$K^*(Ku^\dagger - g_\alpha) + \alpha A^* q^\dagger = 0$$

for $q^\dagger \in \partial H(Au^\dagger + b)$.

MB, Tatiana A. Bubba, Luca Ratti, and Danilo Riccio. "Trust your source: quantifying source condition elements for variational regularisation methods." IMA Journal of Applied Mathematics (2024): hxae008.

Extension to more general functions and range conditions

Consider the range condition

$$K^*(Ku^\dagger - g_\alpha) + \alpha A^* q^\dagger = 0$$

for $q^\dagger \in \partial H(Au^\dagger + b)$.

Multiplying by $1/\alpha$ and using $g_\alpha = \alpha v + Ku^\dagger$ then yields

$$K^* v = A^* q^\dagger$$

$$q^\dagger \in \partial H(Au^\dagger + b)$$

MB, Tatiana A. Bubba, Luca Ratti, and Danilo Riccio. "Trust your source: quantifying source condition elements for variational regularisation methods." IMA Journal of Applied Mathematics (2024): hxae008.

Extension to more general functions and range conditions

Multiplying by $1/\alpha$ and using $g_\alpha = \alpha v + Ku^\dagger$ then yields

$$K^* v = A^* q^\dagger$$

$$q^\dagger \in \partial H(Au^\dagger + b)$$

Similar to before, we relax these problems by introducing $G_H\colon\ Y \to \mathbb{R}$ with

$$G_H(q) = \left(\frac{1}{2}\|\cdot\|^2 + H\right)(Au^\dagger + b) + \left(\frac{1}{2}\|\cdot\|^2 + H\right)^\star \left(q + Au^\dagger + b\right) - \langle Au^\dagger + b, Au^\dagger + b + q\rangle$$

and minimise

$$E_H(v, q^\dagger) = \frac{1}{2}\|K^* v - A^* q^\dagger\|^2 + G_H(q^\dagger)$$

MB, Tatiana A. Bubba, Luca Ratti, and Danilo Riccio. "Trust your source: quantifying source condition elements for variational regularisation methods." IMA Journal of Applied Mathematics (2024): hxae008.

Computing source condition elements

Approach 2: we can formulate the J-minimising solution of $Ku = f$, i.e.

$$\min_u J(u) \qquad \text{subject to} \qquad Ku = f$$

as a primal-dual problem

$$\min_u \sup_v J(u) + \langle v, f - Ku \rangle$$

with saddle point $(u^\dagger, v^\dagger)$ and optimality conditions

$$K^* v^\dagger \in \partial J(u^\dagger) \qquad \text{source condition}$$

$$Ku^\dagger = f$$

Computing source condition elements

Approach 2: we can formulate the J-minimising solution of $Ku = f$, i.e.

$$\min_u J(u) + H(f - Ku)$$

as a primal-dual problem

$$\min_u \sup_v J(u) + \langle v, f - Ku \rangle - H^\star(v)$$

with saddle point $(u^\dagger, v^\dagger)$ and optimality conditions

$$K^* v^\dagger \in \partial J(u^\dagger) \qquad \text{source condition}$$

$$f - Ku^\dagger \in \partial H^\star(v^\dagger)$$

Computing source condition elements

Approach 2: we can formulate the J-minimising solution of $Ku = f$, i.e.

$$\min_u J(u) + \alpha \| f - Ku \|_Y$$

as a primal-dual problem

$$\min_u \sup_v J(u) + \langle v, f - Ku \rangle - \chi_{\|\cdot\|_Y \leq \alpha}(v)$$

with saddle point $(u^\dagger, v^\dagger)$ and optimality conditions

$$K^* v^\dagger \in \partial J(u^\dagger) \qquad \text{source condition}$$

$$f - Ku^\dagger \in \partial \chi_{\|\cdot\|_Y \leq \alpha}(v^\dagger)$$

Computing source condition elements

Approach 2: we can formulate the J-minimising solution of $Ku = f$, i.e.

$$\min_u J(u) + \alpha\| f - Ku \|_Y$$

Example: $K = I$, $J(u) = \mathrm{TV}(u)$

f

u_∞

v_∞ with $\|v_\infty\| \approx 801.88$

Computing source condition elements

Approach 2: we can formulate the J-minimising solution of $Ku = f$, i.e.

$$\min_u J(u) + \alpha \| f - Ku \|_Y$$

Example: $K = I$, $J(u) = \mathrm{TV}(u)$

f

Reconstructed image

u_α

Source condition element

v_α with $\|v_\alpha\| = \alpha = 100$

Computing source condition elements

Approach 2: we can formulate the J-minimising solution of $Ku = f$, i.e.

$$\min_u J(u) + H(f - Ku)$$

as a primal-dual problem

$$\min_u \sup_v J(u) + \langle v, f - Ku \rangle - H^\star(v)$$

Can (for example) be solved with primal-dual hybrid gradient* method, i.e.

$$u^{k+1} = \mathrm{prox}_{\tau J}\left(u^k + \tau K^* v^k\right)$$
$$v^{k+1} = \mathrm{prox}_{\sigma H^\star}\left(v^k - \sigma\left(K(2u^{k+1} - u^k) - f\right)\right)$$

$$\tau\sigma < 1/\|K\|^2$$

*(cf. Chambolle, A., & Pock, T. (2016). An introduction to continuous optimization for imaging. *Acta Numerica*, 25, 161-319.

Numerical results

(a) Shepp-Logan phantom

(b) Eileen Collins

Numerical results

Inverse problem

$$S\mathscr{F}u^\dagger = f$$

Subsampling operator

with discrete 2D Fourier transform $$(\mathscr{F}u)_{pq} = \frac{1}{\sqrt{n_x n_y}} \sum_{l=0}^{n_y-1} \sum_{j=0}^{n_x-1} u_{lj}\, e^{-i\frac{2\pi pl}{n_y}} e^{-i\frac{2\pi qj}{n_x}}$$

Regularisation function:

$$J(u) = H(Au) \quad \text{with} \quad (Au)_{ijp} = \begin{cases} u_{(i+1)j} - u_{ij} & p = 1 \\ u_{i(j+1)} - u_{ij} & p = 2 \end{cases}, \quad H(q) = \sum_{i=1}^{n_y-1} \sum_{j=1}^{n_x-1} \sqrt{\left|q_{ij1}\right|^2 + \left|q_{ij2}\right|^2}\,.$$

(2D discretised isotropic total variation)

Numerical results

Inverse problem

$$S\mathscr{F}u^\dagger = f$$

Subsampling operator

Source condition

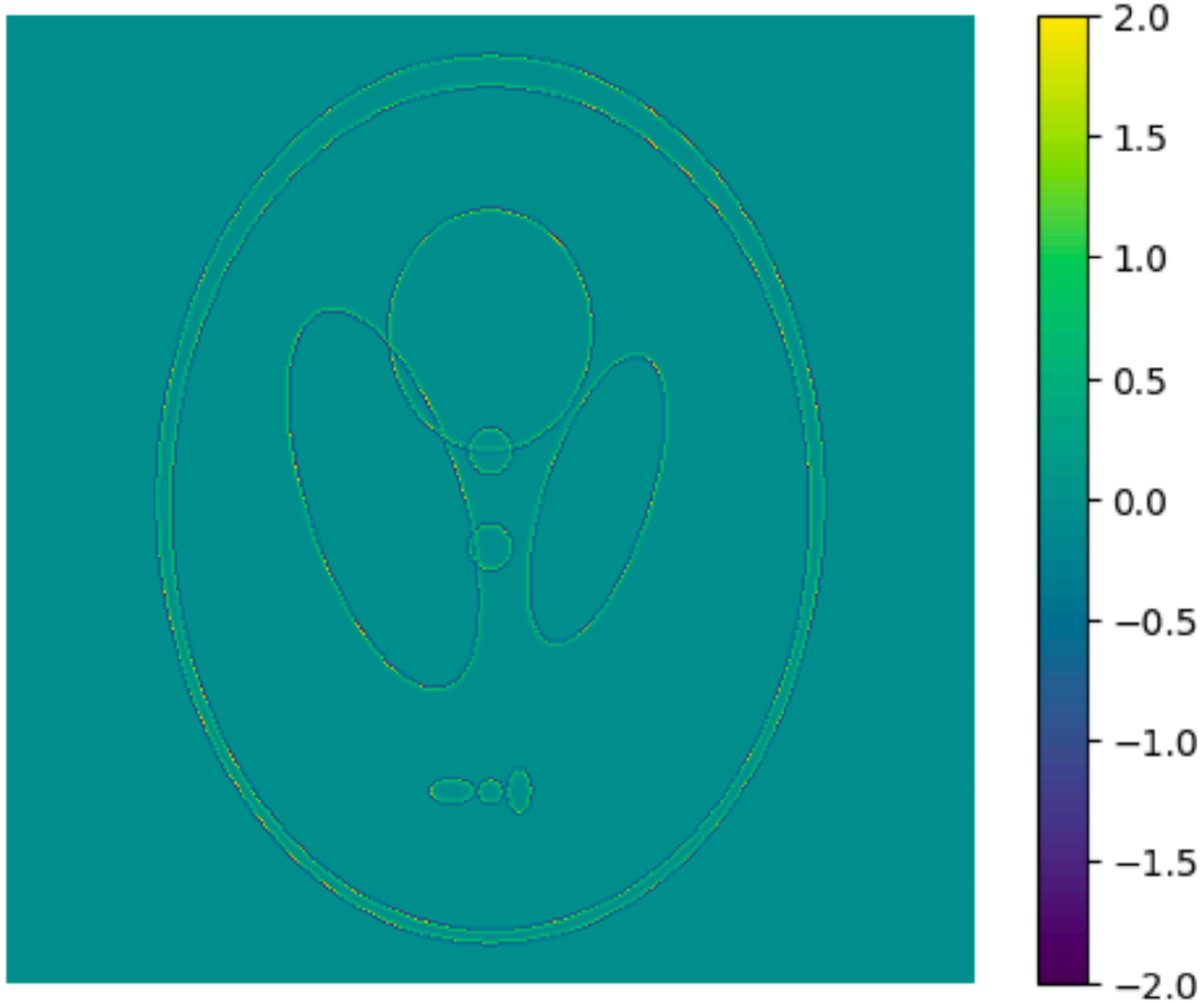
$$\mathscr{F}^{-1}S^\top v \in \partial \mathrm{TV}(u^\dagger)$$

Algorithm

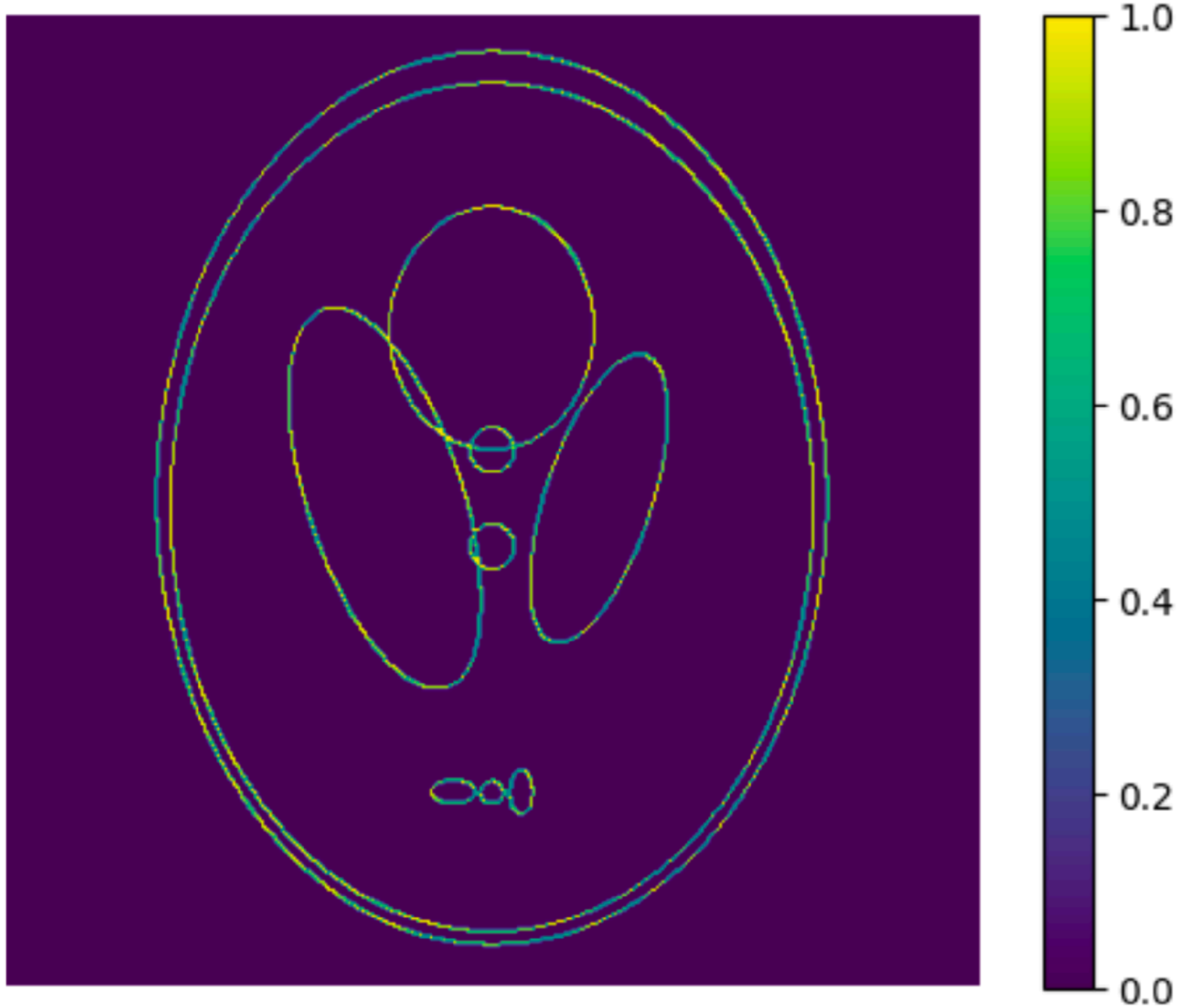
$$v^{k+1} = v^k - \tau S\mathscr{F}\left(\mathscr{F}^{-1}S^\top v^k - A^\top q^k\right),$$

$$q^{k+1} = q^k - \sigma\left(A\left(A^\top q^k - \mathscr{F}^{-1}S^\top v^{k+1}\right) + \mathrm{prox}_{\|\cdot\|_{2,1}}\left(Au^\dagger + q^k\right) - Au^\dagger\right).$$

