

大规模计算重建理论与方法

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摘要 计算成像将高维场景信息压缩编码为低维采集数据,并通过计算重建算法恢复高维场景信息。数据爆炸时代,对高时空分辨率的需求日益迫切,亟需同时满足高精度、低复杂度及适用不同系统的灵活性要求的大规模重建算法。现有大规模计算重建研究,包括交替投影、深度图像先验及即插即用方法,已取得阶段性进展。其中交替投影方法已应用于十亿像素定量相位成像,深度图像先验方法和即插即用方法结合了传统模型优化与深度学习技术的优点,具备大规模重建潜力。系统地梳理3类方法的架构及在大规模计算成像中的应用,展望大规模重建算法的未来发展趋势,以期为后续研究与应用提供有益的指导与借鉴。

关键词 计算成像; 大规模重建; 交替投影; 深度图像先验; 即插即用方法

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Theory and Approach of Large-Scale Computational Reconstruction

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Abstract Computational imaging compressively encodes high-dimensional scene data into low-dimensional measurements and recovers the high-dimensional scene information using computational reconstruction techniques. In the era of big data, the increasing demands for high spatiotemporal resolution have promoted the development of large-scale reconstruction algorithms with high accuracy, low complexity, and flexibility for various imaging systems. The existing large-scale computational reconstruction methods, including alternating projection, deep image prior, and plug-and-play optimization methods, have made great progresses over the past decades. Among the abovementioned methods, the alternating projection has been utilized in gigapixel quantitative phase imaging systems. Besides, the deep image prior and plug-and-play optimization techniques combine the advantages of conventional optimization and deep learning, which hold great potential for large-scale reconstruction. This work reviews the architectures and applications of these methods and prospects for the research trends, which can provide highlights for future works of large-scale computational imaging.

Key words computational imaging; large-scale reconstruction; alternating projection; deep image prior; plug-and-play method

1 引言

光学成像是人类认识、感受与分析世界的重要途径。近年来,传统的光学成像方式逐渐难以满足现代光学探测对多维多尺度的需求,计算成像应运而生。

计算成像技术对高维连续光信号进行优化耦合采集与计算重构,获取高效、高精度的成像结果,有效提升了人类探索世界的深度与广度。顺应数据爆炸时代的发展需求,计算成像对大规模数据采集的需求日益紧迫。近年来,大规模成像系统取得了一定进展,如:2012年

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杜克大学提出的大规模阵列相机^[1-2]实现了 $120^\circ \times 50^\circ$ 的超大视场与 $38 \mu\text{rad}$ 的极高分辨率,成像像素数超亿级;2013年加州理工学院提出的宽视场高分辨傅里叶叠层显微成像(FPM)系统^[3]实现了10亿像素、约 120 mm^2 宽视场成像,对应的空间带宽积(SBP)高达0.23亿;2019年清华大学搭建了RUSH显微系统^[4],对清醒的小鼠进行厘米级视场与微米级分辨率的实时全脑功能性成像。

大规模计算成像的发展对计算重建算法的要求日益提升。计算重建任务一般假设已知观测过程的物理模型和欠定或低维的测量信号,要求重建完整或高维的目标场景。常用的计算成像模型有:线性模型,即 $y = Ax + n$;非线性模型,即 $y = |Ax|^2 + n$ 。其中, y 为测量信号, A 为观测矩阵, x 为待恢复目标场景, n 为干扰或噪声。大规模计算重建的难点在于:由于大规模重建任务数据量大、维度高,重建算法所需的计算资源和存储资源急剧增加,非针对大规模计算重建设计的重建方法在面临高维大规模数据时可能会出现精度较差、计算资源和存储资源消耗负担增大的问题,导致难以在可控的硬件和时间成本内实现目标场景重建。所以,大规模计算重建应至少具有以下两个特性之一:一、适用于大规模计算成像系统,能实现多维度或高分辨率重建,或重建图像的像素数高于系统的SBP限制^[5-6];二、同等数据量下,比现有其他重建算法所消耗的计算资源和存储资源更少,可以实现更大规模的计算重建。

现有的重建算法可以归纳为模型驱动和数据驱动两大类。模型驱动方法对成像的物理过程进行建模,之后通过解析方程、最优化等方式重建数据;数据驱动方法是人工智能时代下的产物,利用大量数据集来学习重建目标与测量值之间的映射关系与统计特性。在计算复杂度方面:模型驱动方法无需训练,因此仅涉及重建复杂度,但算法的迭代过程和迭代不稳定性导致重建复杂度较高;数据驱动方法的重建过程无需迭代,且得益于GPU并行加速技术,因此在重建复杂度方面优于模型驱动方法,但其在大规模数据集上的训练复杂度较高。在灵活性方面:模型驱动方法显式描述成像物理模型,可灵活设置各项系统参数;数据驱动方法从训练数据学习成像模型、系统参数的隐式描述,若迁移至新成像系统或硬件设置则需要重新训练或精调(fine-tuning)重建算法,灵活性较差。近年来,即插即用(plug-and-play)、深度图像先验(deep image prior)等技术试图结合深度神经网络与模型驱动方法,将预训练网络作为先验算子求解目标场景,在一定程度上兼顾计算复杂度与灵活性。综上所述,大规模数据重建须避免高资源需求或重复的算法训练,保障重建的高效性和对不同系统的泛化性。

现有研究已经在大规模、高空间带宽积的计算重建方面取得了阶段性进展:基于模型驱动的交替投影算法计算复杂度低、灵活性高,已在十亿像素定量相位成像等计算重建任务上获得了广泛的应用;深度图像先验算法与即插即用算法结合模型驱动和数据驱动的优势,重建质量高,规避了复杂耗时的训练过程,适用于大规模计算重建。在当前阶段,总结与分析相关技术研究进展对该领域的发展具有重要意义。因此,本文系统地梳理了3类大规模重建算法的特性及适用场景,并对它们的发展趋势和未来工作进行了展望,希望为后续研究与应用提供有益的指导与借鉴。

2 交替投影优化重建

交替投影(AP)^[7-8]源于非线性相位恢复领域,作为经典的计算重建算法被广泛应用近50年,现今已被成功应用于其他线性计算成像领域,如单像素成像^[9]中的图像重建^[10]。1972年,最早的交替投影算法由Gerchberg和Saxton开创,称为GS算法^[7]。两位开创者受电子显微领域能够获取空间域强度和频域强度的启发,在空间域和频域之间交替变换图像,并施加强度约束,最终重建出目标信息。GS算法的流程如图1(a)所示,从随机初始猜测开始,每一次迭代包含以下步骤:

- 1) 对当前迭代信号 $z_i[n]$ 进行傅里叶变换,并投影到频域,得到频域信号 $Z_i[k]$;
- 2) 保留频域估计信号 $Z_i[k]$ 的相位信息,用探测器捕获的频域强度测量值替换估计信号的强度信息,形成一个新的频域信号 $Z'_i[k]$;
- 3) 对新组成的频域信号 $Z'_i[k]$ 进行傅里叶逆变换,并投影到空间域,得到空域信号 $z'_i[n]$;
- 4) 保留空域估计信号 $z'_i[n]$ 的相位信息,用探测器捕获的空域强度测量值替换估计信号的强度信息,形成一个新的空域信号 $z'_{i+1}[n]$ 。

上述4步可以分为两类:步骤1)和步骤3)是对信号在频域和空域的交替投影;步骤2)和步骤4)是对信号施加强度约束。虽然GS算法由来已久,但其收敛性证明仍然是一大难题^[11-12]。其恢复误差被定义为 $E_i = \sum_{k=1}^m \left| |Z_i[k]| - |X[k]| \right|_2^2$,虽然能够证明每次迭代误差在逐渐减小^[8],但在测量噪声较大时,算法往往收敛到局部最优解,无法保证到达全局最优解。

GS算法需要测量两个域的强度信息,但在许多场景中,空域的强度信息是难以获取的,往往仅能探测频域强度。针对这种情况,1978年Fienup进一步扩充了GS算法的理念,他指出GS算法的步骤4)空域约束可以进一步放松,使用其他约束替代(如非零约束等)。基于这种考虑,Fienup^[8]提出了若干种改进算法,这些变体算法都只对GS算法的最后一步进行改进,却显