Numerical results



$S = I$

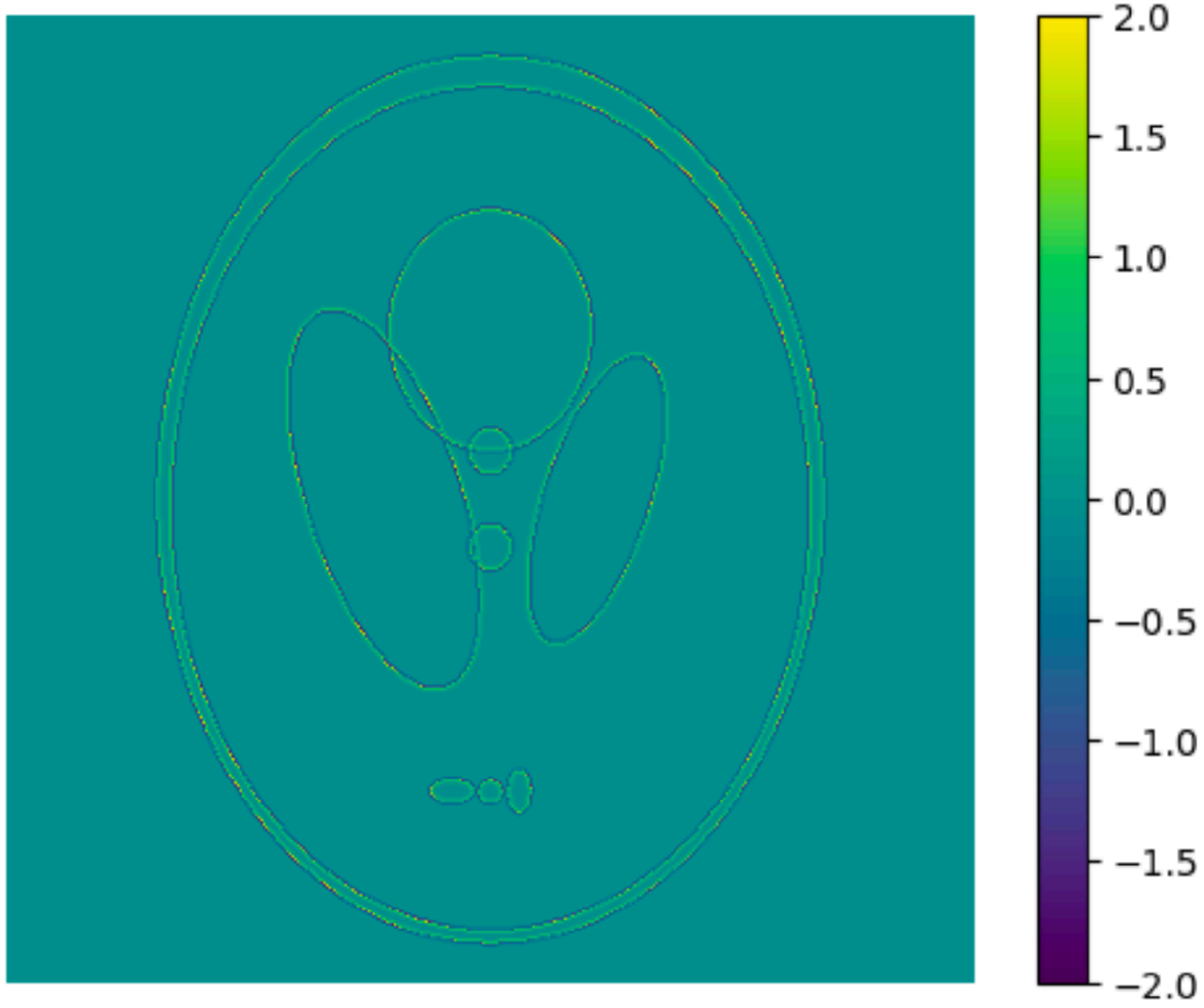


(a) $\mathscr{F}^{-1}v^K$

$\mathscr{F}^{-1}v^K = A^\top q^K$

(b) $\sqrt{|q_1^K|^2 + |q_2^K|^2}$

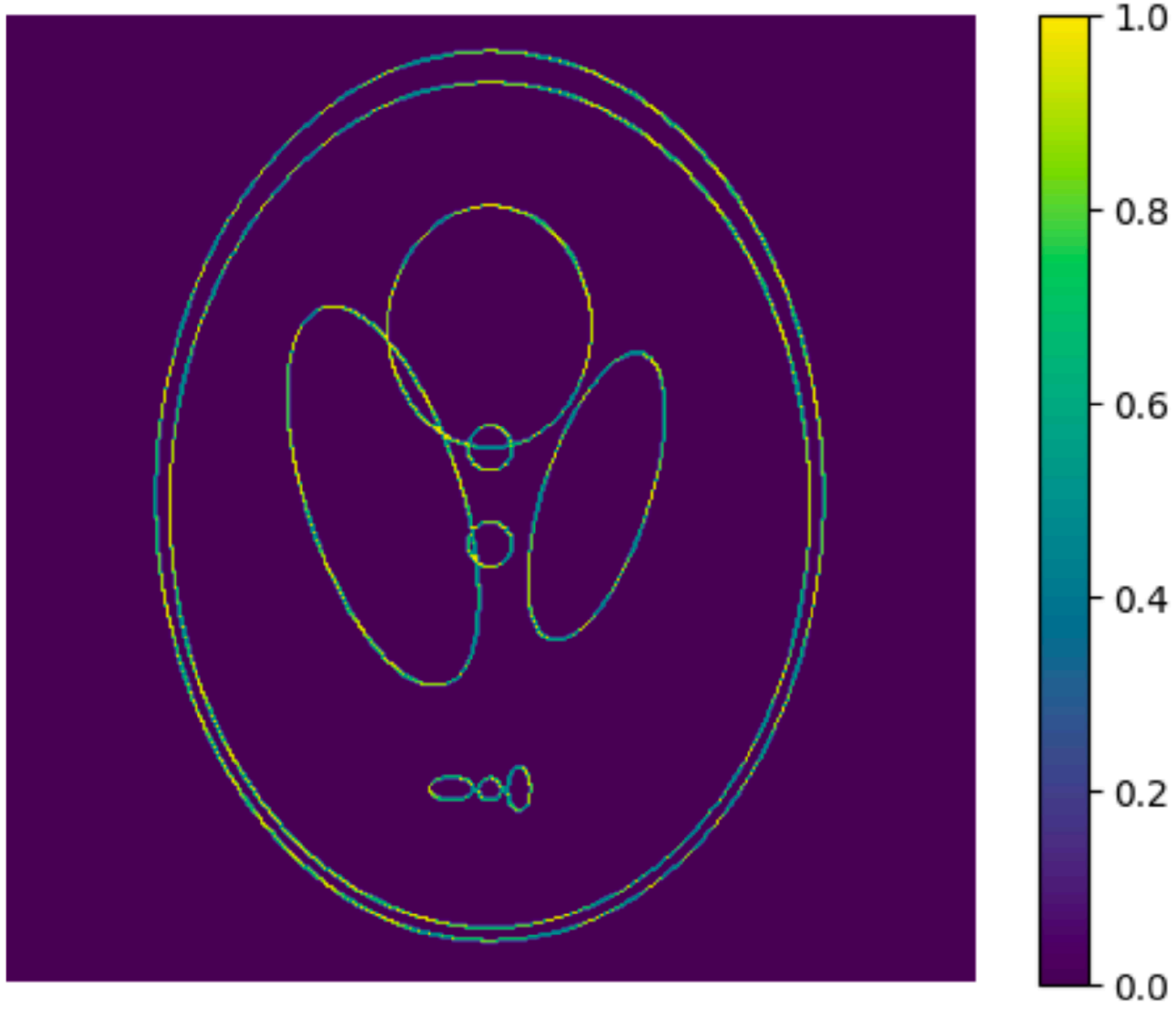
Numerical results



(a) $\mathscr{F}^{-1}v^K$

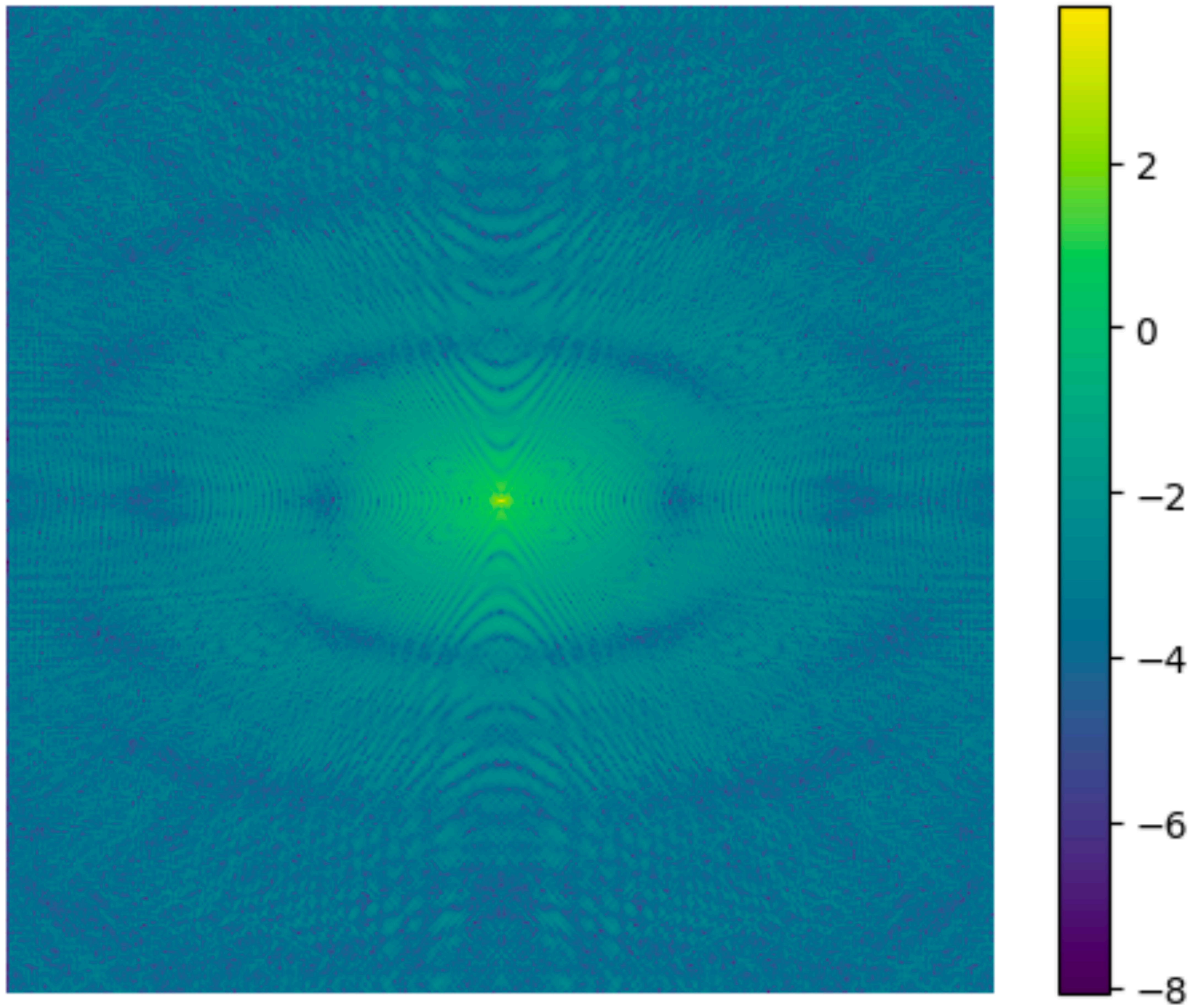
$S = I$

$\|v^K\| \approx 101.78$

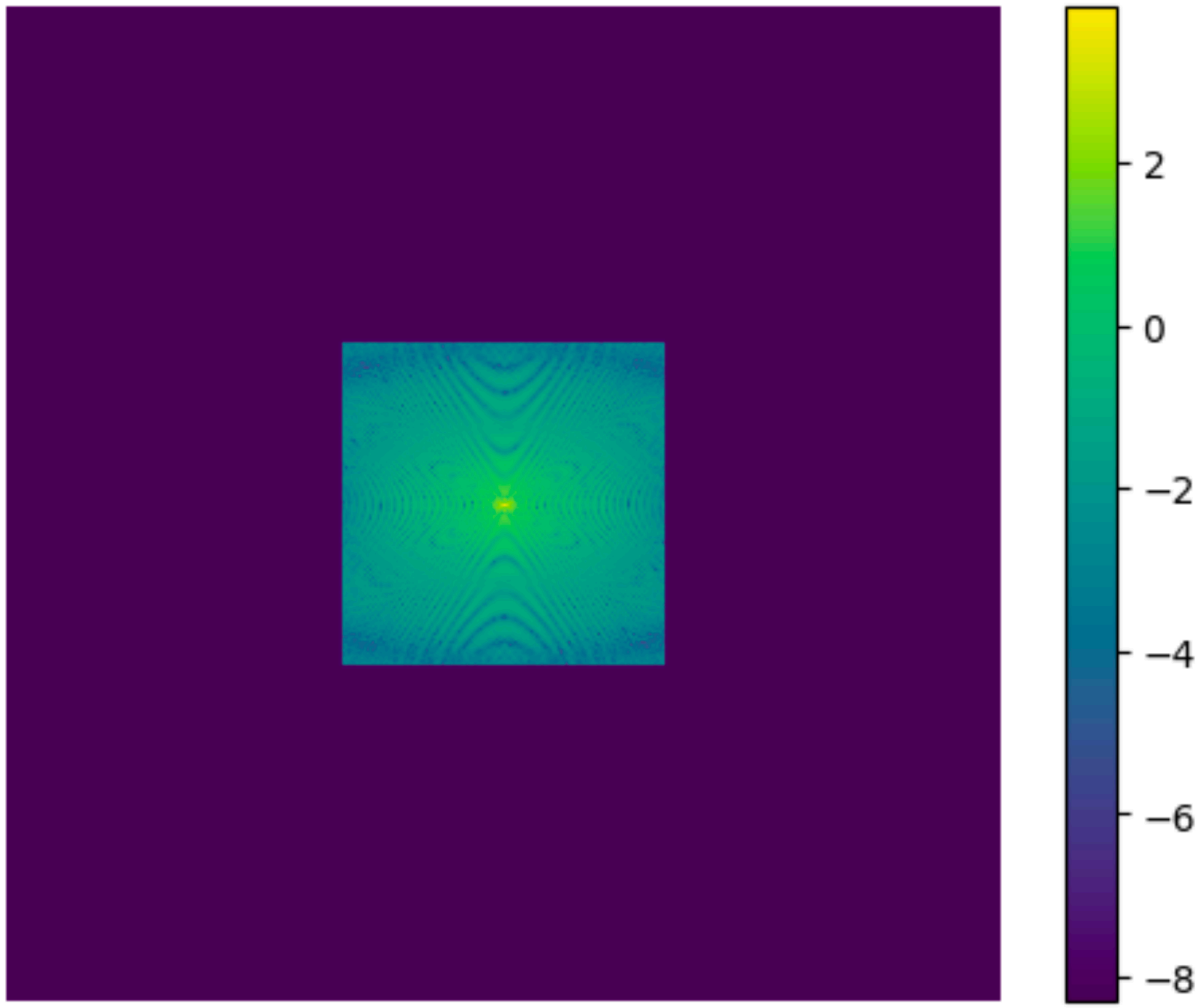


(b) $\sqrt{|q_1^K|^2 + |q_2^K|^2}$

Numerical results

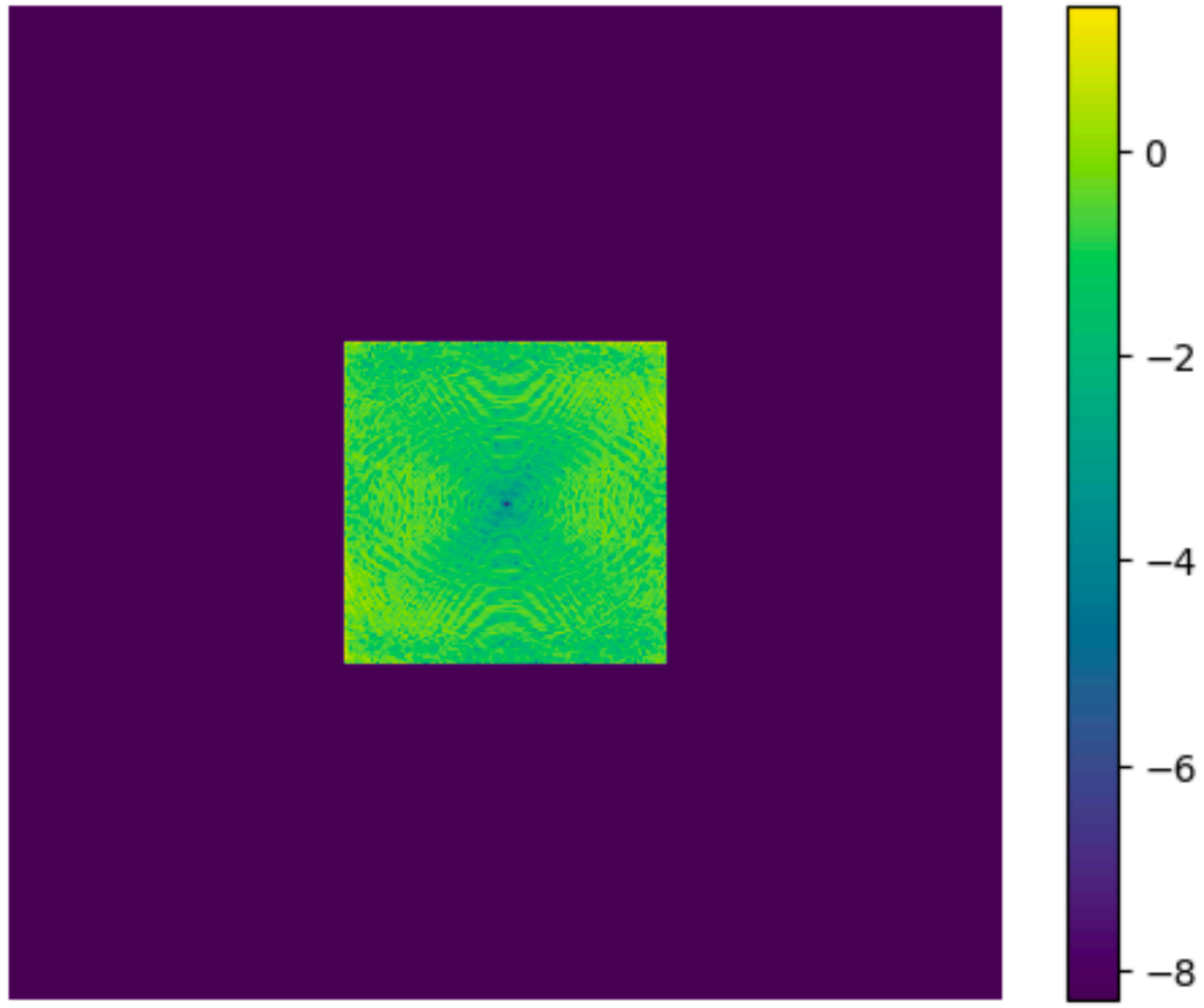


(a) Fourier transformed data

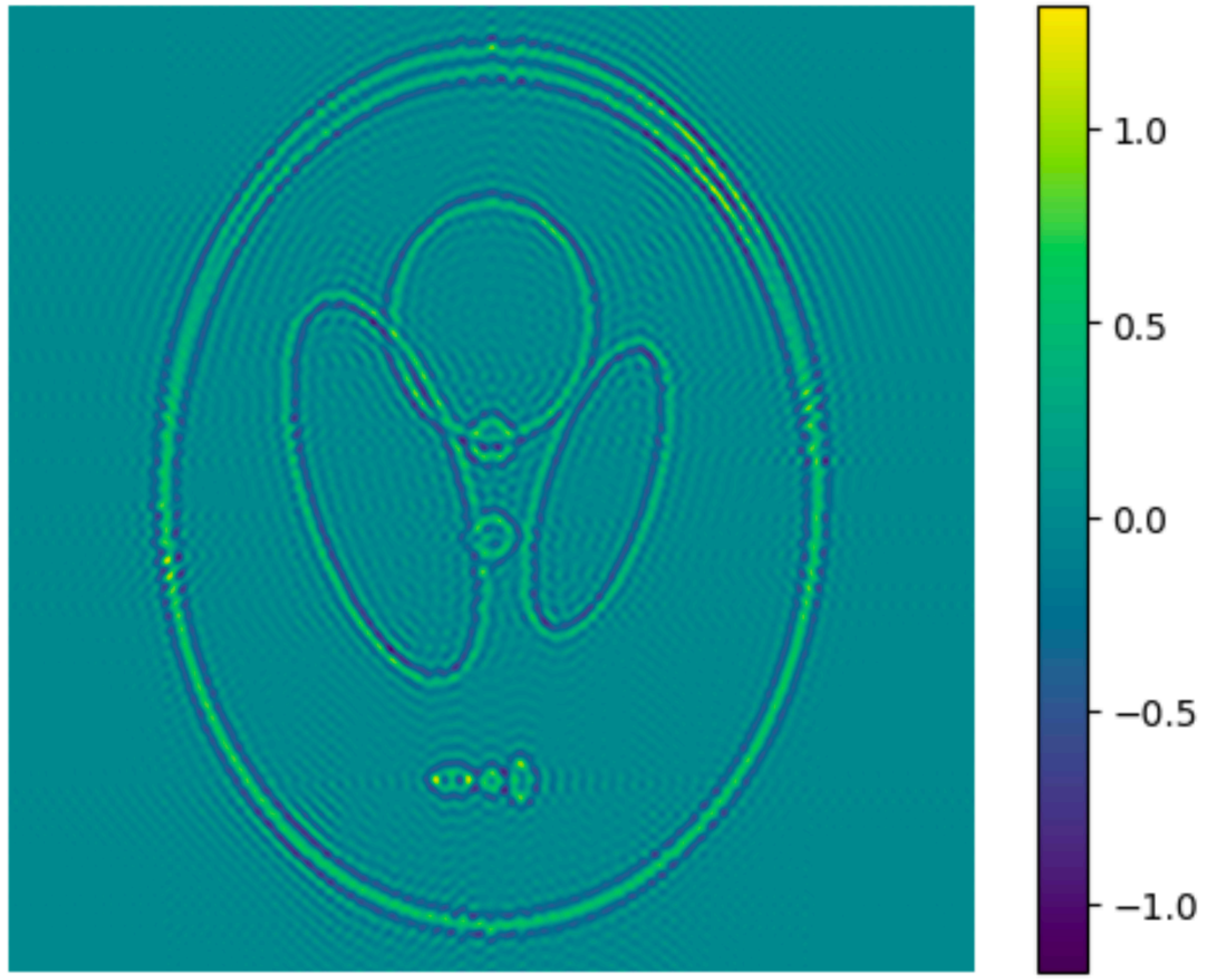


(b) Sub-sampled Fourier transformed data

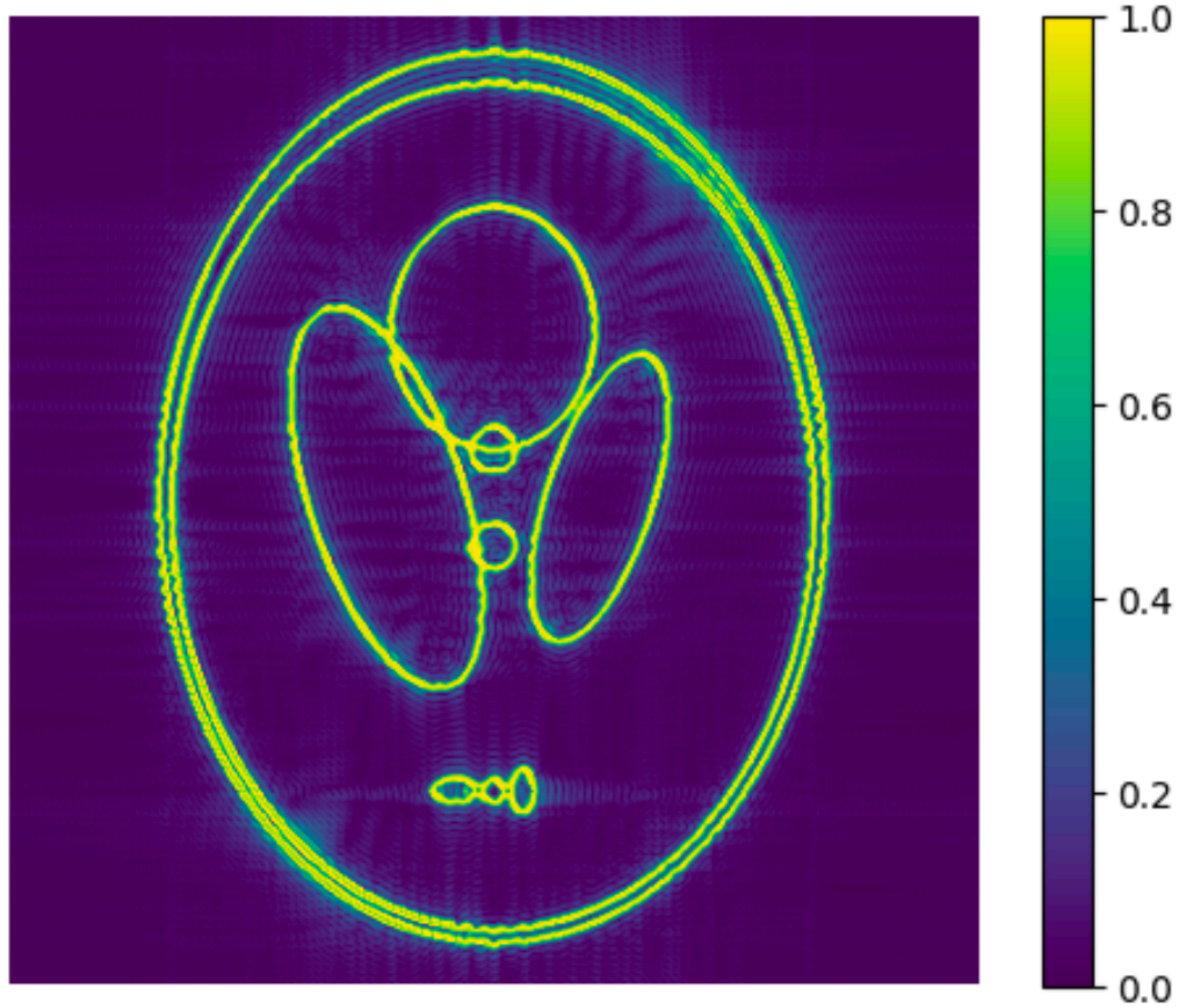
Numerical results



(a) v^K



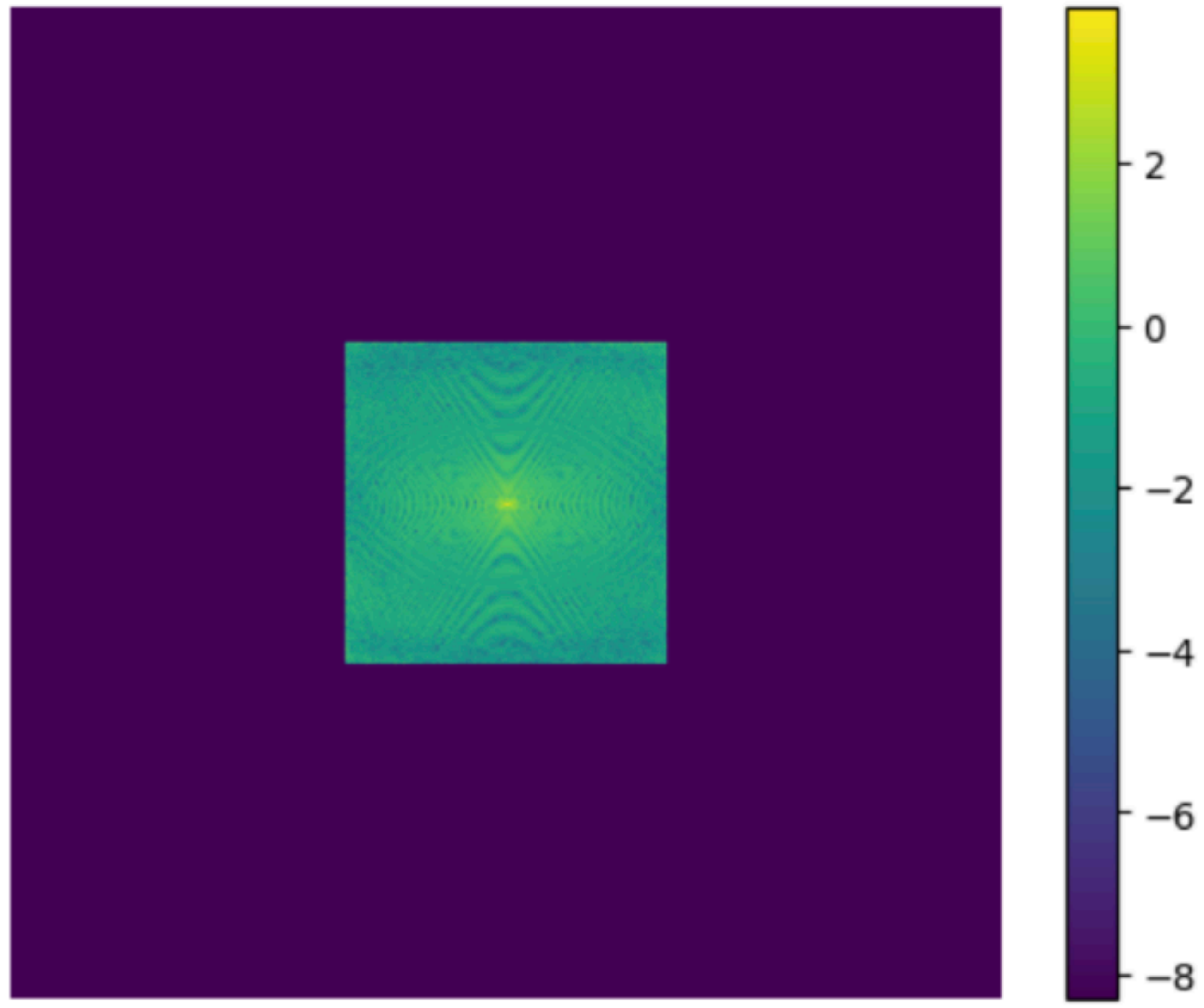
(b) Backprojection $\mathcal{F}^{-1} S^\top v^K$



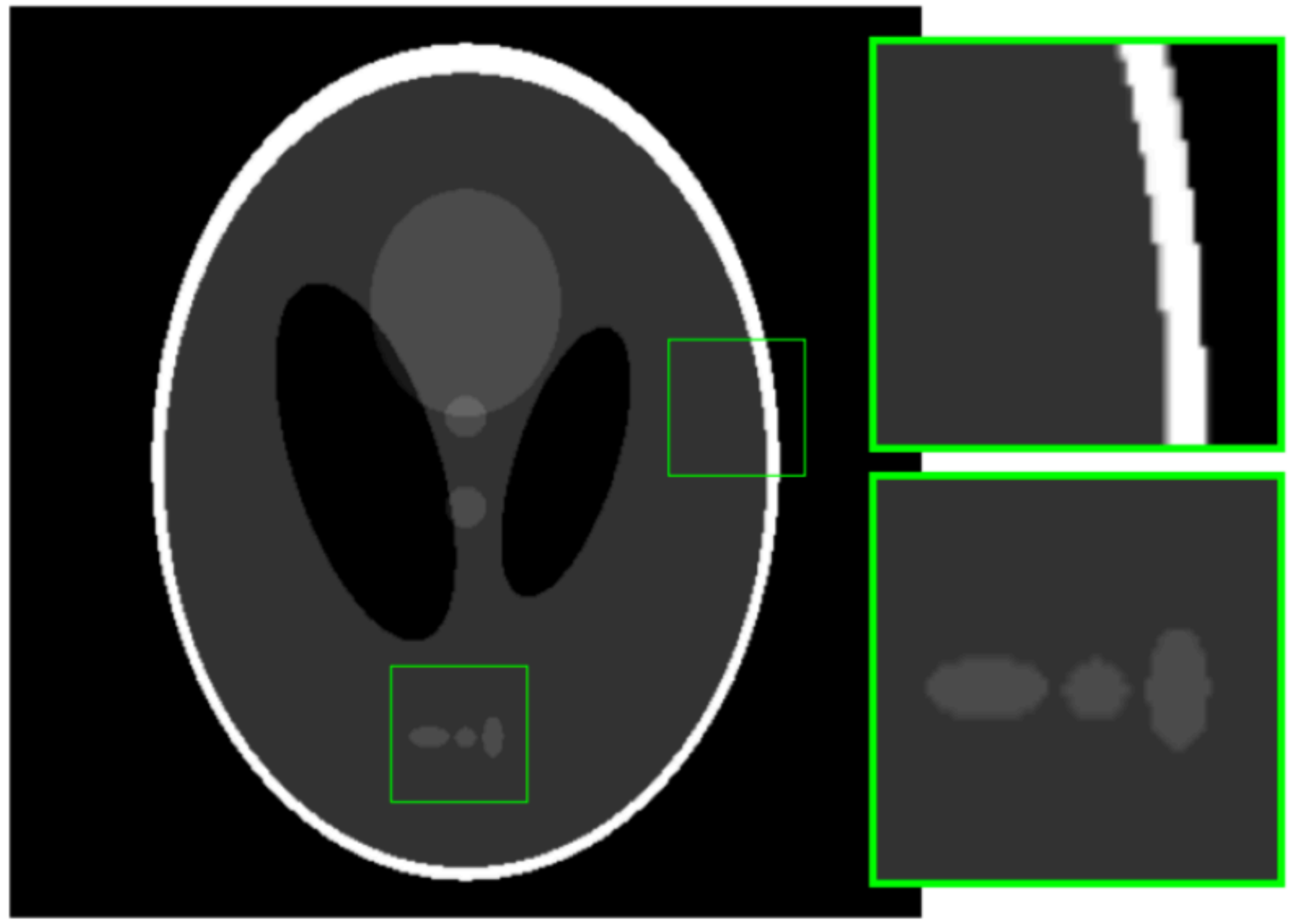
(c) $\sqrt{|q_1^K|^2 + |q_2^K|^2}$

$$\mathscr{F}^{-1} S^T v^K = A^\top q^K$$

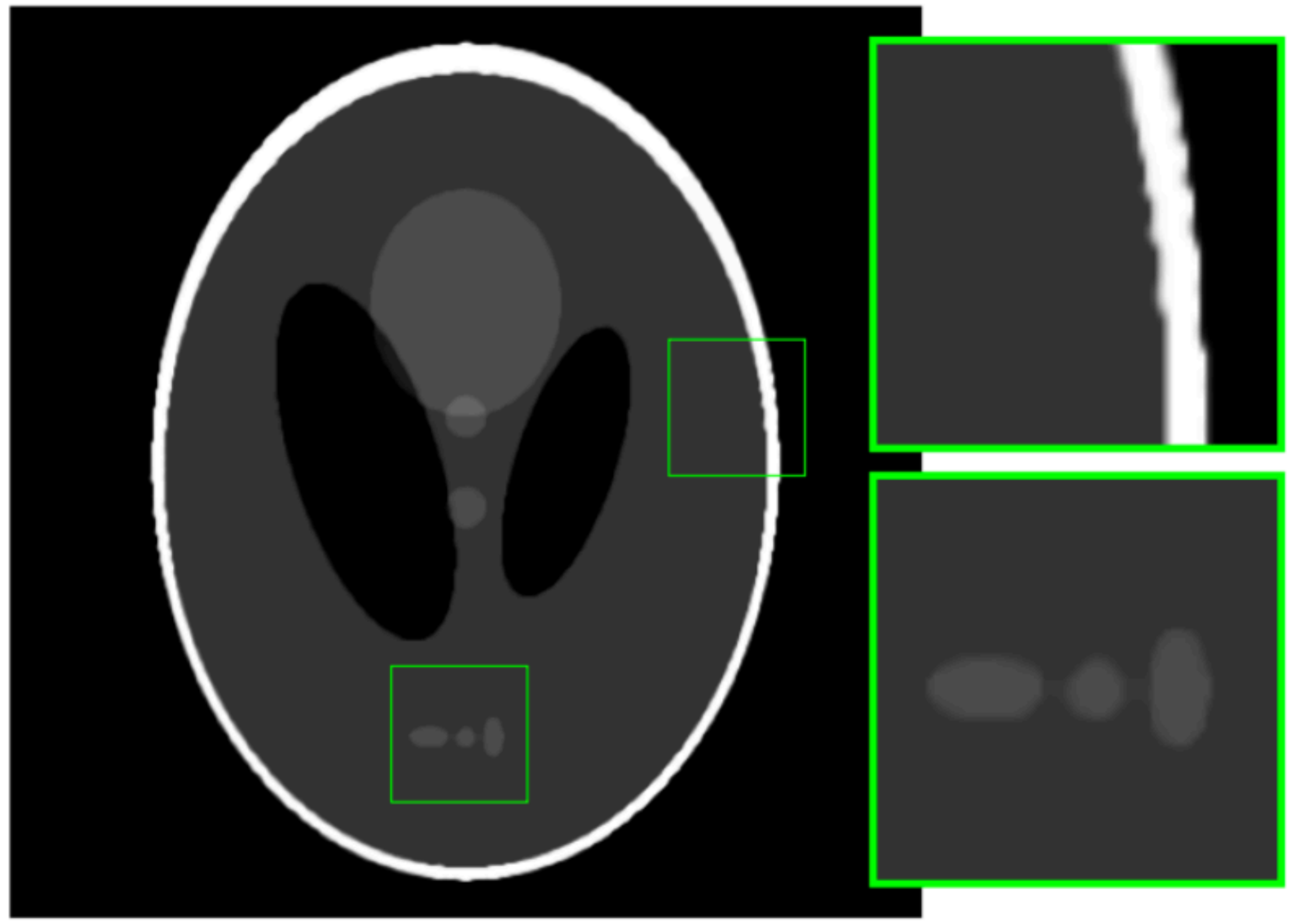
$$\|v^K\| \approx 72.79$$



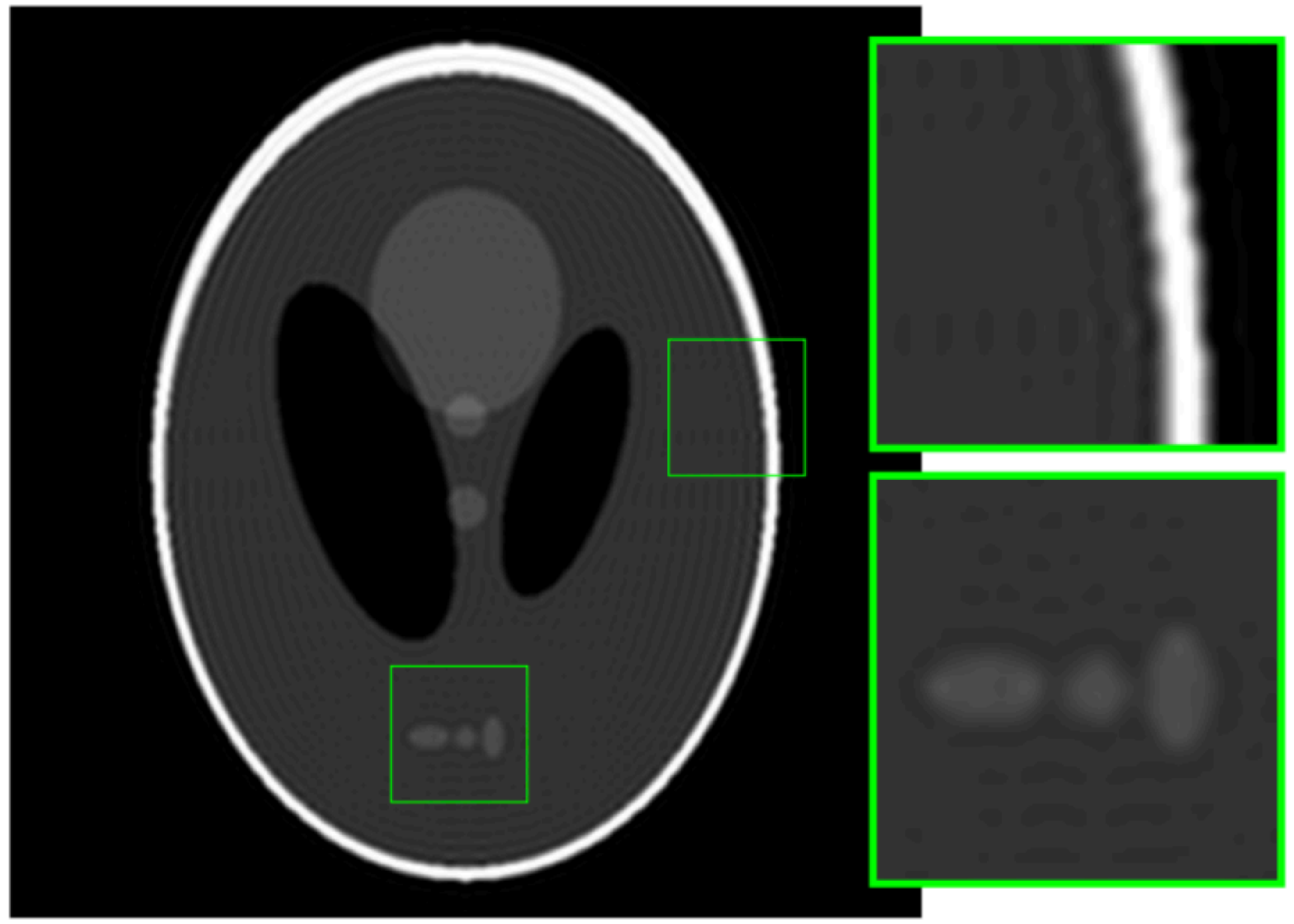
(a) Range cond. data g_α^K



(b) ground truth $u^\dagger$



(c) approximate solution u^N *



(d) low-pass filtered rec. $\mathcal{F}^{-1}S^\top S\mathcal{F}u^\dagger$

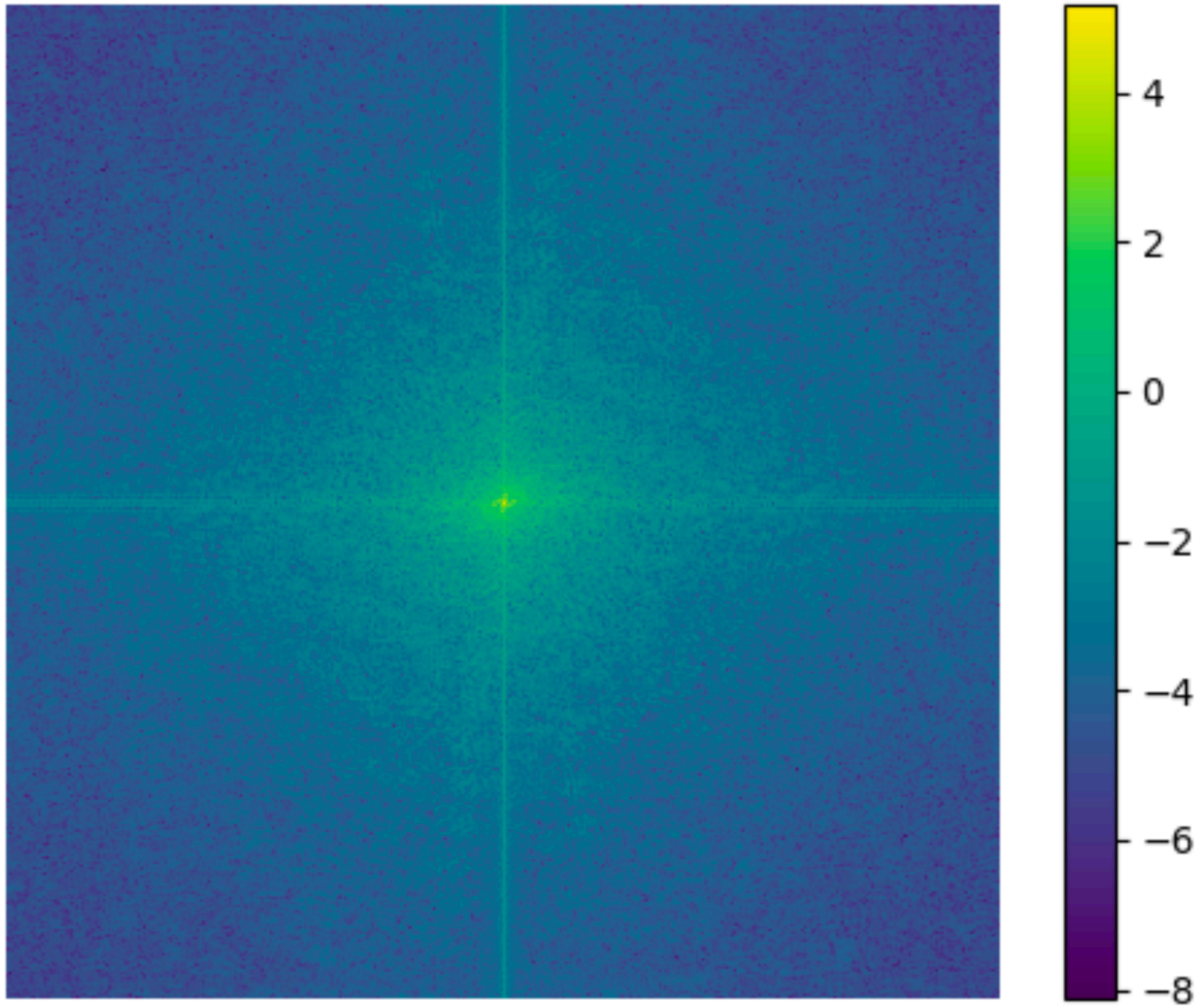
*Sanity check computed with PDHG method (cf. Chambolle, A., & Pock, T. (2016). An introduction to continuous optimization for imaging. *Acta Numerica*, *25*, 161-319.)