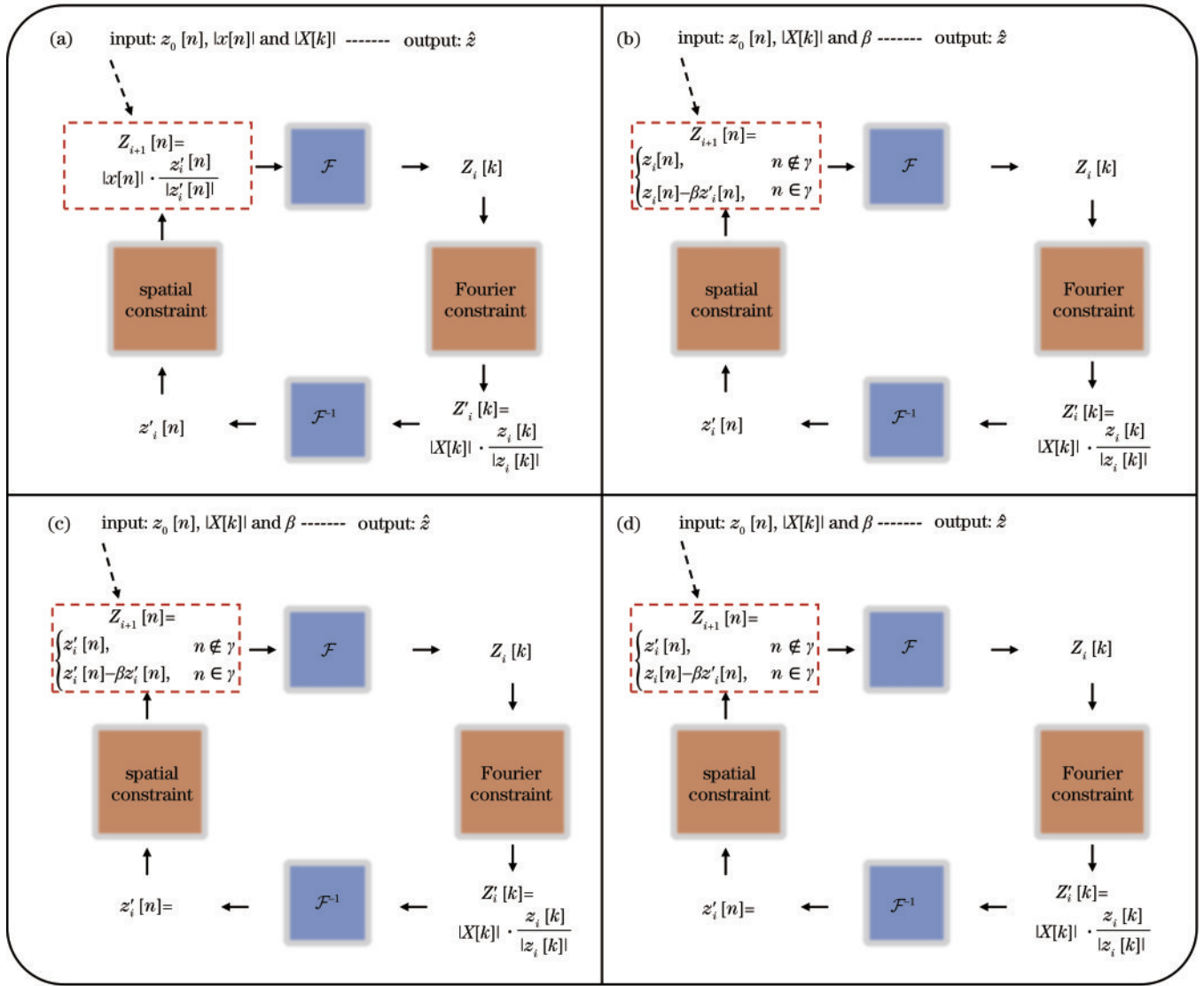


图 1 交替投影算法流程。(a) GS算法;(b) input-output算法;(c)output-output算法;(d) hybrid input-output算法

Fig. 1 Flowchart of alternating projection algorithms. (a) GS algorithm; (b) input-output algorithm; (c) output-output algorithm; (d) hybrid input-output algorithm

著加快了GS算法的收敛速度并提升了性能。以下介绍3种对应步骤4)的关于空域约束的算法。

1. input-output算法,算法流程如图1(b)所示。

$$z_{i+1}[n] = \begin{cases} z_i[n], & n \notin \gamma \\ z_i[n] - \beta z'_i[n], & n \in \gamma \end{cases} \quad (1)$$

2. output-output算法,算法流程如图1(c)所示。

$$z_{i+1}[n] = \begin{cases} z'_i[n], & n \notin \gamma \\ z'_i[n] - \beta z'_i[n], & n \in \gamma \end{cases} \quad (2)$$

3. hybrid input-output(HIO)算法,算法流程如图1(d)所示。

$$z_{i+1}[n] = \begin{cases} z'_i[n], & n \notin \gamma \\ z_i[n] - \beta z'_i[n], & n \in \gamma \end{cases} \quad (3)$$

式中: β 是一个权重超参; γ 是空域约束条件(包括非负性约束等)。HIO算法被大量实验证明,当测量噪声较小时能够收敛到全局最优解。

Finup提出的算法仍缺乏收敛性证明。此外,提出的算法对约束信息的准确性非常敏感。然而,HIO算法在大量研究实践中表现优异,使得它成为光学成像领域恢复相位的首选工具。例如在相干衍射成像中^[13],HIO算法在无噪声/小噪声情况下可以从过采样衍射图中完美重建原始目标。

部分研究者尝试从凸优化角度解释交替投影算法^[14],并以HIO为基础,衍生出了许多算法,例如,误差减小(ER)算法^[8]、差分图(DM)算法^[15]、混合投影映射(HPR)算法^[16]、导向HIO(GHIO)算法^[17]、relaxed averaged alternating reflectors(RAAR)算法^[18]、噪声鲁棒HIO(NR-HIO)算法^[19]、过采样平滑(OSS)算法^[20]。其中,OSS算法在实际中表现出色。OSS算法在HIO算法的第4步之后加入高斯滤波算子,即第5步为

$$z_{i+1}[n] = \begin{cases} z_{i+1}[n], & n \notin \gamma \\ \mathcal{F}\{z_{i+1}[k]W[k]\}, & n \in \gamma \end{cases}, \quad (4)$$

式中: $W[k]$ 是高斯滤波函数, 其噪声方差随着迭代次数增加逐渐减小。此外, 合理的初值对交替投影算法的收敛性和收敛速度会造成显著的影响, 因此对初始解 (initial guess) 的研究也是一个热点方向。

交替投影算法因强泛化性被广泛地应用到了晶体学、光学成像、天文学等众多领域^[12]。在光学成像领域, 由于其低计算复杂性, 因此被应用到大规模、高空间带宽积成像方面。本文重点介绍 AP 在傅里叶叠层显微成像和相干衍射成像中的应用。

2.1 傅里叶叠层显微成像

在传统的成像系统中, 宽视场和高分辨率往往无法同时实现, 互相折中。这源于光学元件的折射问题, 即光圈越大, 校正相差的难度就越大。2013 年加州理工学院 Zheng 等^[3]提出了一种利用低成本小孔径物镜实现高 SBP 成像的显微系统, 称为傅里叶叠层显微成像 (FPM)。基于频域中的移位对应于空域中的角度变化的原理, FPM 系统以不同角度或模式照亮样本^[21], 获得的图像对应于频域不同子孔径的信息。通过这种方式, 实现了 10 亿像素、约 120 mm² 宽视场成像, 对应的空间带宽积高达 0.23 亿。FPM 的光学成

像模型为

$$I = \left| \mathcal{F}^{-1} \left\{ P(k_x, k_y) \mathcal{F} \left[\phi(x, y) e^{i \left(jx \frac{2\pi}{\lambda} \sin \theta_x + jy \frac{2\pi}{\lambda} \sin \theta_y \right)} \right] \right\} \right|^2, \quad (5)$$

式中: ϕ 是样本; (x, y) 是空间坐标; λ 是波长; θ_x 和 θ_y 是入射角; $\phi(x, y) e^{i \left(jx \frac{2\pi}{\lambda} \sin \theta_x + jy \frac{2\pi}{\lambda} \sin \theta_y \right)}$ 为目标样本透射的光场; $P(\cdot)$ 是瞳孔函数; (k_x, k_y) 是在瞳孔平面的空间坐标。