Numerical results

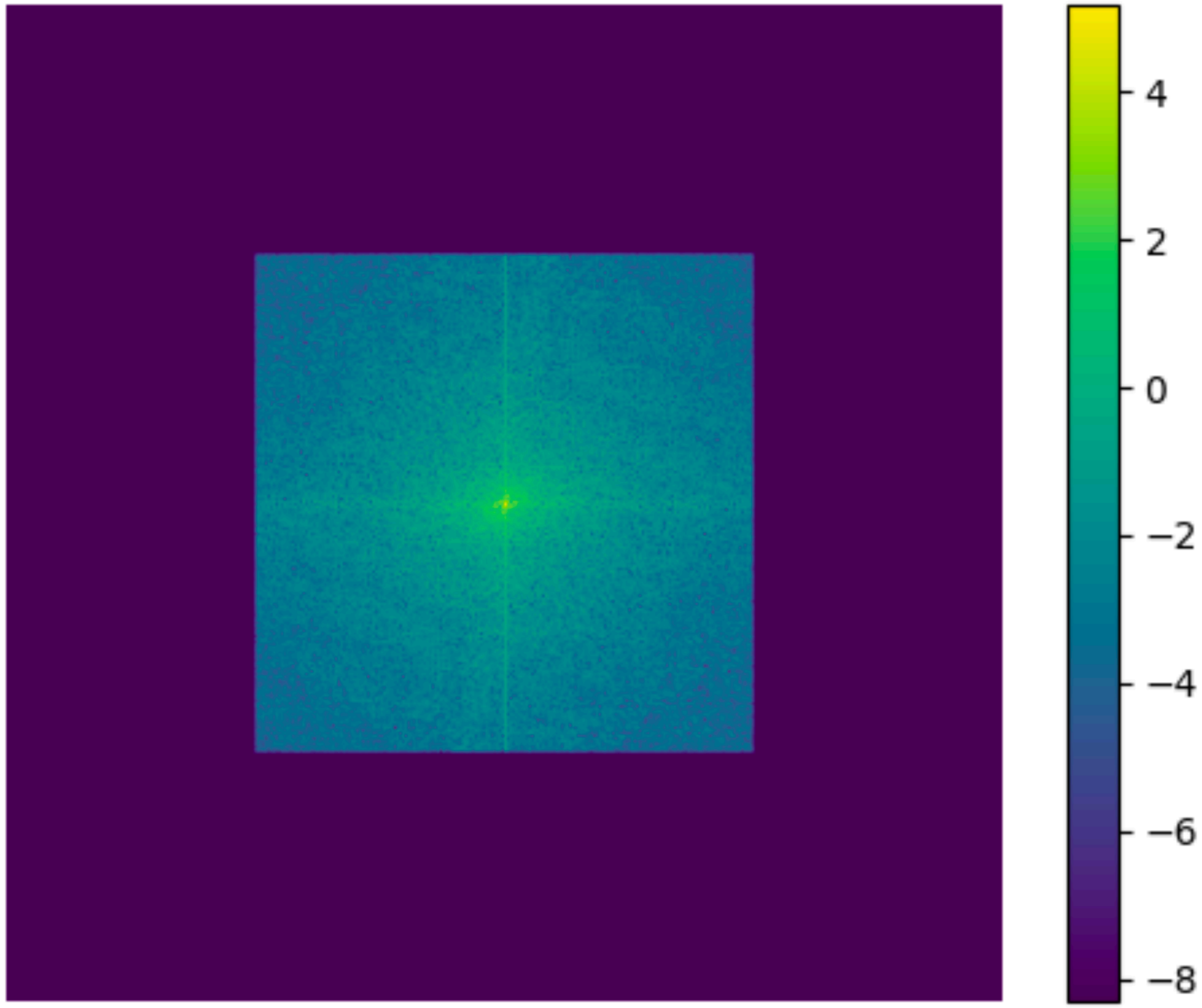
(a) Shepp-Logan phantom

(b) Eileen Collins

Numerical results

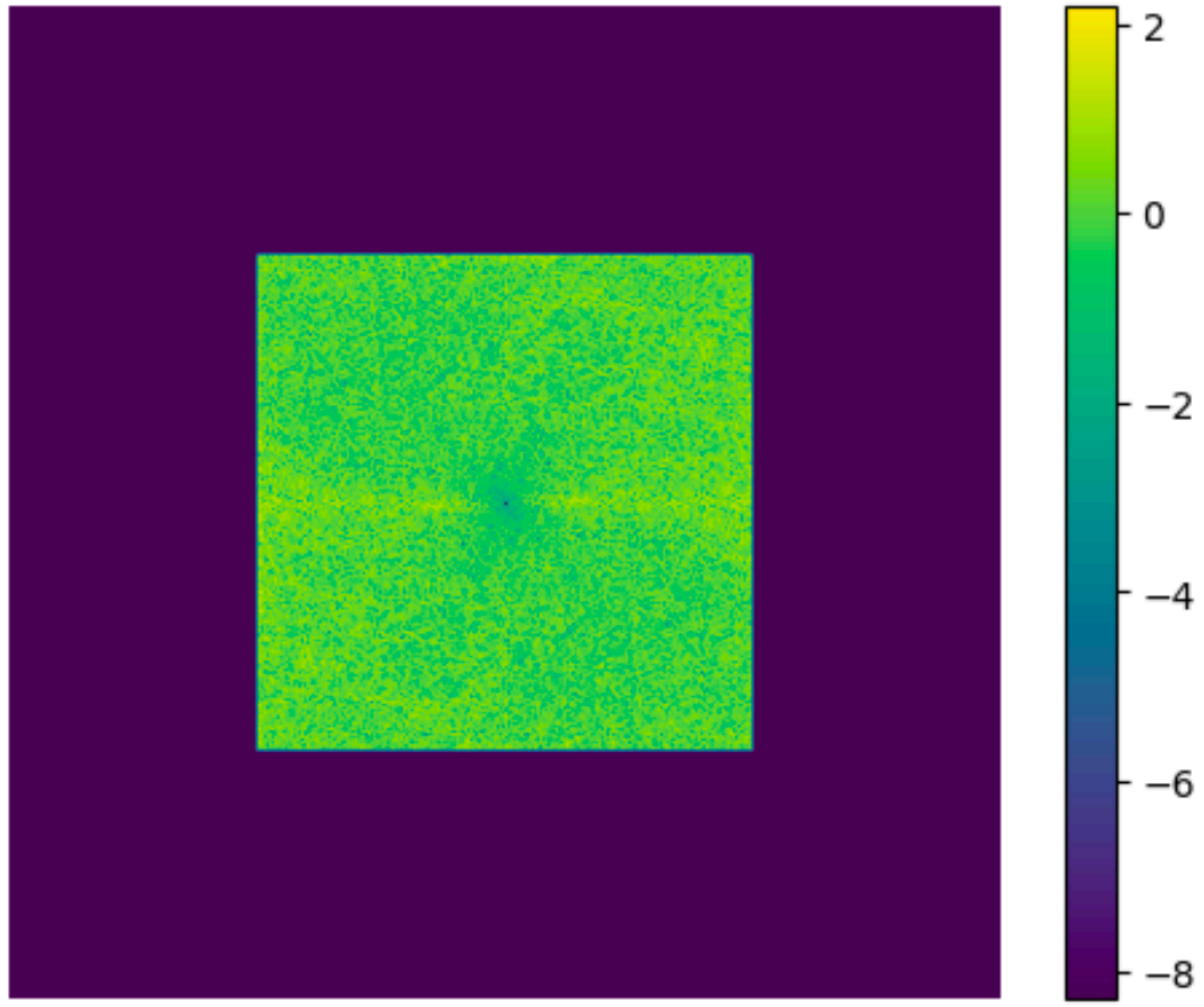


(a) Fourier transformed data

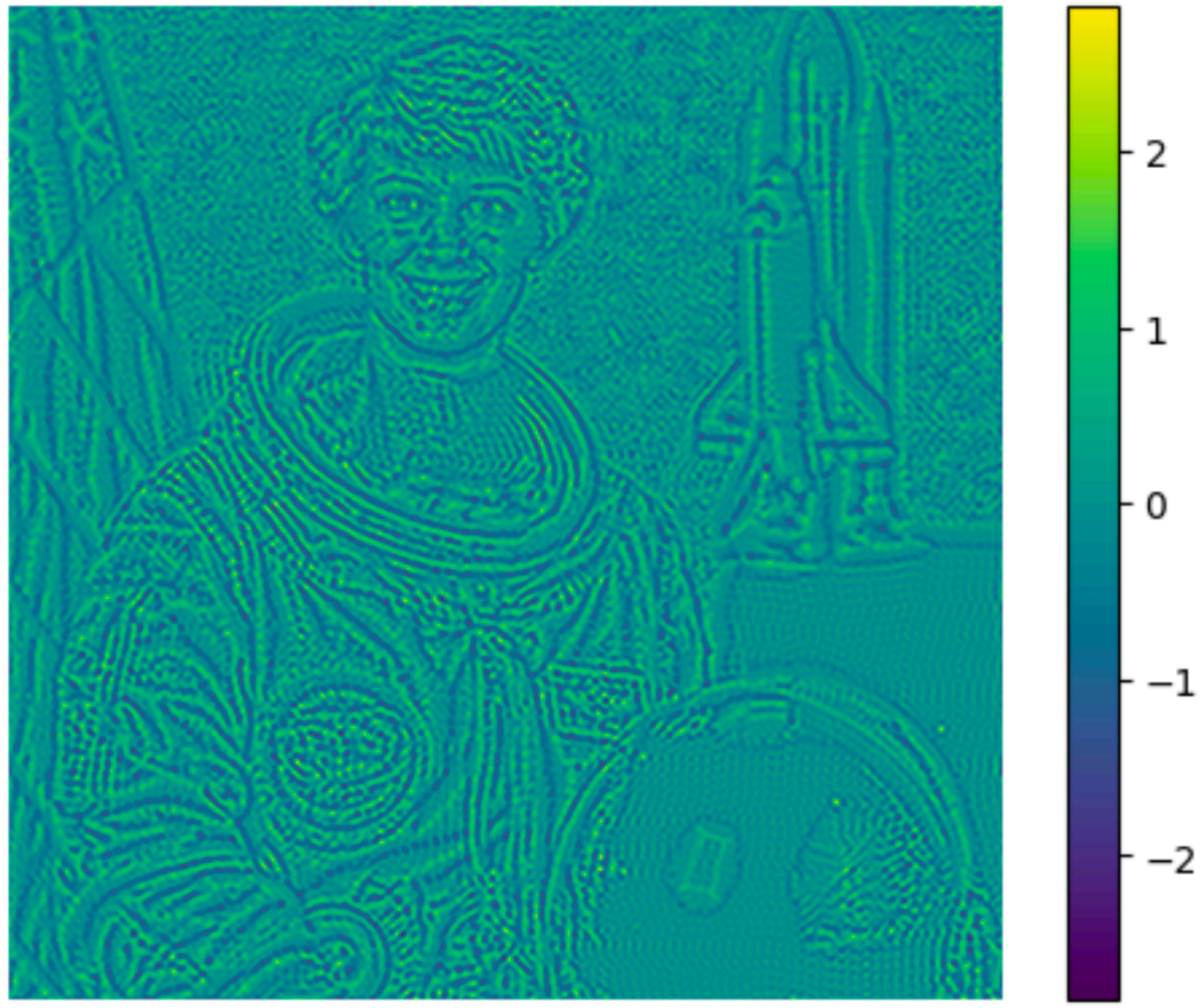


(b) Sub-sampled Fourier transformed data

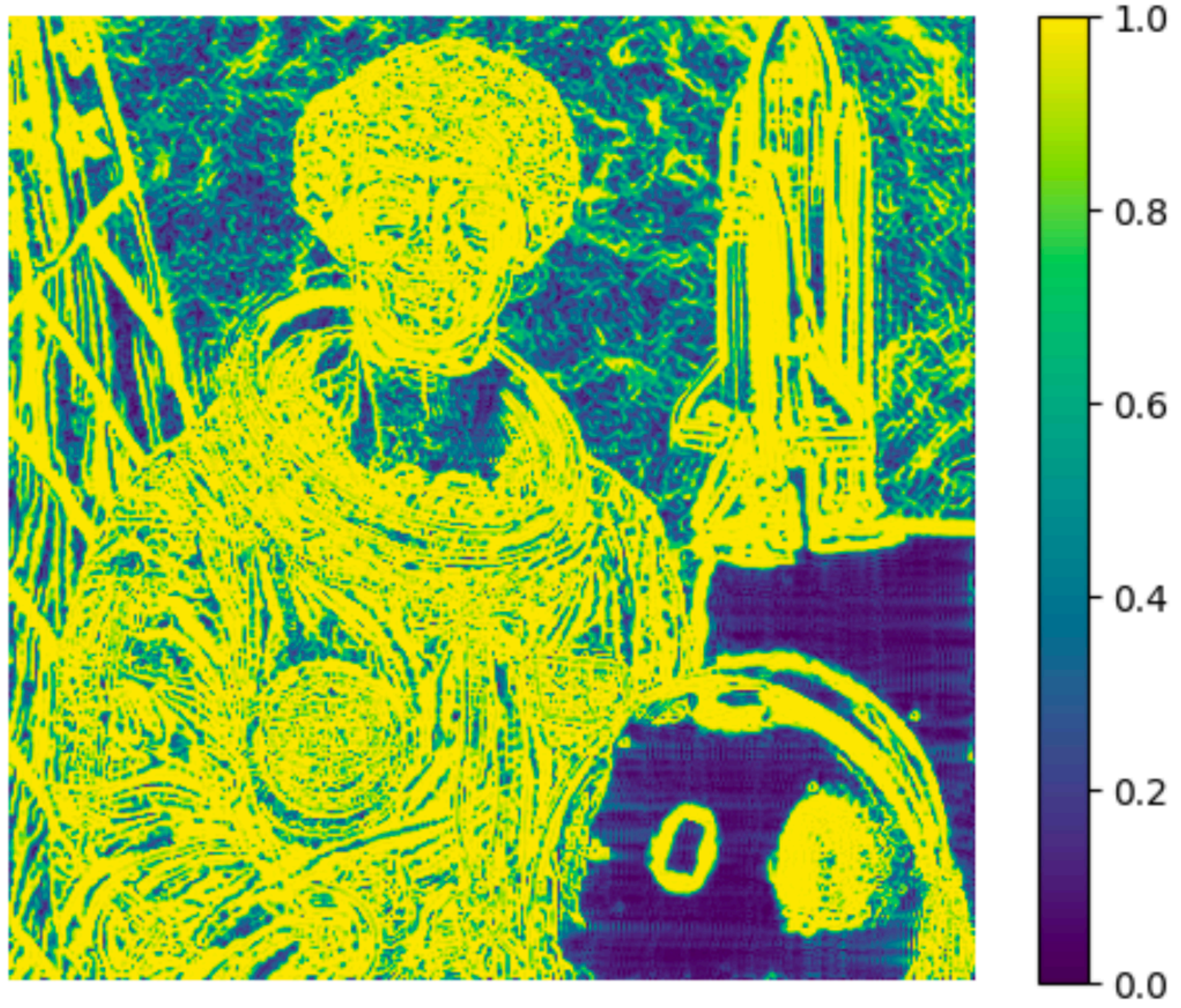
Numerical results



(a) v^K



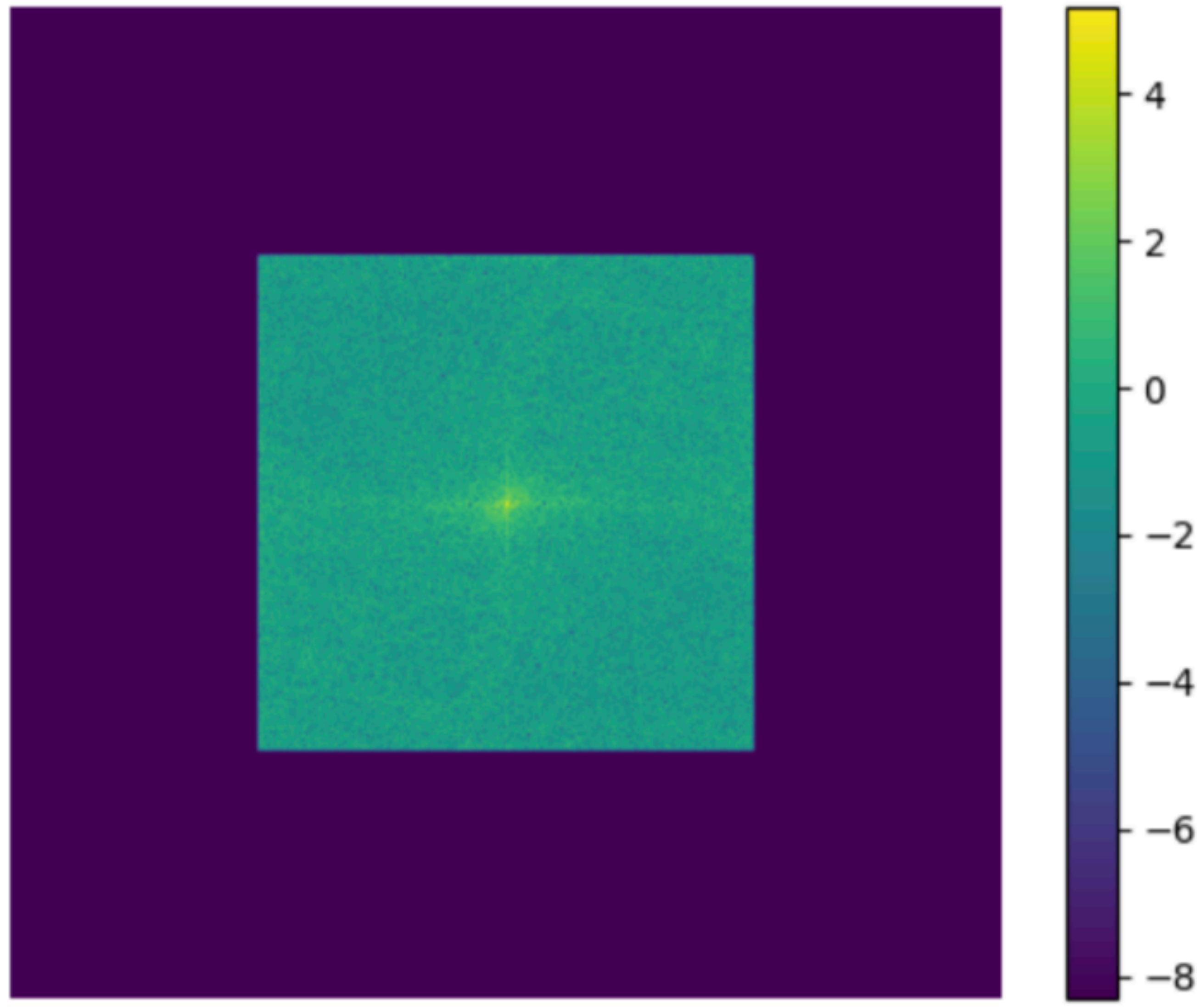
(b) Backprojection $\mathcal{F}^{-1} S^\top v^K$