FPM 通常使用 AP 算法恢复相位并重建目标, 该过程如图 2(d) 所示。首先使用测量值的平方根作为复数目标的初值, 之后迭代地在傅里叶域施加孔径支持域约束并在空间域施加测量值约束。FPM 后续的发展包括成像系统和重建算法的改进, 例如: Dong 等^[22]通过孔径调制的方式改变不同的 LED 照明角度, 能够实现对厚样本成像; Bian 等^[23-24]将 Wirtinger Flow 算法引入 FPM 重建中, 有效提高抗噪性, 降低采集曝光时间, 减少光毒性; Chang 等^[6]引入即插即用优化架构, 实现了低计算复杂度、噪声鲁棒的大规模 FPM 重建。随着对 FPM 技术的深入研究, 其应用场景也进一步拓宽。图 3 展示了 FPM 技术的应用示例, 包括但不限于无标记成像、活细胞实时成像、三维成像等。

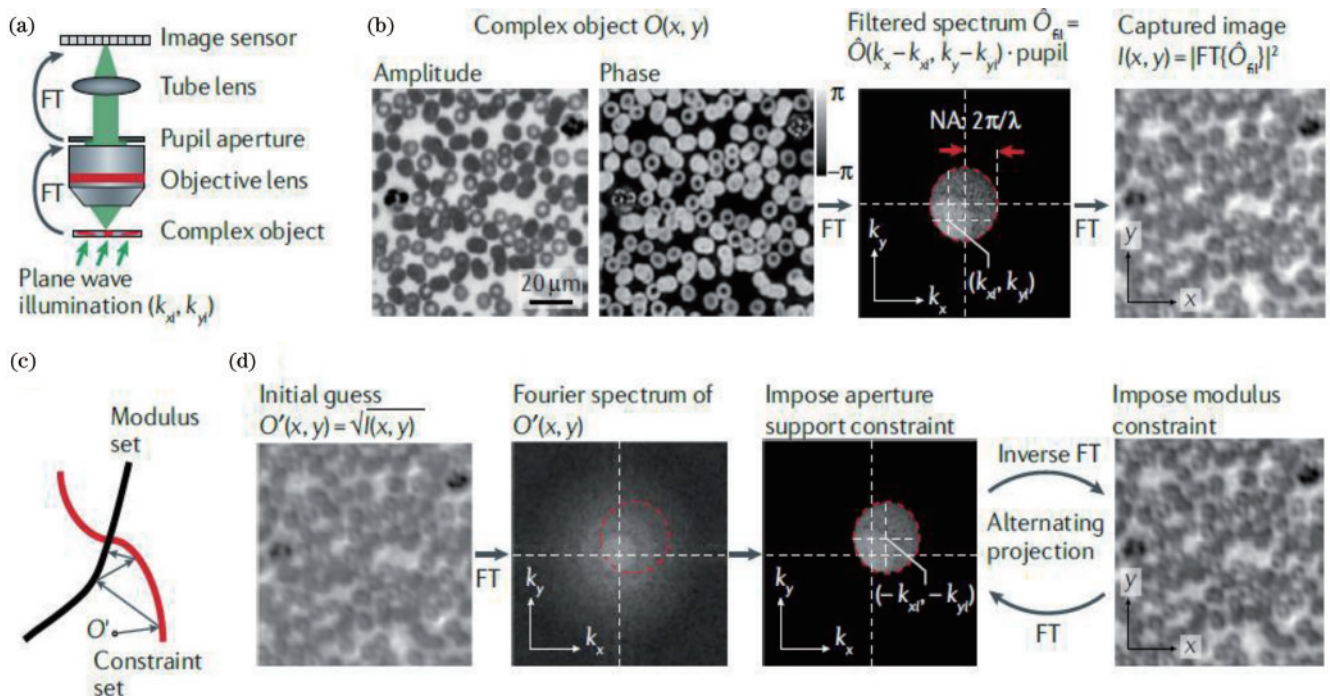


图 2 使用 AP 算法实现 FPM 重建^[25]。(a) FPM 系统结构; (b) FPM 成像模型; (c) AP 算法在解空间中施加强度约束条件; (d) AP 求解 FPM 流程

Fig. 2 FPM reconstruction using AP algorithm^[25]. (a) FPM system structure; (b) FPM imaging model; (c) strength constraints imposed by AP algorithm in solution space; (d) AP solving FPM process

2.2 相干衍射成像

相干衍射成像 (CDI) 技术起源于人们对非晶体材

料结构观测的需求。由于 X 射线的波长和晶体中的原子距离在一个量级 (0.001~10 nm), 因此 X 射线透过

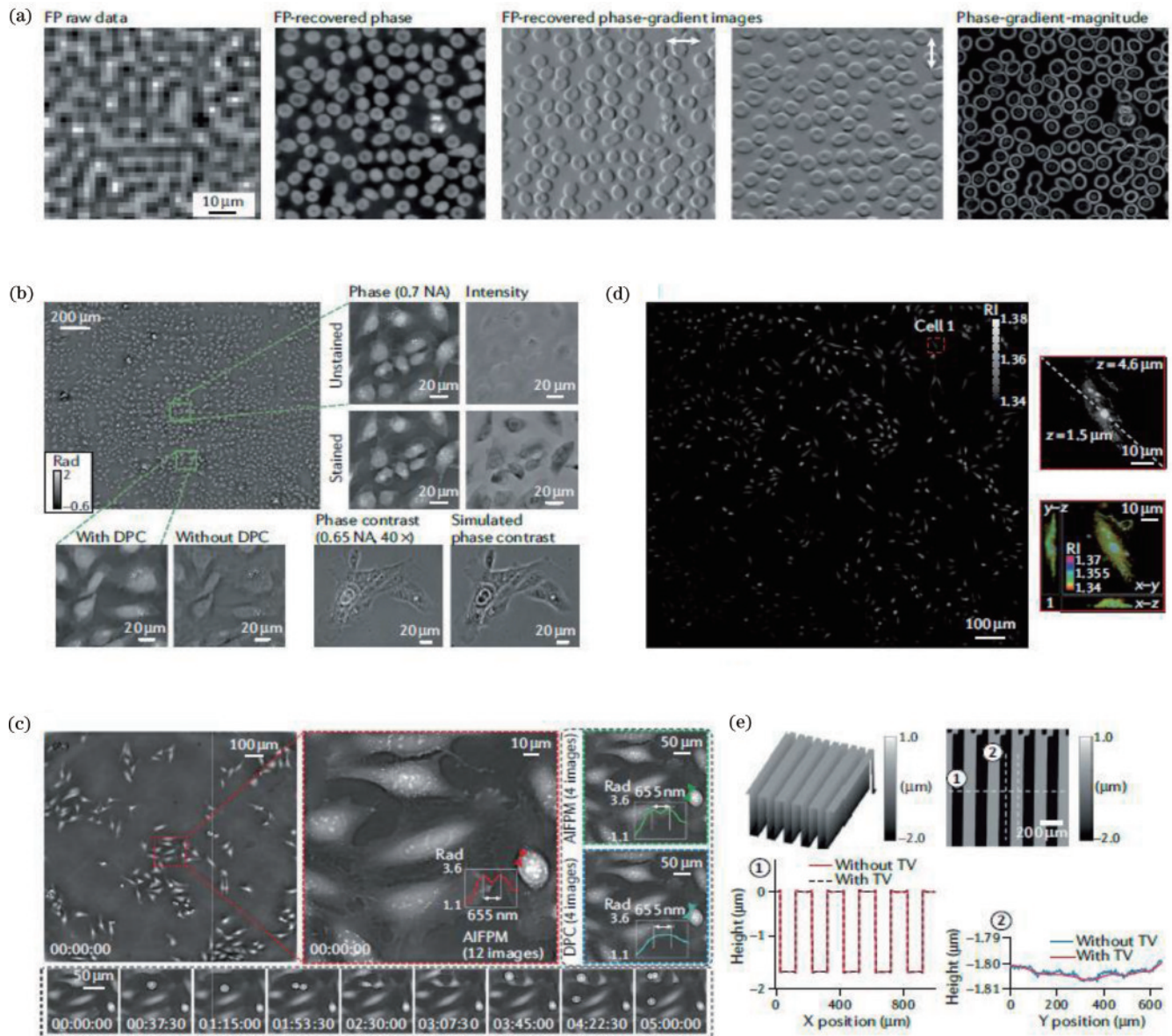


图3 FPM技术的应用^[25]。(a)血细胞定量相位成像；(b)活的HeLa细胞相位图；(c)环形照明FPM技术以25 Hz帧率观测HeLa细胞的有丝分裂和凋亡；(d)FPM技术重建HeLa细胞的三维折射率；(e)FP技术绘制三维曲面地形图