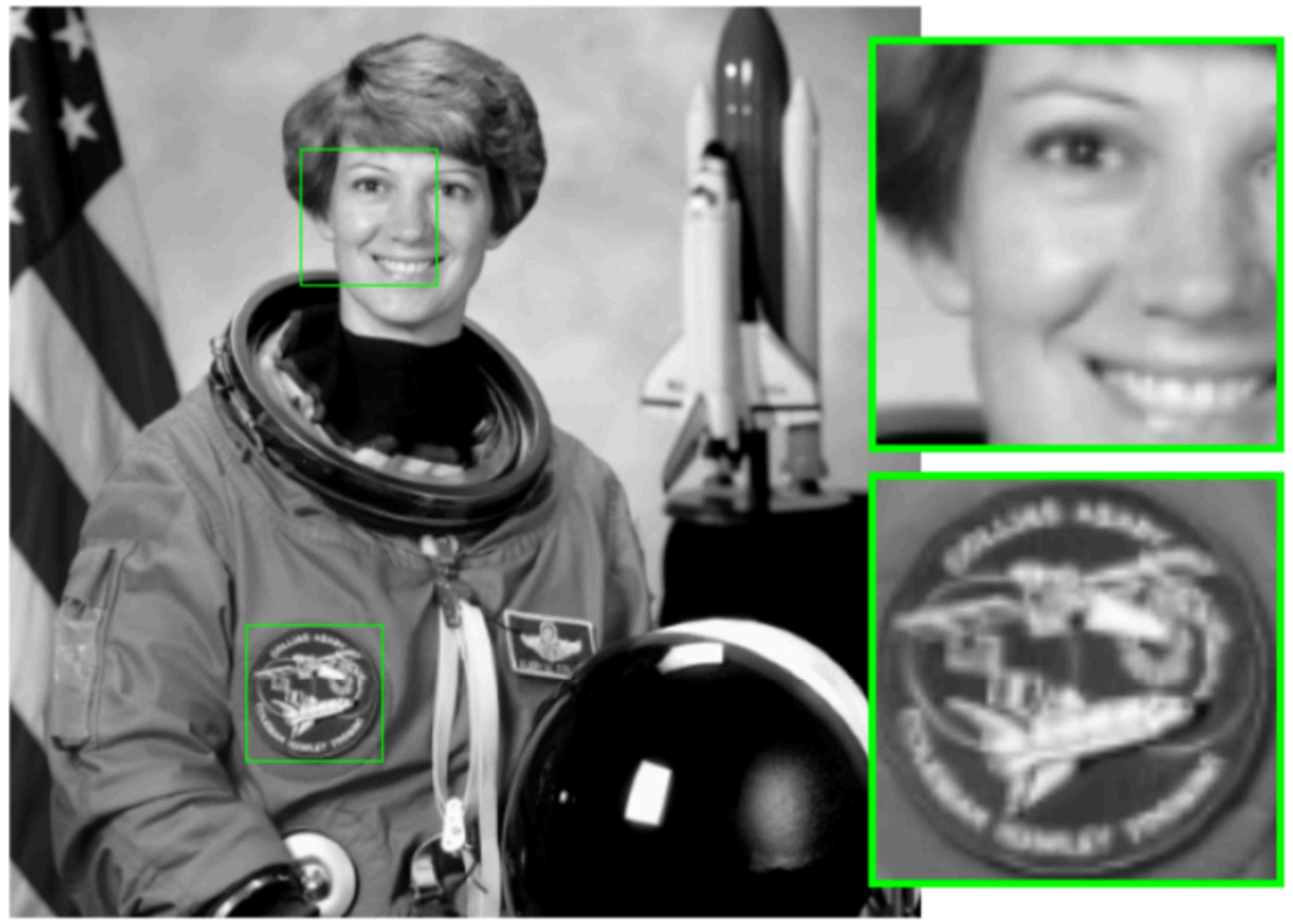
(c) $\sqrt{|q_1^K|^2 + |q_2^K|^2}$

$$\mathscr{F}^{-1} S^T v^K = A^\top q^K$$

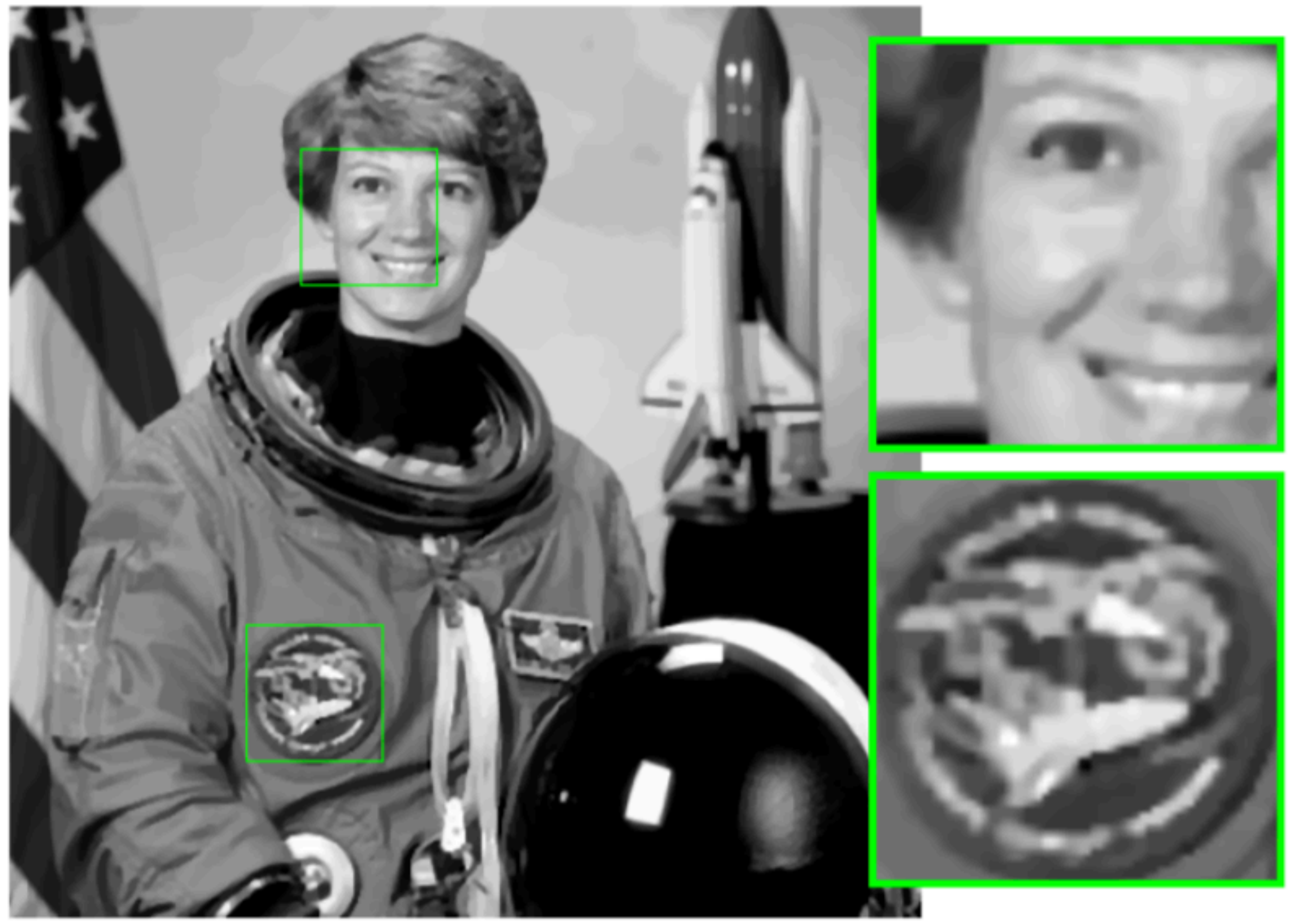
$$\|v^K\| \approx 255.15$$



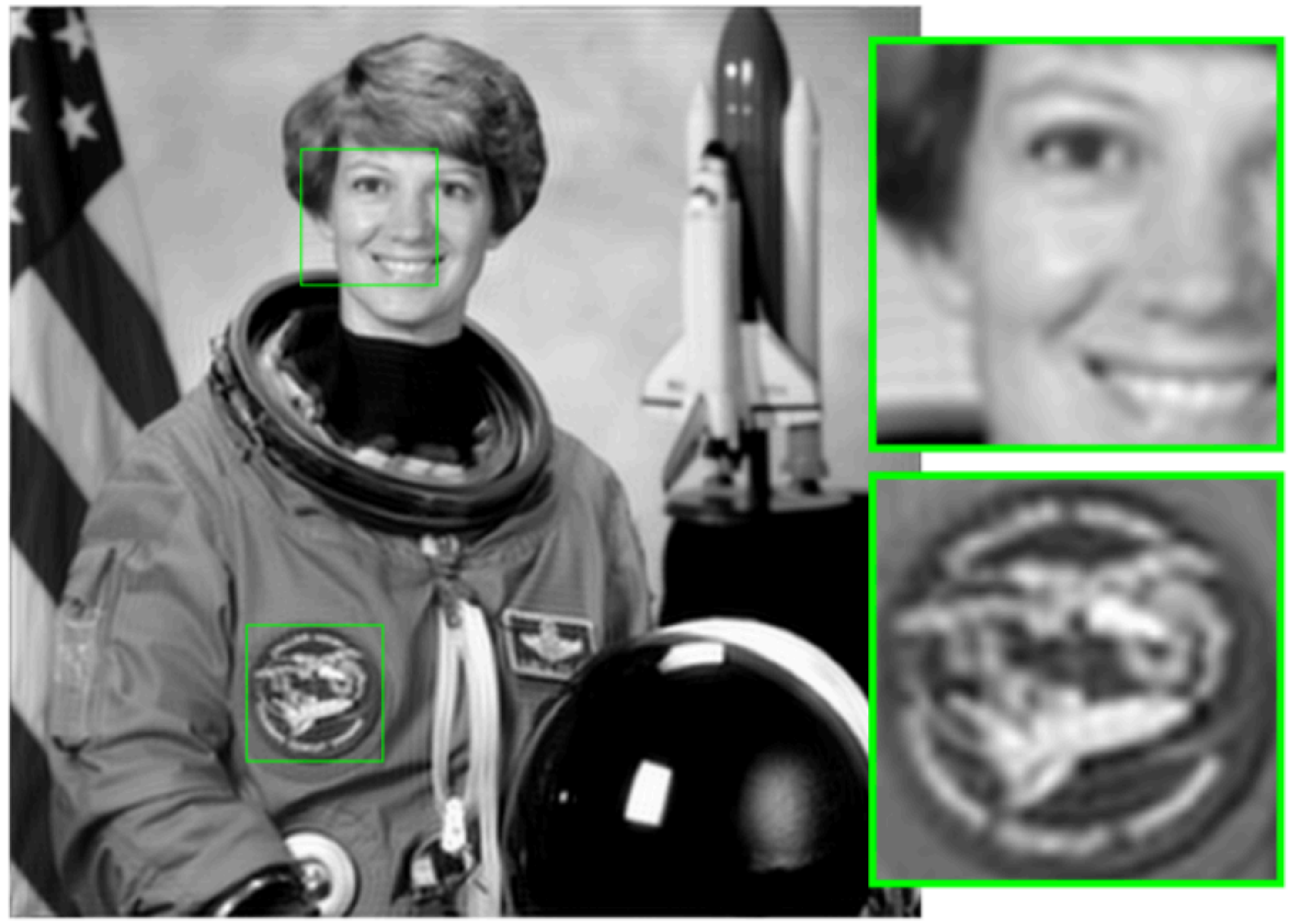
(a) Range cond. data g_α^K



(b) ground truth $u^\dagger$



(c) approximate solution u^N *



(d) low-pass filtered rec. $\mathcal{F}^{-1}S^\top S\mathcal{F}u^\dagger$

*Sanity check computed with PDHG method (cf. Chambolle, A., & Pock, T. (2016). An introduction to continuous optimization for imaging. *Acta Numerica*, *25*, 161-319.)

Learning variational regularisations with optimal error estimates

We could approximate a bilevel problem with trainable regularisation function

$$\min_{\Theta} \frac{1}{2s} \sum_{i=1}^{s} \|u(\Theta) - u^\dagger\|_X^2 + \beta R(\Theta)$$

subject to

$$u(\Theta) \in \arg\min_u \left\{ \frac{1}{2}\|Ku - f^\delta\|_Y^2 + J(u,\Theta) \right\}$$ (Lower level problem)

and check if learned regularisation function $J(\,\cdot\,,\Theta)$ improves norm of source condition elements

Choose $R(\Theta) = 0$ $\quad J(u,A) = \sum_{j=1}^{n} \sqrt{\sum_{l=1}^{m} (Au)_{jl}}$ $\quad K = I$

Approximate lower level problem with finite number of PDHG iterations

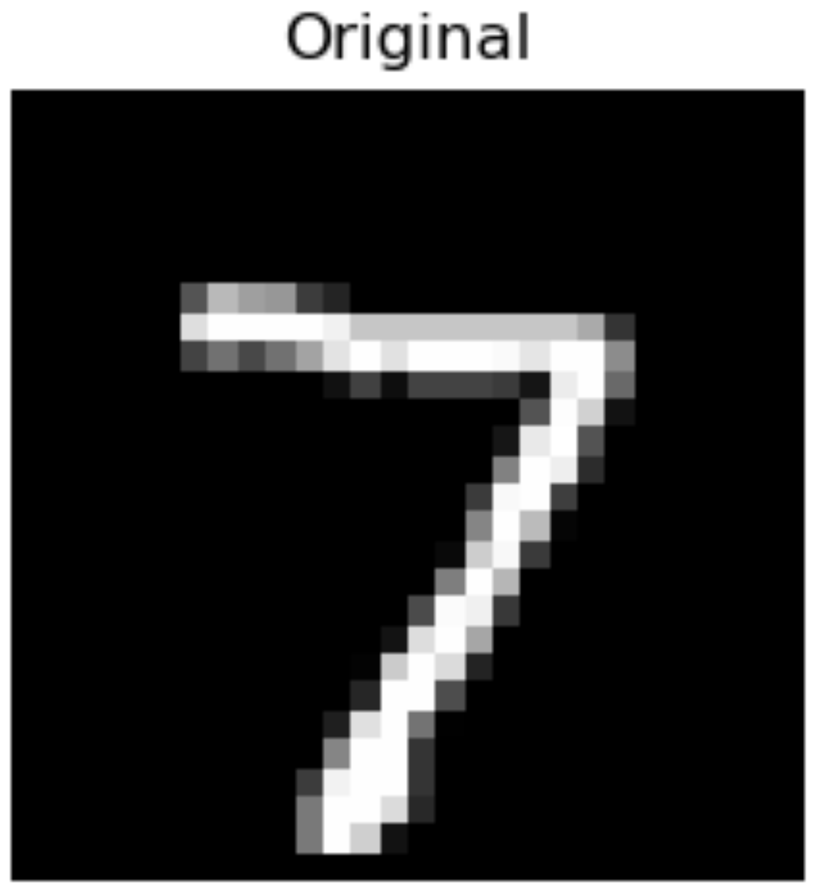
Choose $R(\Theta) = 0$ $J(u, A) = \sum_{j=1}^{n} \sqrt{\sum_{l=1}^{m} (Au)_{jl}}$ $K = I$

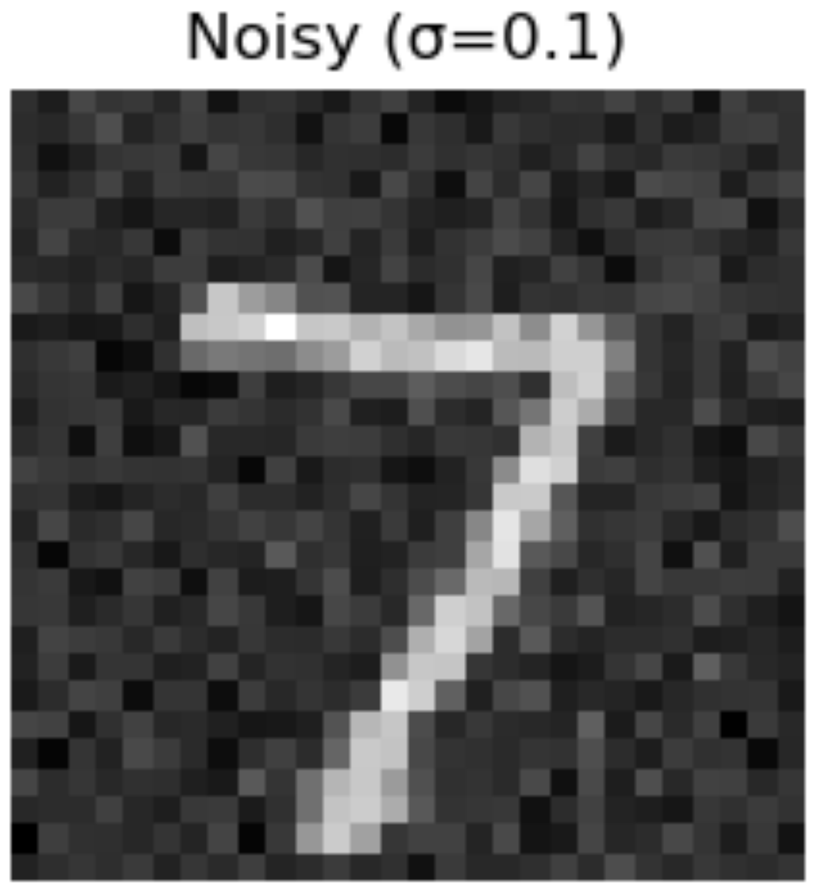
Approximate lower level problem with finite number of PDHG iterations

Example: convolution $Au = \begin{pmatrix} h_1 \\ \vdots \\ h_m \end{pmatrix} * u$

Samples

$u_i^\dagger =$





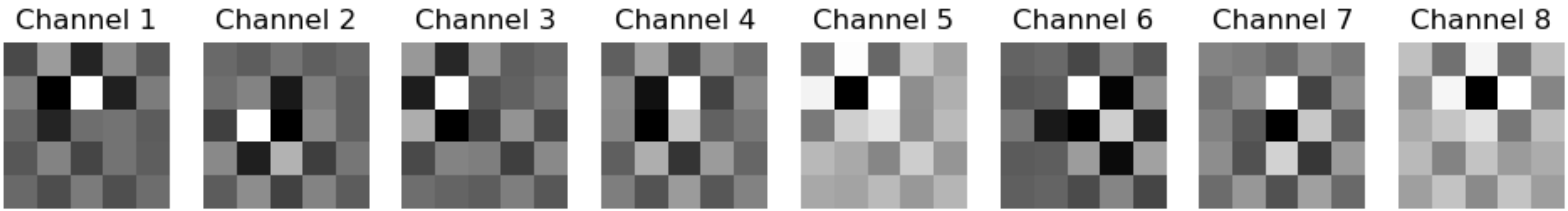
$= f_i^\delta$

Choose $R(\Theta) = 0$ $J(u, A) = \sum_{j=1}^{n} \sqrt{\sum_{l=1}^{m} (Au)_{jl}}$ $K = I$

Approximate lower level problem with finite number of PDHG iterations

Example: convolution $Au = \begin{pmatrix} h_1 \\ \vdots \\ h_m \end{pmatrix} * u$

Optimal kernel ($m = 8$):



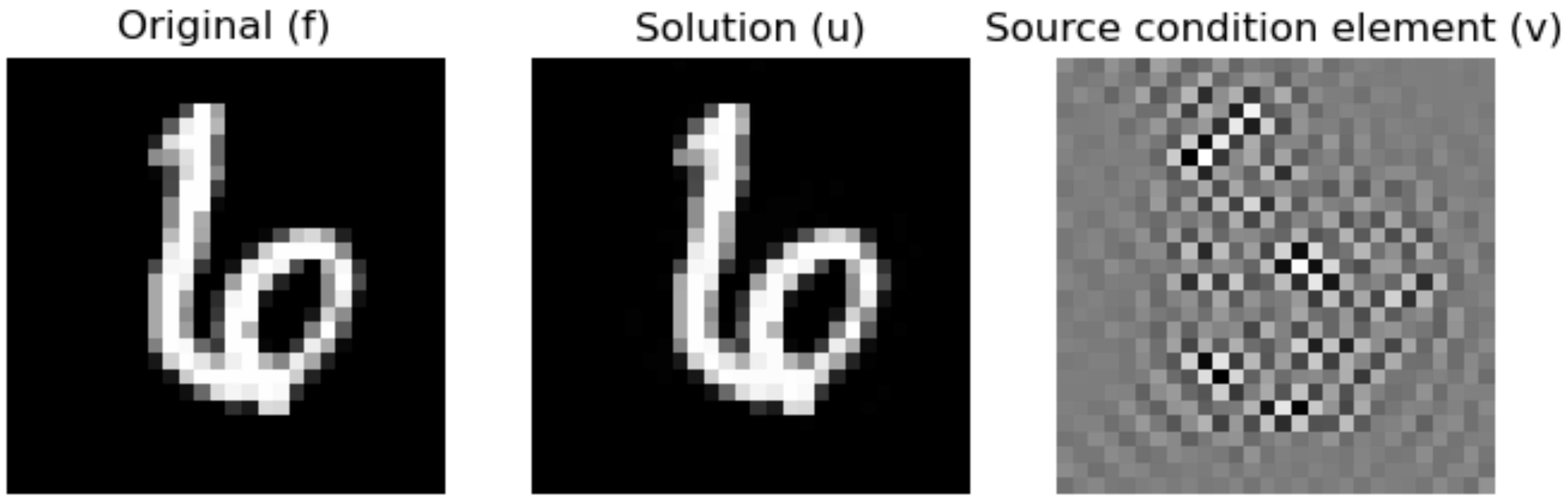
Choose $R(\Theta) = 0$ $\quad J(u, A) = \sum_{j=1}^{n} \sqrt{\sum_{l=1}^{m} (Au)_{jl}}$ $\quad K = I$

Approximate lower level problem with finite number of PDHG iterations

Example: convolution $\quad Au = \begin{pmatrix} h_1 \\ \vdots \\ h_m \end{pmatrix} * u$