Fig. 3 Applications of FPM technique^[25]. (a) Quantitative phase imaging of blood smear; (b) phase images of live HeLa cell; (c) phase images of mitosis and apoptosis events of live HeLa cell captured by annular illumination FPM at a frame rate of 25 Hz; (d) reconstruction of three-dimensional refractive index of HeLa cells by FPM; (e) topographic map of a 3D surface via FP technology

晶体后衍射线的空间分布与晶体结构密切相关,每种晶体所产生的衍射图样都反映出该晶体内部的原子分配规律。然而,有许多材料不能得到足够好的结晶体,甚至根本无法结晶,这严重阻碍了X射线晶体学的进一步发展。在此背景下,相干衍射成像技术应运而生。它由加州大学洛杉矶分校Miao等^[13]于1999年提出,是一种新颖的无透镜成像技术。CDI技术使用相干或者部分相干的光穿透样本,波前会受到调制,在不同厚度或者折射率突变的地方发生传播方向的改变。CDI的光学成像模型可表示为

$$I = \left| \mathcal{F}[\phi(x, y)] \right|^2, \quad (6)$$

式中: \mathcal{F} 为二维傅里叶变换; I 为采集到的远场衍射强度图。AP也是CDI重建的常用算法。具体而言,AP算法通常始于一个随机初始猜测,之后在空间域和傅里叶域之间来回迭代;在每次迭代中,空间域约束通常使用非负约束(即样本分布密度不能为负),在傅里叶域中保留相位,使用测量值更新幅度;经过数千次的迭代后,即可恢复出样本图像。在此基础上,后续又发展出了图4所展示的菲涅耳CDI^[26]、布拉格CDI^[27]、叠层CDI^[28]、编码CDI^[29]等多种形态,它们进一步拓展了CDI技术的应用范围。图5展示了CDI技术在晶体学、材料科学、生命科学等众多领域的应用。

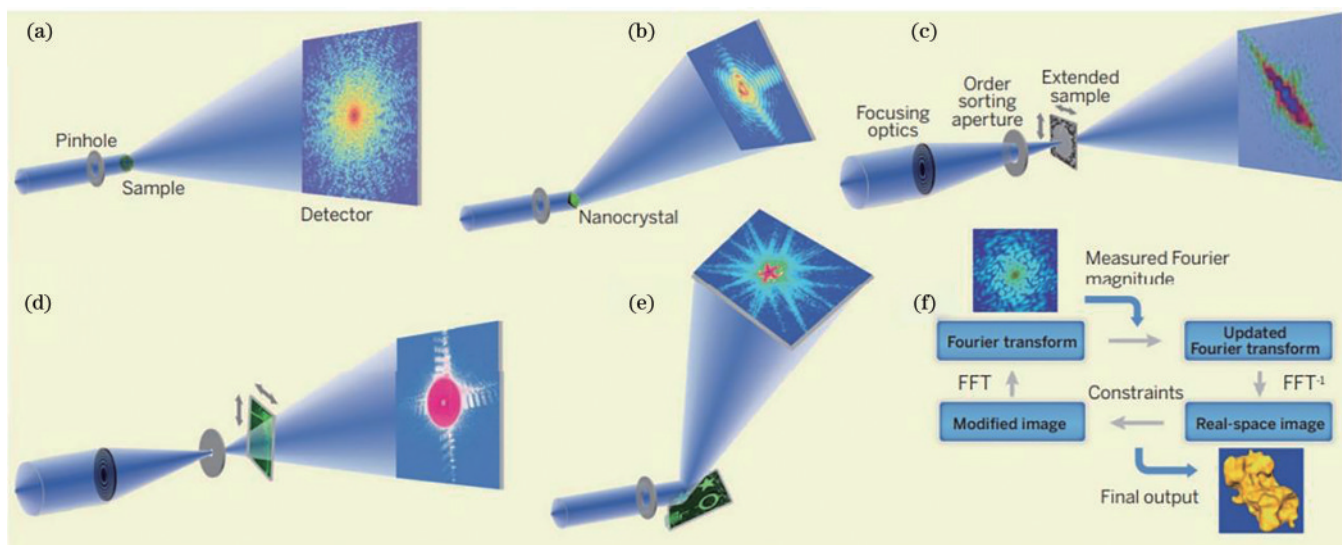


图4 CDI技术及重建算法^[30]。(a)平面波 CDI; (b)布拉格 CDI; (c)叠层 CDI; (d)菲涅耳 CDI; (e)反射 CDI; (f)基于交替投影的 CDI 重建算法流程

Fig. 4 CDI techniques and reconstruction algorithms^[30]. (a) Plane-wave CDI; (b) Bragg CDI; (c) ptychographic CDI; (d) Fresnel CDI; (e) reflection CDI; (f) flowchart of alternating-projection-based CDI reconstruction algorithm

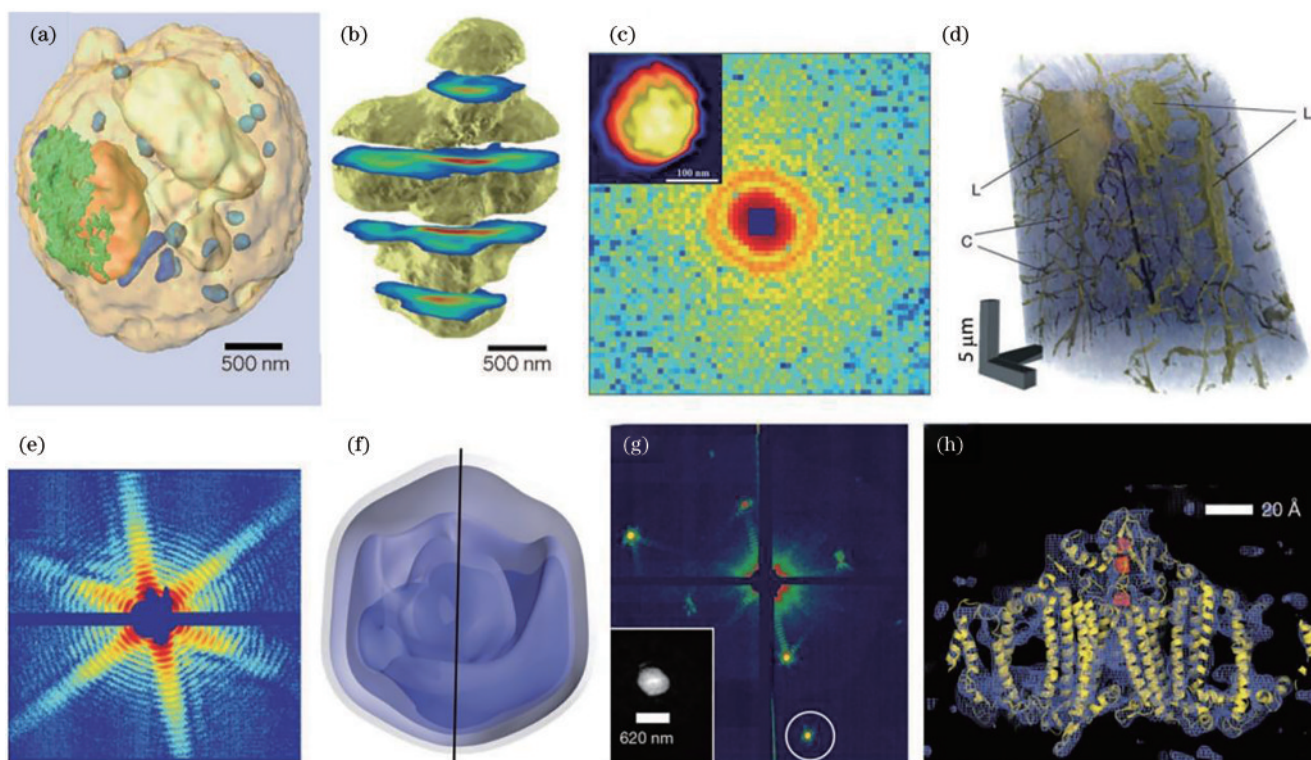


图5 CDI技术的应用^[30]。(a)未染色的酵母孢子细胞三维密度分布; (b)未染色的人类染色体三维图像; (c)未染色的疱疹病毒粒子重建; (d)骨基质三维定量测量; (e)米米病毒的相干衍射图样; (f)米米病毒的三维重建; (g)纳米晶体的衍射图样; (h)2mFo-DFc 电子密度图

Fig. 5 Applications of CDI technique^[30]. (a) 3D mass density distribution of an unstained yeast spore cell; (b) 3D image of an unstained human chromosome; (c) reconstruction of an unstained herpesvirus virion; (d) quantitative 3D measurement of osteocyte; (e) representative diffraction pattern of a giant mimivirus particle; (f) 3D reconstruction of a mimivirus; (g) diffraction pattern of a nanocrystal; (h) electron density map of 2mFo-DFc

3 深度图像先验

2018年, Ulyanov 等^[31]提出深度图像先验(DIP),

DIP 输入受损的图像到未训练的 UNet^[32], 令 UNet 学习受损图像到受损图像自身的映射, 在一定迭代次数后, UNet 能够修补受损图像或去除图像中的噪声。

DIP证明人为设计的深度神经网络结构本身也可以作为一种图像先验。深度图像先验算法适用于多类线性与非线性成像模型。对于线性成像过程,基于DIP的拓展研究在图像去噪^[33-34]、超分辨^[35-40]、去雾^[41]、去模糊^[42-43]、图像修补^[44-45]、分割^[46]等计算机视觉任务上取得了一定的进展。同时,DIP的提出与应用掀起了深度神经网络与传统优化技术深层次结合的研究热潮。

利用深度网络作为图像生成模型,与传统优化方式联合进行计算重建,目标函数表示为

$$\min_{\theta} \| \mathbf{y} - f[\text{Net}(\mathbf{z}, \theta)] \|_2^2, \quad (7)$$

式中: $\text{Net}(\cdot)$ 为神经网络操作; θ 为网络参数; \mathbf{z} 为神经网络的输入信号; \mathbf{y} 为测量信号; f 为正向成像模型。输入信号 \mathbf{z} 可以是随机噪声,可以是测量信号,或利用其他方法求解的初始值。如图6所示,深度图像先验算法通过优化网络参数 θ 获得重建图像。深度图像先验算法的计算复杂度与mini-batch为1的端到端深度学习训练阶段的计算复杂度相同,适用于较大规模计算重建。相比于端到端深度学习方法,深度图像先验算法无需预训练,对缺少大规模数据集的计算重建任务更加鲁棒,泛化性更强。

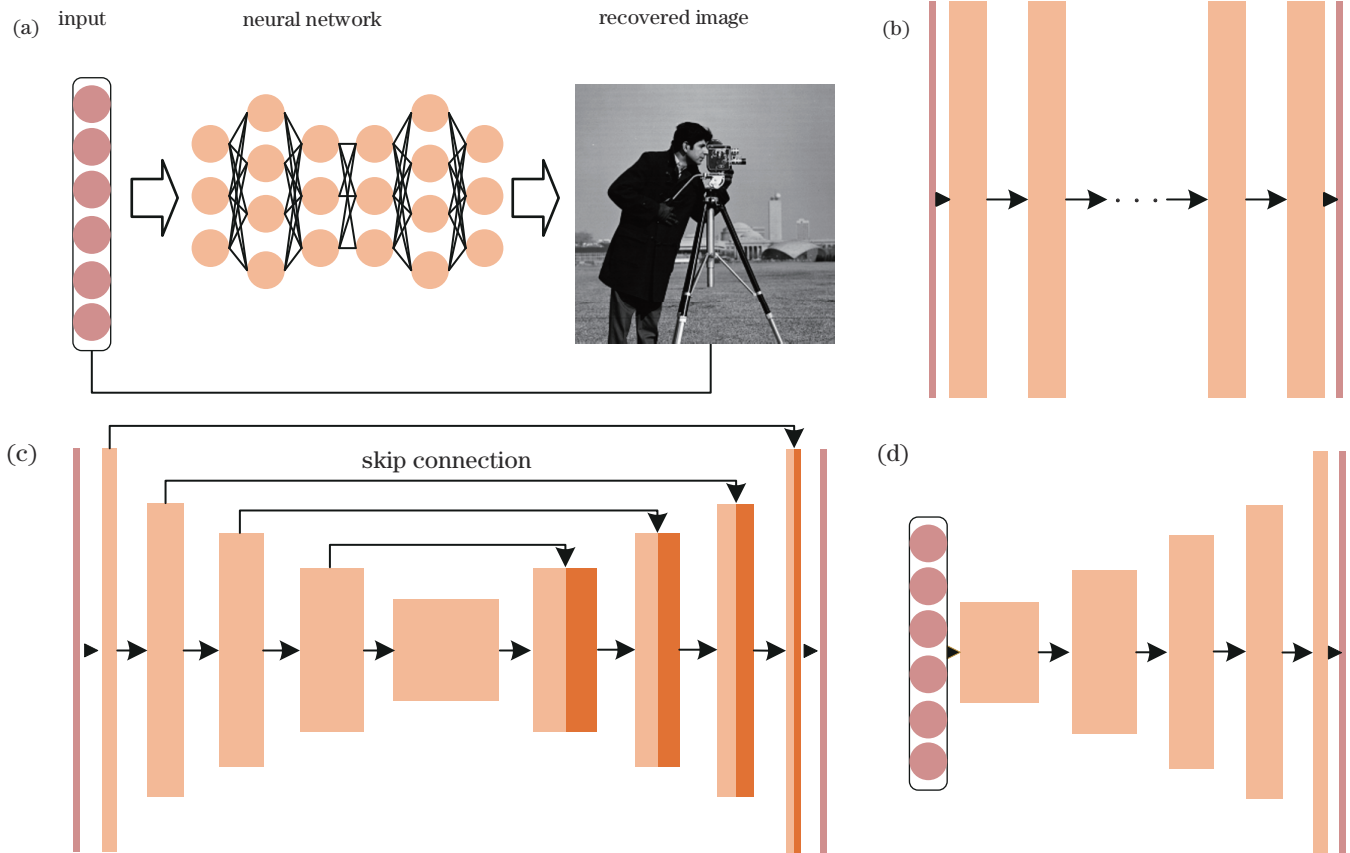


图6 深度图像先验算法架构。(a) 深度图像先验算法框架;(b) 常规卷积神经网络结构;(c) UNet结构;(d) 深度解码器结构

Fig. 6 Framework of DIP algorithm. (a) Principle of DIP; (b) common CNN structure; (c) UNet structure; (d) deep decoder structure

3.1 深度网络结构

Ulyanov等^[31]指出,深度图像先验与网络结构相关,合适的网络会带来更好的重建效果。如图6所示,较常使用的网络结构有三种:常规卷积结构、UNet结构、深度解码器(DD)结构。常规卷积结构是使用特征图尺度不变的多个卷积层组成的网络结构,卷积层中可以包含二维卷积层、标准化层、激活函数层等子层。Jagatap等^[47]利用深度图像先验算法处理相位恢复(PR)问题,对于不同类型的图像,使用不同的网络进行重建,如对于MNIST手写数字图像^[48]使用两层常规卷积网络,而对于更加复杂的CelebA人脸图像^[49]使用三层网络。Jiang等^[50]将傅里叶叠层显微成像中物

镜的点扩展函数(PSF)作为卷积网络的输入,将卷积层的参数作为重建图像的亮度值,优化网络参数直接获得重建图像。UNet由Ronneberger等^[32]提出,是经典的图像生成网络。UNet结构的网络一般利用解码子网络生成多分辨率特征图,然后通过跨层连接将对应分辨率的特征图输入编码子网络,实现浅层特征与深层特征的复用。Wang等^[51]以UNet为基础网络,提出了一个统一的非训练相位恢复网络模型(PhysNet),恢复图像的相位信息。Wang等证明基于UNet结构的深度图像先验算法的成像质量相比于迭代恢复算法和端到端深度学习重建算法更高。Gong等^[52]将非局部层引入UNet以进行计算机断层扫