$\|v\| \approx 8.59$

Source condition computation



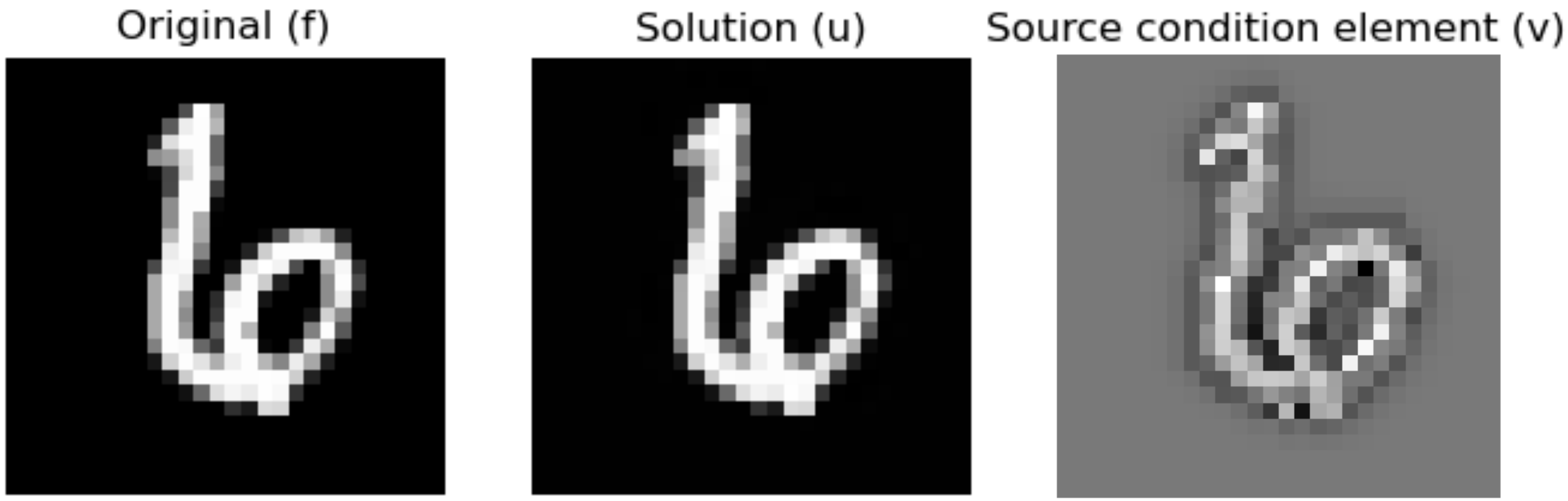
Choose $R(\Theta) = 0$ $\mathrm{TV}(u) = \sum_{j=1}^{n} \sqrt{\sum_{l=1}^{m} (\nabla u)_{jl}}$ $K = I$

Approximate lower level problem with finite number of PDHG iterations

Comparison with total variation

$\|v\| \approx 17.376$

Source condition computation



Learning the sampling pattern in MRI

Numerical results

Back to the source condition $\mathscr{F}^{-1}S^\top v \in \partial \mathrm{TV}(u^\dagger)$

Idea: define $\tilde{v} := S^\top v \in \mathbb{C}^{n_y \times n_x}$

and estimate sparse $\tilde{v}$ instead of v by solving

$$\min_{\tilde{v},q^\dagger} \frac{1}{2}\|\mathscr{F}^{-1}\tilde{v} - A^\top q^\dagger\|^2 + G_{\|\cdot\|_{2,1}}(q^\dagger) + \beta\|\tilde{v}\|_1$$

e.g. via PALM*, i.e.

$$\tilde{v}^{k+1} = \mathrm{prox}_{\beta\|\cdot\|_1}\left(\tilde{v}^k - \tau\left(\tilde{v}^k - \mathscr{F}A^\top q^k\right)\right),$$

$$q^{k+1} = q^k - \sigma\left(A\left(A^\top q^k - \mathscr{F}^{-1}\tilde{v}^{k+1}\right) + \mathrm{prox}_{\|\cdot\|_{2,1}}\left(q^k + Au^\dagger\right) - Au^\dagger\right).$$

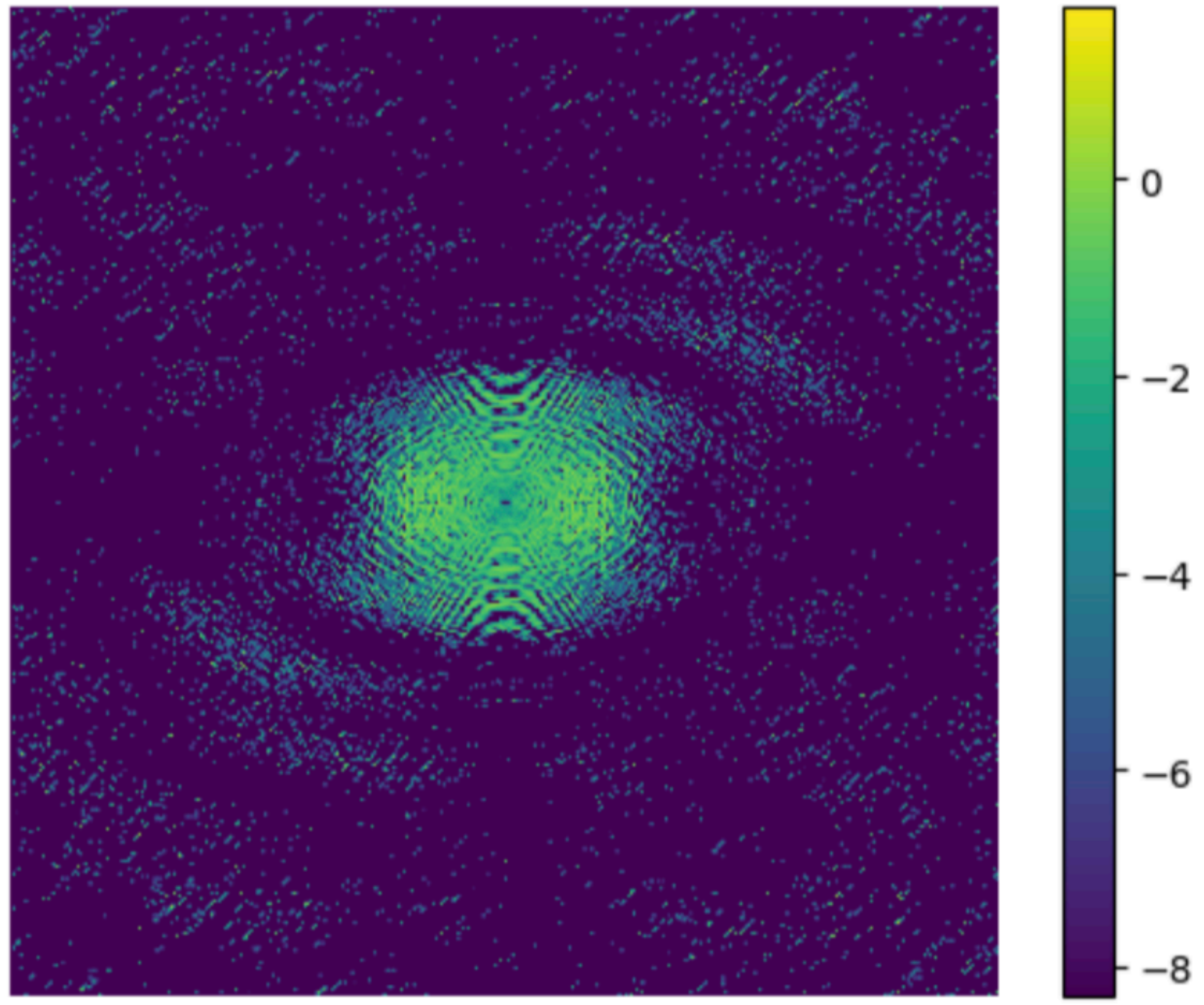
*Bolte, J., Sabach, S., & Teboulle, M. (2014). Proximal alternating linearized minimization for nonconvex and nonsmooth problems. *Mathematical Programming*, *146*(1-2), 459-494.