描(CT)图像重建。解码器结构输入一段低维信号,通过上采样层逐级提高特征图分辨率,最后输出高分辨率重建图像,一般低维信号为固定的随机噪声。Darestani等^[53]讨论了多种解码器结构,进行核磁共振成像以加速计算重建。深度图像先验算法的收敛性已被证明与网络架构本身有关^[54],所以探究合适的网络结构对深度图像先验算法具有重要的意义。随着深度学习中网络可解释性理论的发展,更加灵活高效、更高重建质量的网络结构会被引入深度图像先验算法中,进一步提升性能。

3.2 额外的图像先验

在目标函数中引入额外的图像先验会避免过拟合,使得优化更鲁棒^[55],假设先验正则项为 R ,目标函数为

$$\min_{\theta} \left\| \mathbf{y} - f[\text{Net}(\mathbf{z}, \theta)] \right\|_2^2 + R[\text{Net}(\mathbf{z}, \theta)]. \quad (8)$$

常用的先验正则项包含全变分(TV)正则项、非局部(Nonlocal)去噪正则项、初始值先验等。由于自然图像具有一定的平滑性,其变分图在大多数情况下是稀疏的,引入TV正则项可以去掉图像中过度的畸变与噪声,使得输出图像更加平滑。Liu等^[56]通过加入TV正则项指导深度图像先验算法重建,在图像去噪与去模糊任务上相比传统TV去噪或DIP去噪,重建质量更高。Bager等^[57]也指出DIP+TV可以更精确地重建CT图像。Fan等^[58]结合非局部去噪与DIP网络进行光学相干断层扫描(OCT)重建。Bager等^[57]将端到端网络的结果作为初值,该值可视为施加了基于统计的初始值先验,此时深度图像先验算法能够得到收敛速度更快且比端到端网络泛化性更强的CT重建结果。Zhao等^[59]将一张高分辨核磁共振图像(MRI)作为初始值输入DIP网络,利用脑部核磁共振图像的结构相似性,加快深度图像先验算法重建。

3.3 多网络并行优化

当需要使用网络预测多个中间变量时,部分研究会采用多网络结构。Li等^[41]利用深度图像先验算法进行去雾,所采用的光照模型存在三个变量,即清晰场景图像、透射率图与环境光照图。采用三个DIP网络分别预测上述三个变量,其中通过常规卷积网络预测清晰场景图像与透射率图,利用变分网络预测环境光照图。Qayyum等^[60]采用了相同的光照模型,与Li等^[41]提出的方法的主要区别是,采用深度解码网络作为DIP网络进行视网膜图像的增强。Yokota等^[61]通过非负矩阵分解利用多个UNet并行重建动态计算机断层扫描(PET)图像,验证了多网络结构重建在大噪声下的鲁棒性。Han等^[62]引入贝叶斯推断框架,利用两个DIP网络分别重建清晰图像与不均匀性场,以进行MR图像校正。

综上所述,深度图像先验算法所用的网络结构、输入信号、额外正则项与场景分类总结如图7和表1

所示。近年来,由于结合神经网络且无需预训练的特点,深度图像先验算法在医学计算成像领域受到了大量关注。根据众多研究实践可知,深度图像先验算法在大噪声情况下的重建效果优于其他方法。深度图像先验算法的关键在于神经网络的结构与收敛判定。UNet因为结构简单、恢复质量高成为较为常用的网络结构。探究更适合深度图像先验算法的轻量级网络结构是未来研究的基础。同时,由于DIP网络需要特定的迭代次数达到收敛,过少或过多的迭代次数会带来欠拟合与过拟合现象,导致成像质量较低,所以研究DIP网络的收敛性与最佳收敛方法具有重要的意义。

4 即插即用优化

即插即用优化重建在传统优化基础上结合了深度神经网络的发展成果,通过深度神经网络作为正则先验,将深度神经网络与传统优化有机地结合起来。即插即用优化分解计算重建问题分为数据项和先验正则项等若干子问题,迭代求解数据项与正则项。数据项子问题的更新一般通过近端梯度法或闭式解法,正则项则由深度去噪网络求解。目前,即插即用优化重建方法已经在众多成像与计算视觉任务(如图像去模糊^[65]、超分辨^[66-69]、相位恢复^[70-74]、核磁共振成像^[73,75]、光学断层重建^[76-77]等)中展现出了先进的性能和强大的泛用性。

4.1 即插即用优化框架

对于计算摄像问题,即插即用优化建构的目标函数为

$$\min_{\mathbf{x}} R(\mathbf{x}) \quad \text{s. t.} \quad \mathbf{y} = f(\mathbf{x}), \quad (9)$$

式中: \mathbf{x} 是待求信号; \mathbf{y} 是观测信号; $f(\mathbf{x})$ 代表信号传输过程; $R(\mathbf{x})$ 是关于 \mathbf{x} 的正则项。可进行大规模计算重建的优化框架有半二次分裂法、快速迭代收缩阈值法、交替方向乘法、广义交替投影法等。

4.1.1 半二次分裂法

半二次分裂法^[78]利用变量分裂的方法将原目标函数分解为两个子目标函数,首先原目标函数需要改写为

$$\min_{\mathbf{x}} \left\| \mathbf{y} - f(\mathbf{x}) \right\|_2^2 + R(\mathbf{x}). \quad (10)$$

将变量 \mathbf{x} 分裂为 \mathbf{x} 和 \mathbf{z} 两个变量,得到

$$\min_{\mathbf{x}} \left\| \mathbf{y} - f(\mathbf{x}) \right\|_2^2 + R(\mathbf{z}) + \mu \left\| \mathbf{z} - \mathbf{x} \right\|_2^2. \quad (11)$$

新目标函数式(11)可以迭代地分别求解 \mathbf{x} 和 \mathbf{z} ,更新形式为

$$\begin{cases} \mathbf{x}_{k+1} = \arg \min_{\mathbf{x}} \left\| \mathbf{y} - f(\mathbf{x}) \right\|_2^2 + \mu \left\| \mathbf{z} - \mathbf{x} \right\|_2^2 \\ \mathbf{z}_{k+1} = \arg \min_{\mathbf{z}} R(\mathbf{z}) + \mu \left\| \mathbf{z} - \mathbf{x} \right\|_2^2 \end{cases}. \quad (12)$$