Numerical results

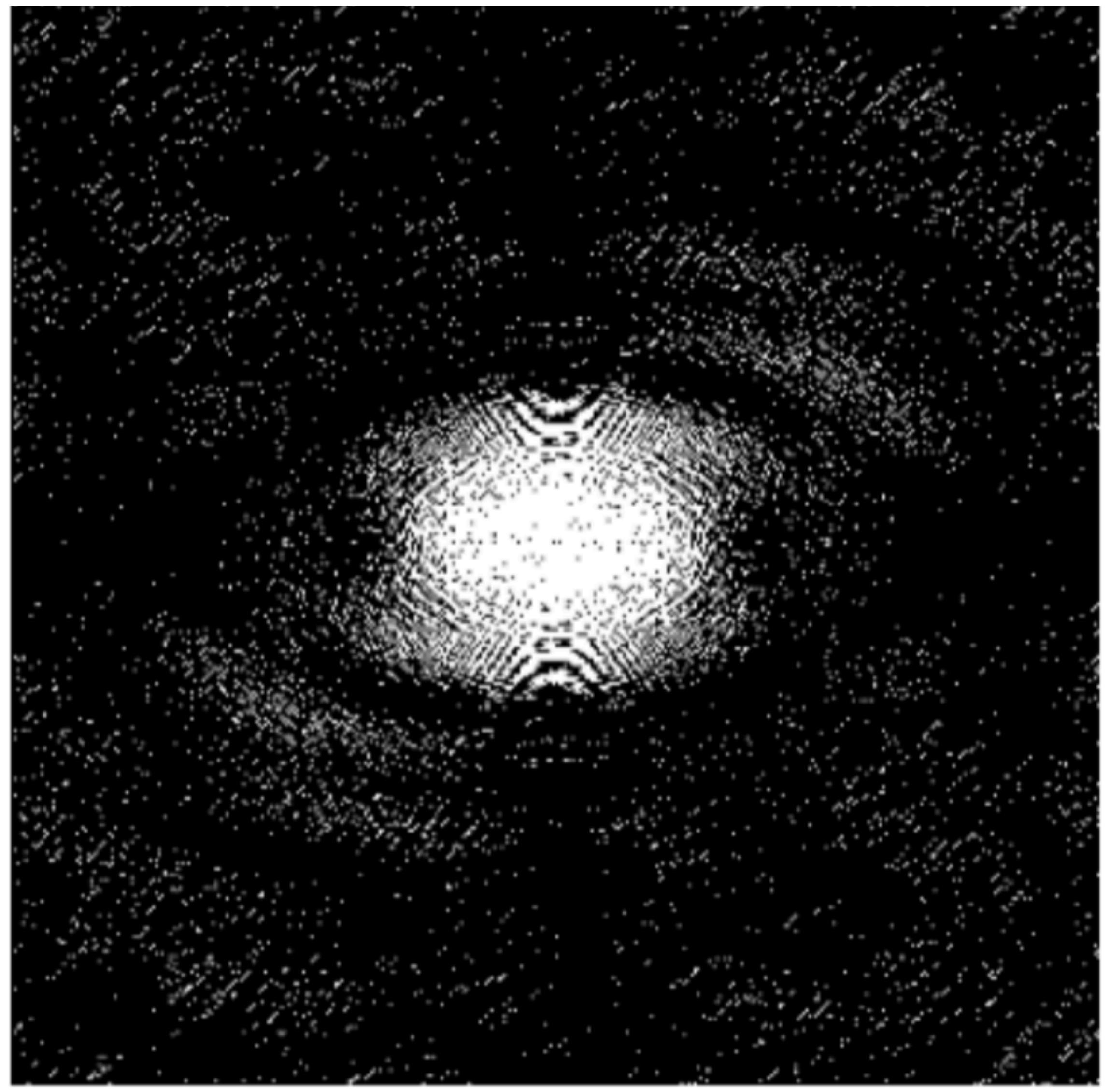
(a) Shepp-Logan phantom

(b) Eileen Collins

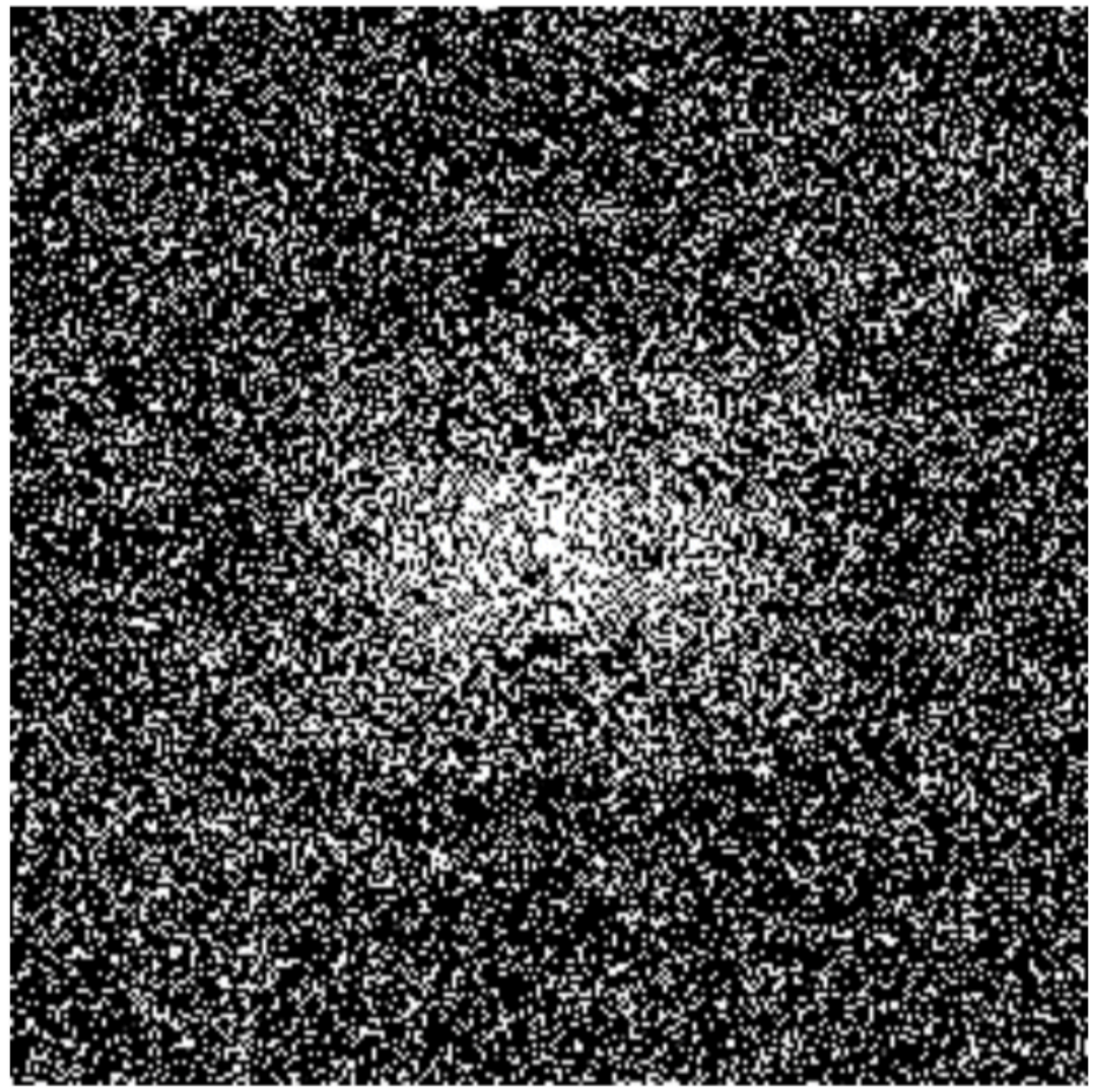
$\beta = 0.1$



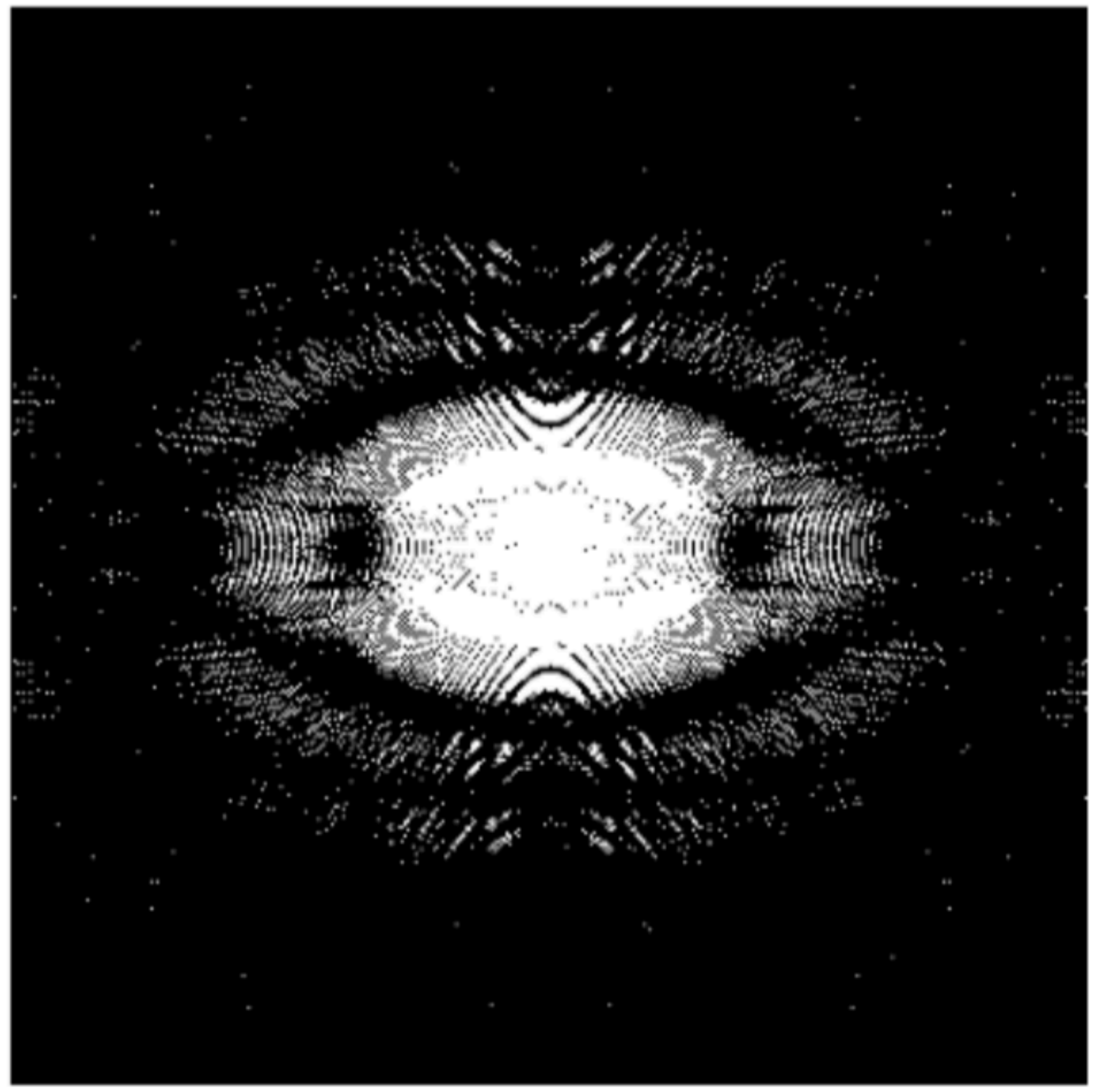
(a) $\tilde{v}^K$



(b) Sampling pattern

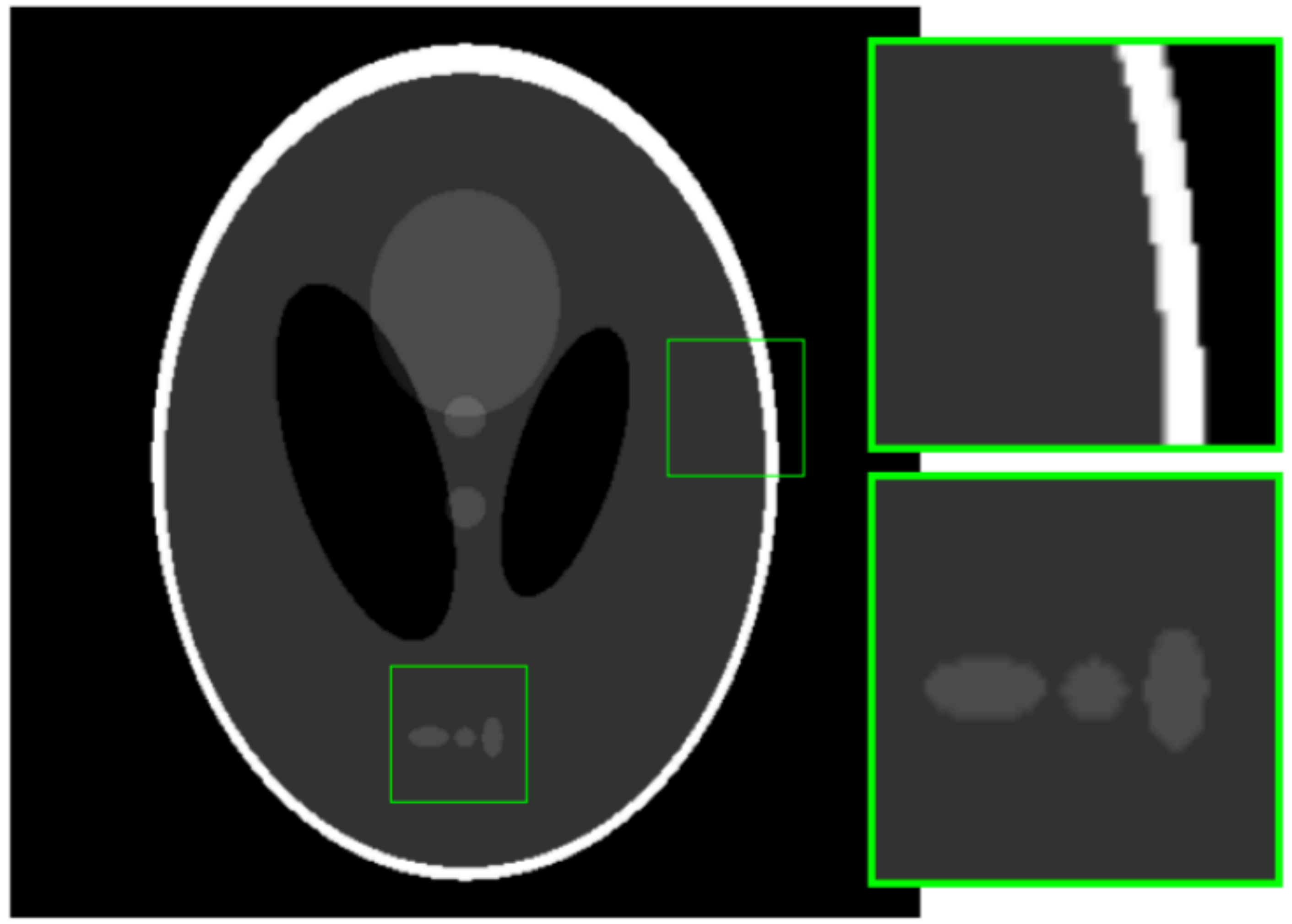


(c) Learned sampling pattern from *

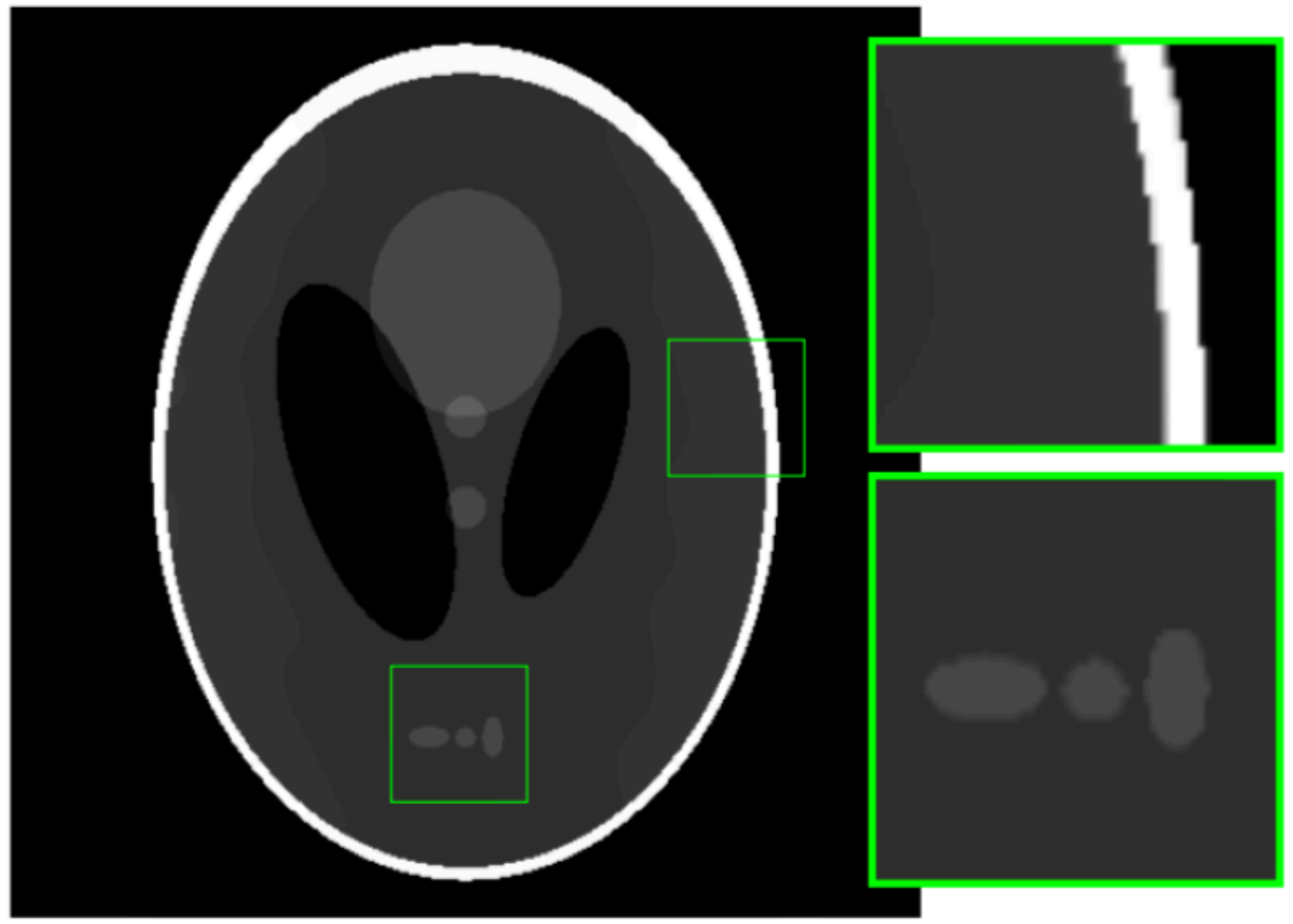


(d) Largest Fourier coefficients

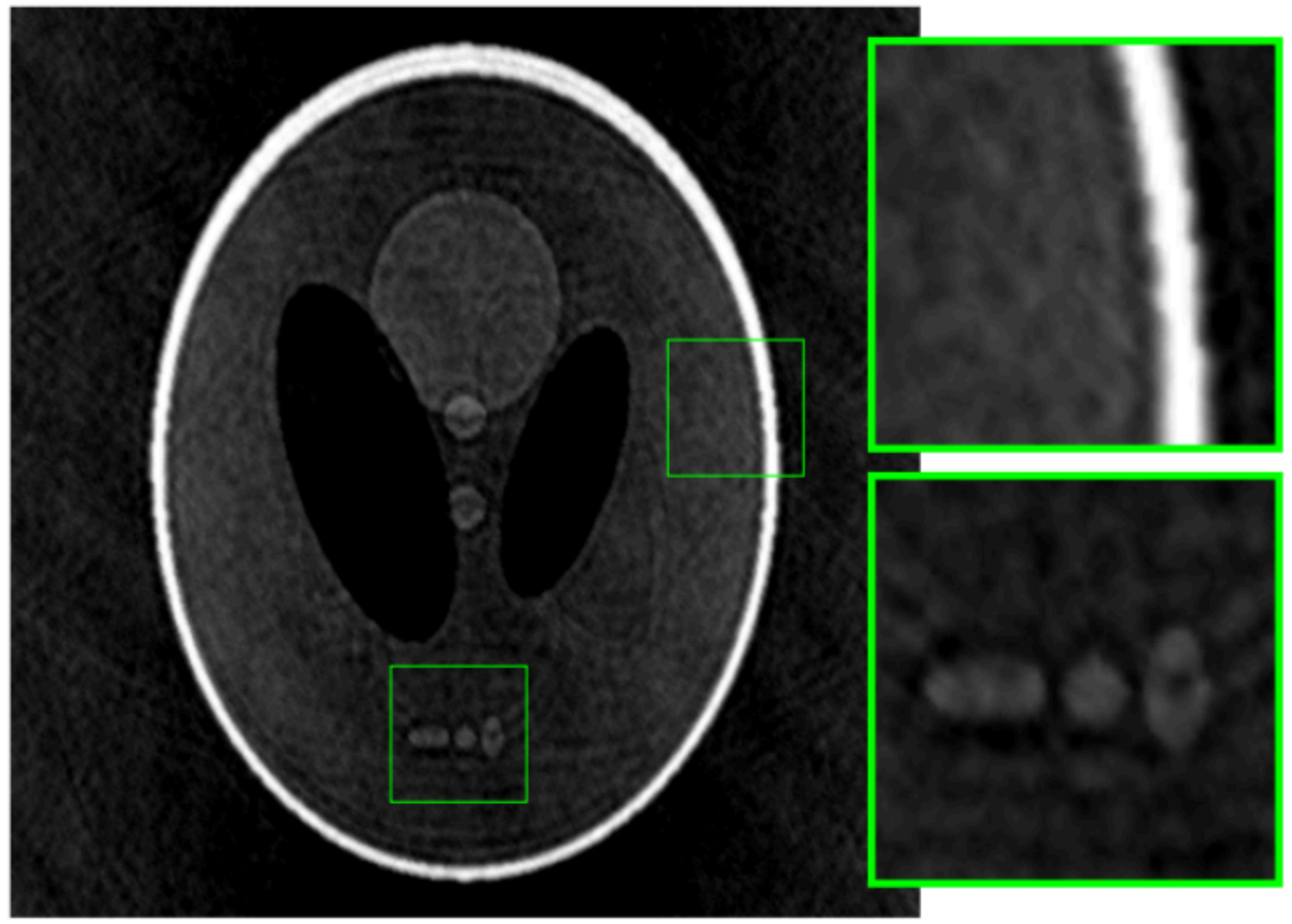
*F. Sherry et al. (2020). Learning the sampling pattern for MRI. *IEEE Transactions on Medical Imaging*, 39(12), 4310-4321.



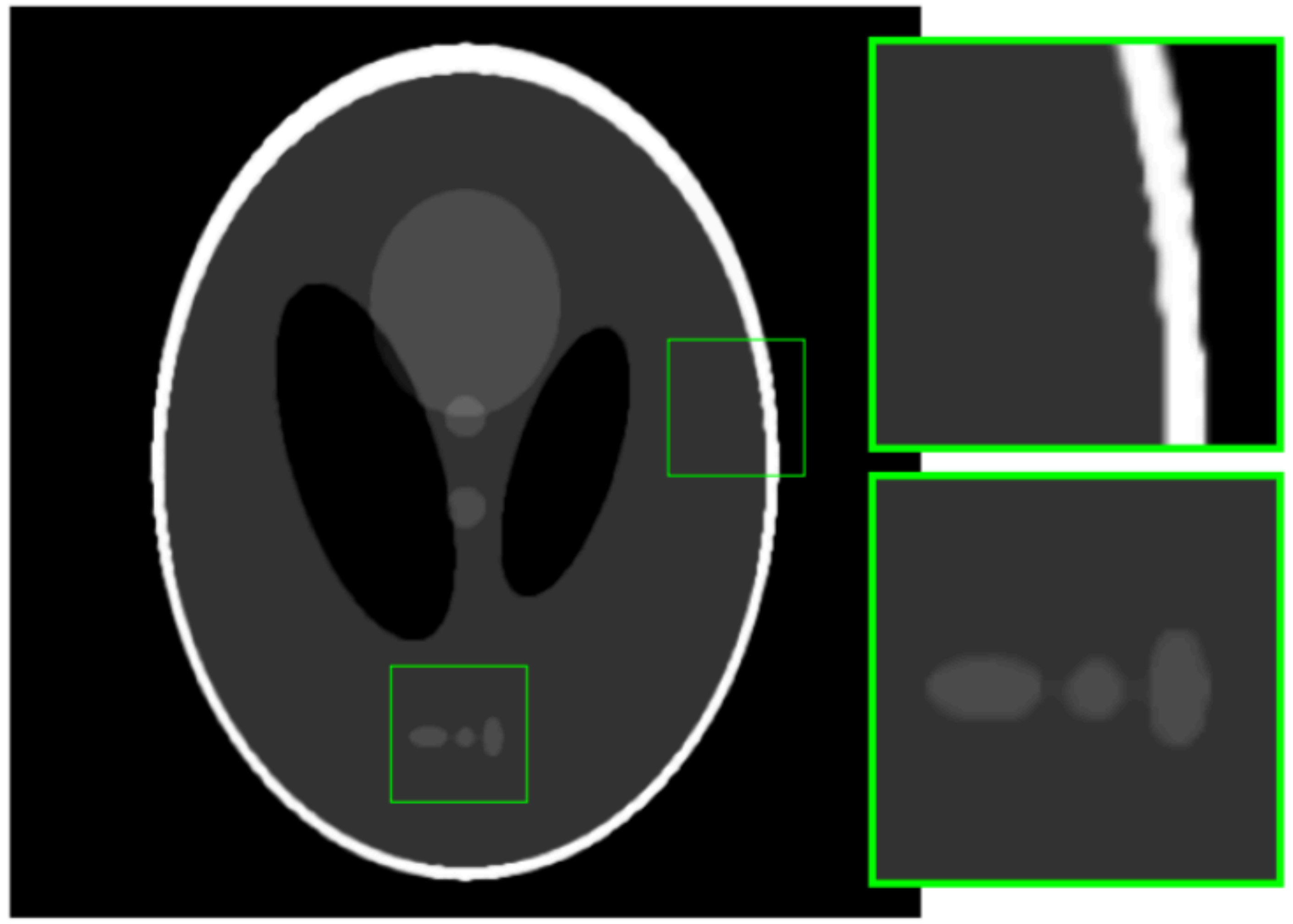
(a) ground truth $u^\dagger$



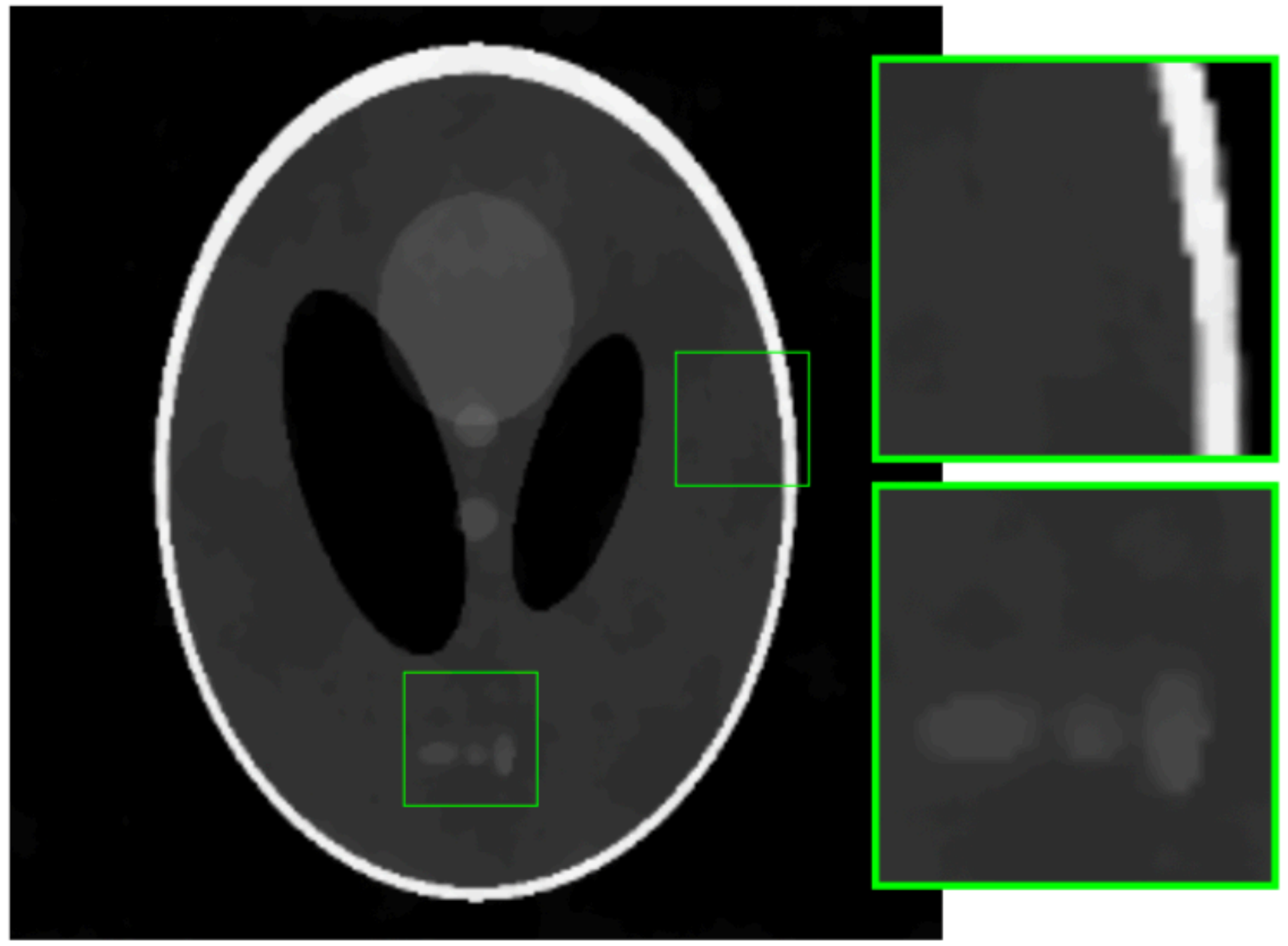
(b) approximate solution u^N



(c) projection $\mathcal{F}^{-1}S^\top S\mathcal{F}u^\dagger$



(d) low-pass filtered rec.



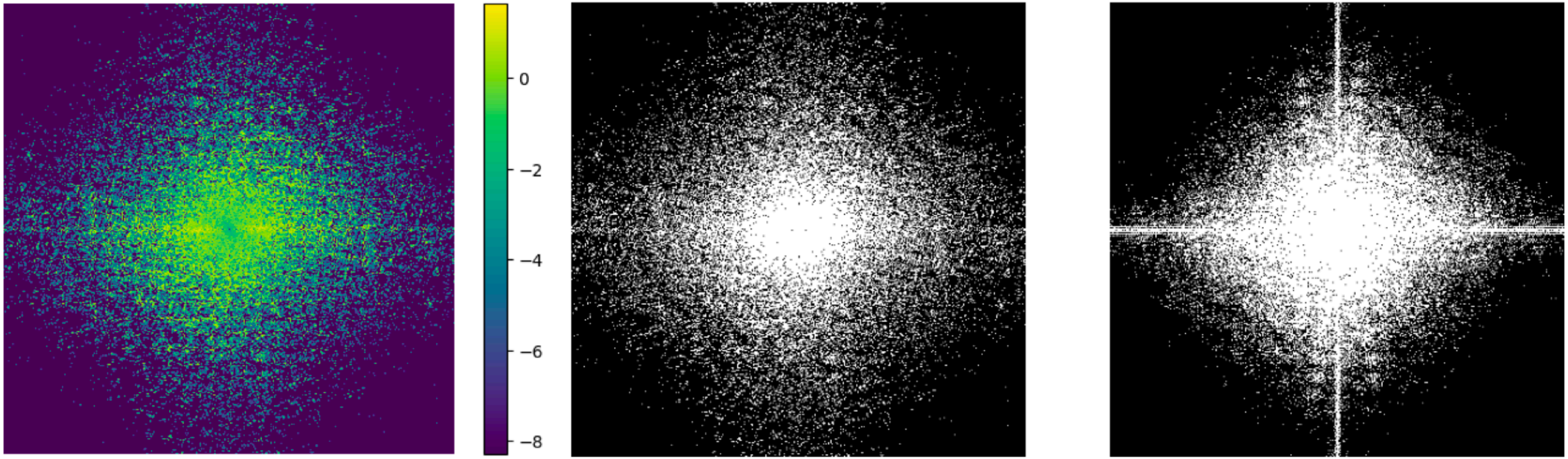
(e) reconstruction from Sherry et al.