4.1.2 迭代收缩阈值法

迭代收缩阈值法(ISTA)^[79]是基于近端梯度下降

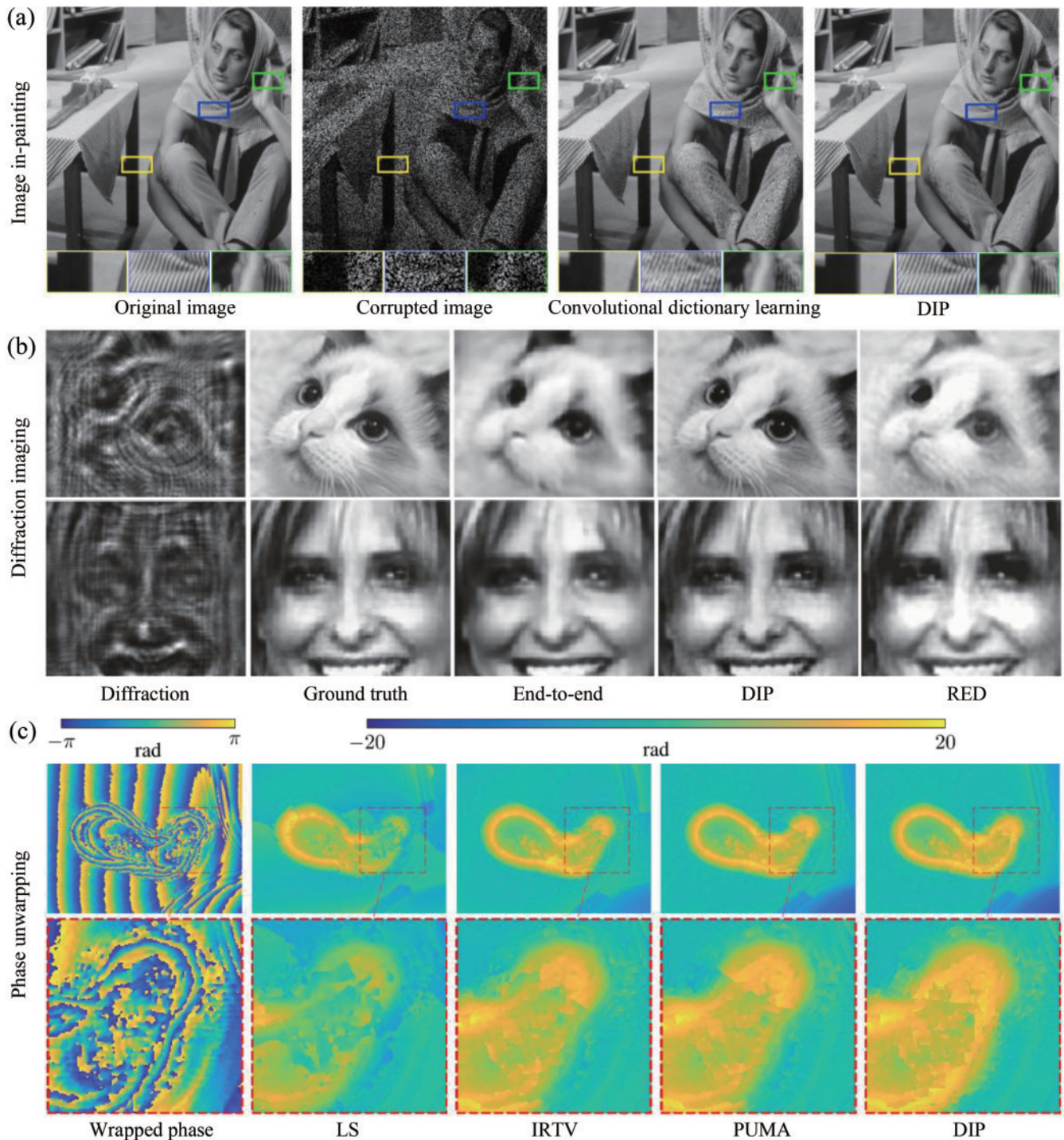


图 7 DIP 算法结果及在各任务上与其他算法的对比。(a) 图像修复^[31]; (b) 衍射成像^[51]; (c) 相位解包裹^[63]

Fig. 7 Results of DIP algorithm and comparisons with other algorithms in each task. (a) Inpainting^[31]; (b) diffraction imaging^[51]; (c) phase unwrapping^[63]

思想的。ISTA 定义的近端函数为

$$\text{prox}_L(\mathbf{z}) = \arg \min_{\mathbf{x}} R(\mathbf{x}) + \frac{L}{2} \left\| \mathbf{x} - \left[\mathbf{z} - \frac{1}{L} \nabla f(\mathbf{z}) \right] \right\|_2^2. \quad (13)$$

在求解过程中,每一次迭代都是基于近端函数的:

$$\mathbf{x}_k = \text{prox}_L(\mathbf{x}_{k-1}), \quad (14)$$

式中: L 为迭代步长。选定初始值 $y_1 = x_0, t_1 = 1$, 快速

迭代收缩阈值法(FISTA)的迭代过程为

$$\begin{cases} \mathbf{x}_k = \text{prox}_L(\mathbf{z}_k) \\ t_{k+1} = \frac{1 + \sqrt{1 + 4t_k^2}}{2} \\ \mathbf{z}_{k+1} = \mathbf{x}_k + \frac{t_k - 1}{t_{k+1}} (\mathbf{x}_k - \mathbf{x}_{k-1}) \end{cases}. \quad (15)$$

表 1 深度图像先验算法及其应用场景
Table 1 DIP algorithms and their applications

Algorithm	Network	Input	Regularization	Application
Algorithm in Ref. [31]	UNet	Degraded image	/	Denosing & Inpainting & SR
Algorithm in Ref. [50]	CNN	PSF	/	FPM
Algorithm in Ref. [47]	CNN	Measurement	/	PR
Algorithm in Ref. [52]	UNet	Measurement	/	CT
Algorithm in Ref. [56]	UNet	Degraded image	TV	Denosing & Deblurring
Algorithm in Ref. [51]	UNet	Measurement	/	PR
Algorithm in Ref. [53]	DD	Noise	/	MRI
Algorithm in Ref. [61]	2×CNN	Noise	/	MR correction
Algorithm in Ref. [60]	3×DD	Noise	Dark channel prior	Retinal image enhancement
Algorithm in Ref. [57]	UNet	Initial reconstruction	TV	CT
Algorithm in Ref. [58]	UNet	Noise	Nonlocal	OCT
Algorithm in Ref. [59]	UNet	Reference image	/	MRI
Algorithm in Ref. [41]	2×CNN+VAE	Haze image	HSV loss & Smooth loss on air-light map	Dehaze
Algorithm in Ref. [61]	3×UNet	Noise	TV	Dynamic PET
Algorithm in Ref. [63]	UNet	Measurement	/	Phase unwarping
Algorithm in Ref. [64]	DNN	To-be-updated image	/	SCI

4.1.3 交替方向乘法

交替方向乘子 (ADMM) 法^[80]是一种通用的优化框架,适用于求解凸优化问题。ADMM 法将目标函数改写为

$$\min_{\mathbf{x}, \mathbf{z}} \|\mathbf{y} - f(\mathbf{x})\|_2^2 + R(\mathbf{z}) \quad \text{s. t.} \quad \mathbf{x} = \mathbf{z}。 \quad (16)$$

根据式(16)建立增广拉格朗日函数:

$$L_\rho(\mathbf{x}, \mathbf{z}, \boldsymbol{\lambda}) = \|\mathbf{y} - f(\mathbf{x})\|_2^2 + R(\mathbf{z}) + \boldsymbol{\lambda}^\top(\mathbf{x} - \mathbf{z}) + \frac{\rho}{2} \|\mathbf{x} - \mathbf{z}\|_2^2, \quad (17)$$

式中: $\boldsymbol{\lambda}$ 为对偶变量; ρ 为常数,用于调整收敛速率。ADMM 法的迭代更新形式为

$$\begin{cases} \mathbf{x}_{k+1} = \arg \min_{\mathbf{x}} L_\rho(\mathbf{x}, \mathbf{z}_k, \boldsymbol{\lambda}_k) \\ \mathbf{z}_{k+1} = \arg \min_{\mathbf{z}} L_\rho(\mathbf{x}_{k+1}, \mathbf{z}, \boldsymbol{\lambda}_k) \\ \boldsymbol{\lambda}_{k+1} = \boldsymbol{\lambda}_k + \rho(\mathbf{x}_{k+1} - \mathbf{z}_{k+1}) \end{cases} \quad (18)$$

交替方向乘子法对弱凸甚至是非凸优化问题的许多模型具有较好的全局收敛性。

4.1.4 广义交替投影法

广义交替投影 (GAP) 法由 Yuan^[81]于 2016 年提出, GAP 主要针对线性模型 $\mathbf{y} = f(\mathbf{x}) = \mathbf{A}\mathbf{x}$, 其目标函数写作

$$\min_{\mathbf{x}, \mathbf{z}} \|\mathbf{y} - \mathbf{A}\mathbf{x}\| + \lambda R(\mathbf{z}) \quad \text{s. t.} \quad \mathbf{x} = \mathbf{z}。 \quad (19)$$

利用欧几里得投影法求解目标函数式(19), GAP 的迭代更新形式为

$$\begin{cases} \mathbf{x}_{k+1} = \mathbf{z}_k + \mathbf{A}^\top(\mathbf{A}\mathbf{A}^\top)^{-1}(\mathbf{y} - \mathbf{A}\mathbf{z}_k) \\ \mathbf{z}_{k+1} = \arg \min_{\mathbf{z}} R(\mathbf{x}_{k+1}) \end{cases} \quad (20)$$

广义交替投影法相比交替方向乘法收敛速度更

快^[82], 在小噪声或者无噪声的情况下精度与交替方向乘法接近。

4.1.5 近似消息传递法

对于线性模型 $\mathbf{y} = f(\mathbf{x}) = \mathbf{A}\mathbf{x}$, 近似消息传递 (AMP) 法^[83-84]的迭代求解过程为

$$\begin{cases} \mathbf{x}_{k+1} = \mathfrak{R}(\mathbf{x}_k + \mathbf{A}^* \mathbf{z}_k) \\ \mathbf{z}_k = \mathbf{y} - \mathbf{A}\mathbf{x}_k + \frac{1}{\delta} \mathbf{z}_{k-1} \mathfrak{R}'(\mathbf{x}_{k-1} + \mathbf{A}^* \mathbf{z}_{k-1}) \end{cases}, \quad (21)$$