Numerical results

(a) Shepp-Logan phantom

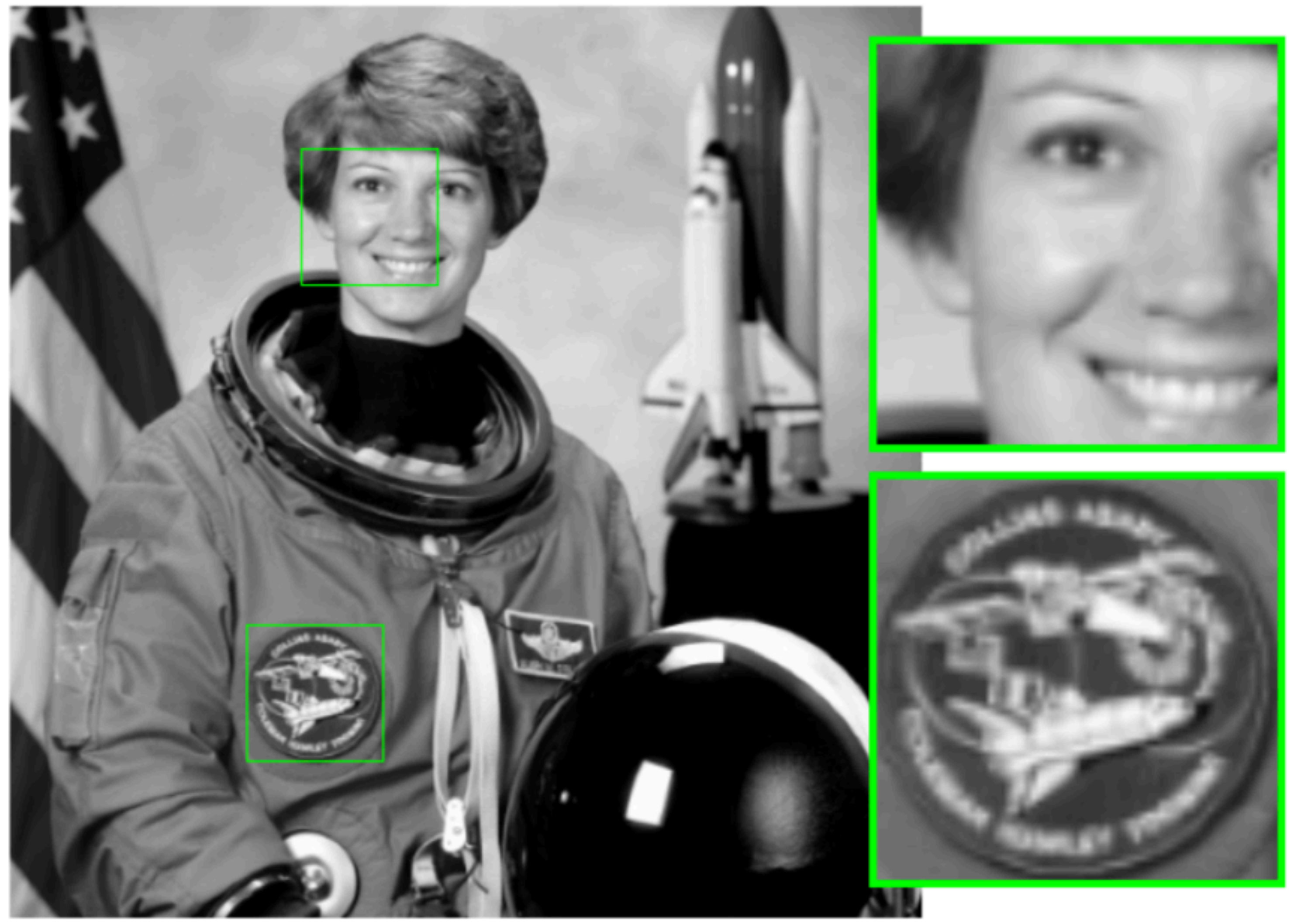
(b) Eileen Collins

Numerical results

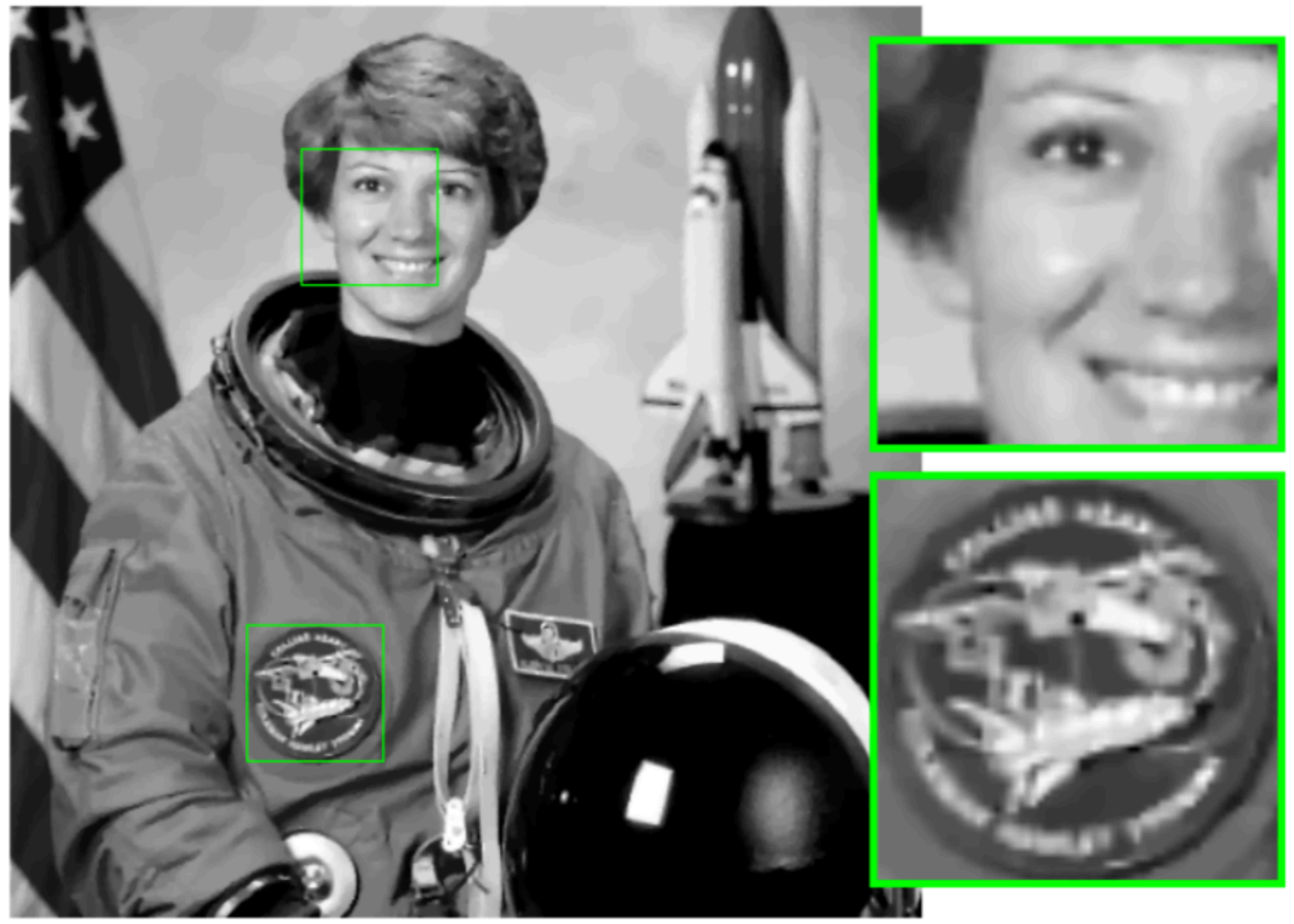


(a) $\tilde{v}^K$ (b) Sampling pattern (c) Largest Fourier coefficients

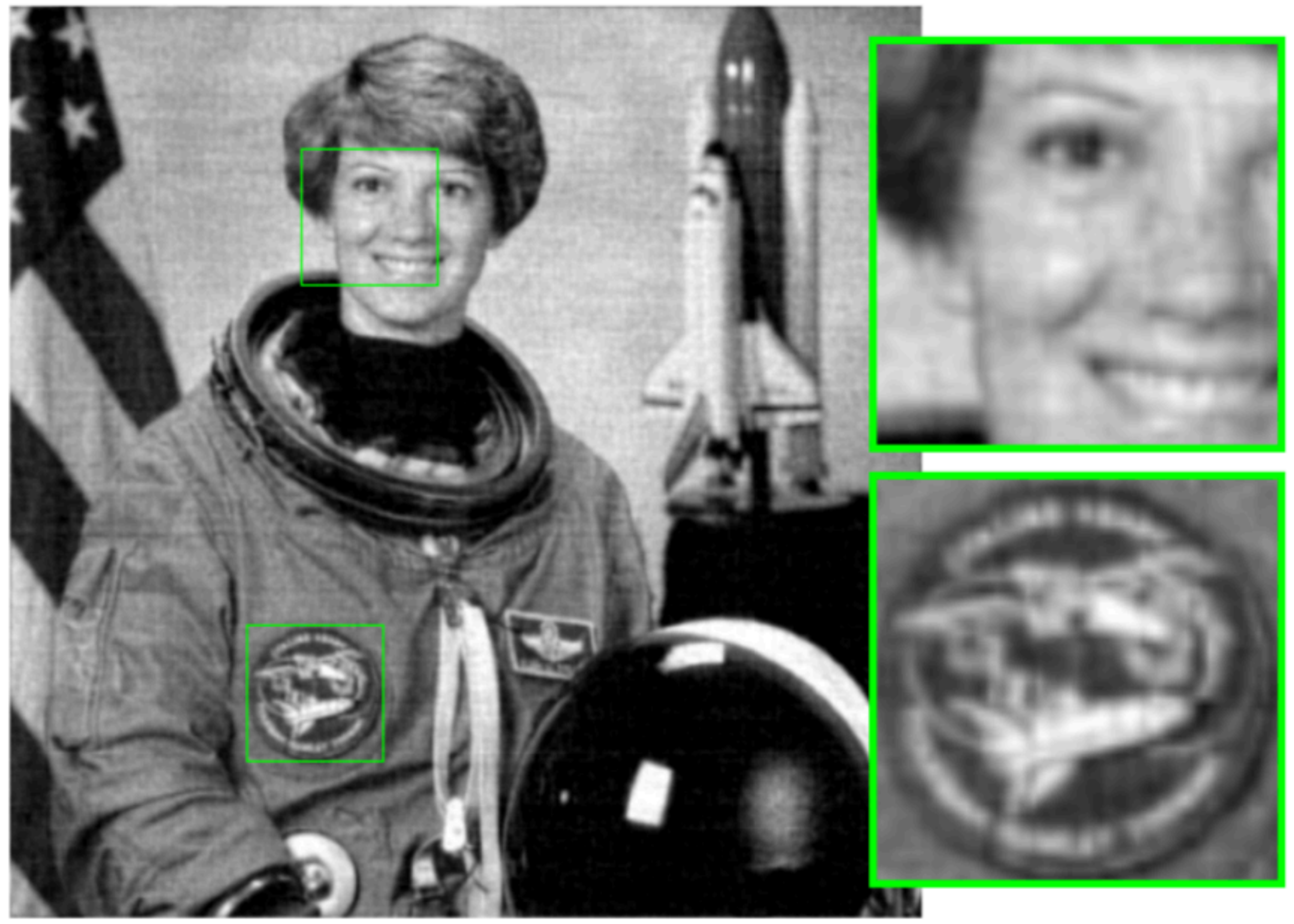
$$\beta = 0.24$$



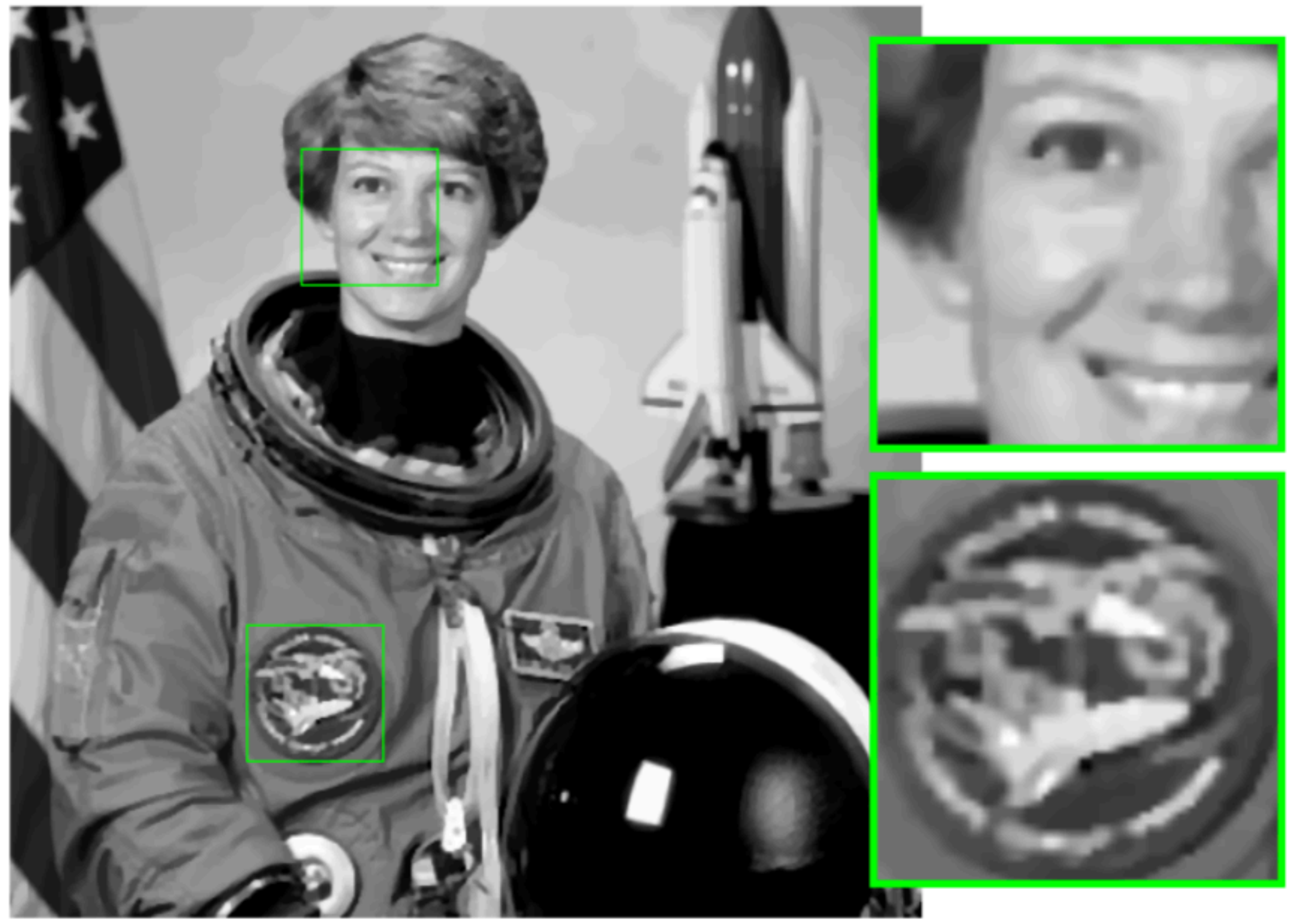
(a) ground truth $u^\dagger$



(b) approximate solution u^N



(c) projection $\mathcal{F}^{-1}S^\top S\mathcal{F}u^\dagger$



(d) low-pass filtered rec.

Conclusions & Outlook

Conclusions & outlook

Conclusions: we have

- reformulated source and range conditions as the solution of convex minimisation problems
- provided iterative algorithms for their numerical approximation
- made an attempt at supervised learning of regularisation functions with optimal error constants

Outlook:

- Higher-order or variational source conditions, gen. eigenfunctions
- Optimal sampling in various domains (e.g. MRI, single-pixel camera)
- Supervised learning for more general operator correction
- Use framework in other contexts (e.g., training deep neural networks)

Thank you for your attention!

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https://doi.org/10.1093/imamat/hxae008

Trust your source: quantifying source condition elements for variational regularisation methods

Error estimates in inverse problems

Example: variational regularisation

$$R_\alpha : Y \rightrightarrows X, \quad R_\alpha : f \mapsto u_\alpha \in \arg\min_{u \in X} \left\{ \frac{1}{2} \|Ku - f\|_Y^2 + \alpha J(u) \right\}$$

Assume source condition:

$$\exists\, v \in Y: \qquad K^* v \in \partial J(u^\dagger)$$

We can then show the following (well-known) estimate:

Optimality condition $u_\alpha \in R_\alpha(f^\delta)$ if and only if

$$\exists\, p_\alpha \in \partial J(u_\alpha): \qquad K^*(Ku_\alpha - f^\delta) + \alpha p_\alpha = 0$$

Burger, M., Resmerita, E., & He, L. (2007). Error estimation for Bregman iterations and inverse scale space methods in image restoration. *Computing*, *81*(2-3), 109-135.
Scherzer, O., Grasmair, M., Grossauer, H., Haltmeier, M., & Lenzen, F. (2009). Variational methods in imaging.
MB, & Burger, M. (2018). Modern regularization methods for inverse problems. *Acta Numerica*, *27*, 1-111.

Error estimates in inverse problems

$$K^*(Ku_\alpha - f^\delta) + \alpha p_\alpha - \alpha K^* v = -\alpha K^* v$$

Dual product with $u_\alpha - u^\dagger$:

$$\langle Ku_\alpha - f^\delta, Ku_\alpha - f\rangle_Y + \alpha \underbrace{\langle u_\alpha - u^\dagger, p_\alpha - K^* v\rangle_*}_{= D_J^{p_\alpha}(u^\dagger, u_\alpha) + D_J^{K^* v}(u_\alpha, u^\dagger)} = -\alpha\langle K^* v, u_\alpha - u^\dagger\rangle_*$$

where

$$D_J^p(v,u) = J(v) - J(u) - \langle p, v - u\rangle \qquad \text{for} \qquad p \in \partial J(u)$$

is the Bregman distance (divergence) w.r.t. J for arguments v, u

$D_J^{\text{symm}}(u,v) = D_J^p(v,u) + D_J^q(u,v)$ is a symmetric Bregman distance

Bregman, L. M. (1967). The relaxation method of finding the common point of convex sets and its application to the solution of problems in convex programming. *USSR computational mathematics and mathematical physics*, *7*(3), 200-217.
Kiwiel, K. C. (1997). Proximal minimization methods with generalized Bregman functions. *SIAM journal on control and optimization*, *35*(4), 1142-1168.

Error estimates in inverse problems

$$\langle Ku_\alpha - f^\delta, Ku_\alpha - f\rangle_Y = \frac{1}{2}\|Ku_\alpha - f\|_Y^2 + \frac{1}{2}\|Ku_\alpha - f^\delta\|_Y^2 - \frac{1}{2}\|f - f^\delta\|_Y^2$$

Hence,

$$\frac{1}{2}\|Ku_\alpha - f\|_Y^2 + \frac{1}{2}\|Ku_\alpha - f^\delta\|_Y^2 + \alpha D_J^{\text{symm}}(u_\alpha, u^\dagger) = \frac{1}{2}\|f - f^\delta\|_Y^2 - \alpha\langle v, Ku_\alpha - f\rangle_Y$$

Using the identity

$$\langle \alpha v, f - Ku_\alpha\rangle_Y = \frac{\alpha^2}{2}\|v\|_Y^2 + \frac{1}{2}\|Ku_\alpha - f\|_Y^2 - \frac{1}{2}\|\alpha v - f + Ku_\alpha\|_Y^2$$

then yields

$$\frac{1}{2}\|Ku_\alpha - f + \alpha v\|_Y^2 + \frac{1}{2}\|Ku_\alpha - f^\delta\|_Y^2 + \alpha D_J^{\text{symm}}(u_\alpha, u^\dagger) = \frac{1}{2}\|f - f^\delta\|_Y^2 + \frac{\alpha^2}{2}\|v\|_Y^2$$

Error estimates in inverse problems

$$\frac{1}{2}\|Ku_\alpha - f + \alpha v\|_Y^2 + \frac{1}{2}\|Ku_\alpha - f^\delta\|_Y^2 + \alpha D_J^{\text{symm}}(u_\alpha, u^\dagger) = \frac{1}{2}\|f - f^\delta\|_Y^2 + \frac{\alpha^2}{2}\|v\|_Y^2$$

Dividing by α and using $\|f - f^\delta\| \leq \delta$ yields the estimate

$$\frac{1}{2\alpha}\|Ku_\alpha - f + \alpha v\|_Y^2 + \frac{1}{2\alpha}\|Ku_\alpha - f^\delta\|_Y^2 + D_J^{\text{symm}}(u_\alpha, u^\dagger) \leq \frac{\alpha}{2}\|v\|_Y^2 + \frac{\delta^2}{2\alpha}$$

Hence, if we choose $\alpha(\delta) = \delta / \|v\|_Y$, we obtain

$$D_J^{\text{symm}}(u_{\alpha(\delta)}, u^\dagger) \leq \|v\|_Y \, \delta$$

How do we compute v in order to estimate (or even control) $\|v\|_Y$?