式中: \mathbf{A}^* 为 \mathbf{A} 的共轭转置; \mathfrak{R} 为去噪项; \mathfrak{R}' 表示去噪项的一阶导数; $\frac{1}{\delta} \mathbf{z}_{k-1} D'_{\sigma^{k-1}}(\mathbf{x}_{k-1} + \mathbf{A}^* \mathbf{z}_{k-1})$ 称为 Onsager 校正项, 能够加速算法收敛。

4.1.6 去噪正则法

2017 年 Romano 等^[85]提出了一种显式的自适应正则化泛函 Regulation by Denoiser (RED)。RED 建立的目标函数为

$$\min_{\mathbf{x}} \frac{1}{2\sigma^2} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|^2 + \frac{\lambda}{2} \mathbf{x}^\top [\mathbf{x} - \mathfrak{R}(\mathbf{x})], \quad (22)$$

式中: σ 为估计噪声水平; λ 为正则项权重。迭代求解过程为

$$\begin{cases} \mathbf{x}_{k+1} = \mathfrak{R}(\mathbf{x}_k) \\ \mathbf{x}_{k+1} = \mathbf{x}_k - \mu \left[\frac{1}{\sigma^2} \mathbf{A}^\top(\mathbf{A}\mathbf{x}_k - \mathbf{y}) + \lambda(\mathbf{x}_k - \mathbf{x}_{k+1}) \right], \end{cases} \quad (23)$$

式中: $\mu = 2/(1/\sigma^2 + \lambda)$ 。RED 可以单独使用, 也可作为 ADMM 中的正则约束项更新使用。即插即用优化框架的总结如表 2 所示, 框架的收敛性已经经过了理论分析与大量实例论证。Ryu 等^[86]证明了 ADMM 网络联合优化在 Lipschitz 条件下的收敛性。Sun 等^[87]提

出增量式 ADMM 联合优化形式,该形式可以更高效地求解非平滑数据项,且在大规模计算重建应用上复杂度更低、收敛更快。文献[88-89]则完成了 ISTA 网络联合优化在线性逆问题上的收敛性分析,RED 的收敛也经过了理论与实例验证^[85]。Wei 等^[73]提出了一种

强化学习方式,该方式自适应地调节每一次迭代的超参数,达到高效收敛的效果。随着即插即用优化理论成果的丰富,可以期待收敛速度更快、更鲁棒的即插即用优化框架。

表 2 即插即用优化框架
Table 2 Plug-and-play optimization framework

Model	Framework	Fidelity term	Regularization term
$y=f(x)$	HQS	$\mathbf{x}_{k+1} = \arg \min_x \ \mathbf{y} - f(\mathbf{x})\ _2^2 + \mu \ \mathbf{z} - \mathbf{x}\ _2^2$	$\mathbf{z}_{k+1} = \arg \min_z R(\mathbf{z}) + \mu \ \mathbf{z} - \mathbf{x}\ _2^2$
	FISTA	$\mathbf{x}_k = \text{prox}_L(\mathbf{z}_k)$	$\mathbf{z}_{k+1} = \mathbf{x}_k + \frac{t_k - 1}{t_{k+1}}(\mathbf{x}_k - \mathbf{x}_{k-1})$
	ADMM	$\mathbf{x}_{k+1} = \arg \min_x L_{\rho}(\mathbf{x}, \mathbf{z}_k, \lambda_k)$	$\mathbf{z}_{k+1} = \arg \min_z L_{\rho}(\mathbf{x}_{k+1}, \mathbf{z}_k, \lambda_k)$
$y = \mathbf{A}\mathbf{x}$	GAP	$\mathbf{x}_{k+1} = \mathbf{z}_k + \mathbf{A}^T(\mathbf{A}\mathbf{A}^T)^{-1}(\mathbf{y} - \mathbf{A}\mathbf{z}_k)$	$\mathbf{z}_{k+1} = \arg \min_x R(\mathbf{x}_{k+1})$
	AMP	$\mathbf{z}_k = \mathbf{y} - \mathbf{A}\mathbf{x}_k + \frac{1}{\delta} \mathbf{z}_{k-1} \Re(\mathbf{x}_{k-1} + \mathbf{A}^* \mathbf{z}_{k-1})$	$\mathbf{x}_{k+1} = \Re(\mathbf{x}_k + \mathbf{A}^* \mathbf{z}_k)$
	RED	$\mathbf{x}_{k+1} = \mathbf{x}_k - \mu \left[\frac{1}{\sigma^2} \mathbf{A}^T(\mathbf{A}\mathbf{x}_k - \mathbf{y}) + \lambda(\mathbf{x}_k - \mathbf{x}_{k+1}) \right]$	$\mathbf{x}_{k+1} = \Re(\mathbf{x}_k)$

4.2 深度正则算子

伴随着图像分辨率和数据量的快速增加,去噪器需要在去噪速度和去噪质量之间进行权衡。传统的基于非局部自相似性的去噪器虽然去噪效果较好,但其中块匹配操作会消耗大量时间和内存资源^[90],不利于大规模重建。近年来发展出的基于深度学习技术的去噪器能够有效解决速度和质量的权衡问题,且即插即用优化重建相比传统去噪器具有显著的优势^[71]。随着深度学习理论的发展,深度神经网络已成为解决计算重建问题的热点方法之一。LeCun 等^[48]提出卷积神经网络(CNN)并利用 CNN 解决了手写数字识别问题,推动了深度学习理论真正走向实用化。2009 年 Deng 等^[91]搜集了 ImageNet 大规模图像数据集,为统计学习与神经网络的发展提供了坚实的数据基础。2016 年深度残差网络 ResNet^[92]的提出标志着 CNN 迈向了大规模时代,深度神经网络开始蓬勃发展。至今,深度神经网络已经不限于卷积网络结构,还包括循环(recurrent)网络结构^[93]、基于注意力(attention)机制^[94-95]的结构以及基于多层感知机(MLP)^[96]的深度网络结构。2015 年 Liang 等^[97]与 Xu 等^[98]提出基于深度卷积神经网络的图像去噪方法。2017 年 Zhang 等^[99]提出了应用于高斯去噪、超分辨以及 JPEG 图像增强等低层视觉任务的深度卷积网络(DnCNN),DnCNN 利用批归一化层^[100]与残差学习^[92]加速收敛,提高去噪性能。Bae 等^[101]、Wang 等^[102]、Jifara 等^[103]也验证了残差学习在深度网络去噪上的有效性。

2017 年 Zhang 等^[99,104]在去噪网络中引入噪声引导图(noise map),用于调控网络的去噪程度,允许用户人为权衡图像平滑程度和细节保留程度,进一步拓展了神经网络去噪的自由度。2019 年 Guo 等^[105]利用网

络生成噪声引导图,将噪声引导图与含噪图像同时送入去噪网络模块进行去噪。对于非成对噪声数据集,Chen 等^[106]利用生成对抗网络估计图像的噪声分布,并利用无噪图与噪声分布生成有噪图-无噪图数据对用于训练神经网络。对于数据较少的场景如高光谱图像去噪,Yuan 等^[107]利用多尺度网络结构与残差学习提高网络泛化性。合适的网络架构对提升图像质量具有重要的意义^[108],随着网络架构的丰富,去噪网络的结构越来越多元^[109-112]。

由于 DnCNN 提出时间较早,泛化性较强,所以 prDeep^[71]首次将 DnCNN 作为深度正则项使用。Yuan 等^[90]利用 FFDNet 作为深度正则项,如图 8 所示,该架构充分利用了 FFDNet 根据噪声引导图生成清晰图像的优势,将去噪项权重作为引导图参数,并且去噪项权重随着迭代逐渐收敛而递减。相比于传统的正则项,FFDNet 计算复杂度更低且重建质量更高,所以普遍应用于大规模计算重建。Chang 等^[6]利用基于 FFDNet 的即插即用优化方法实现了分钟级 8K 分辨率(7680×4320)的大规模相位成像,如图 9 所示。表 3 展示了近年来不同应用场景下即插即用优化框架与多种深度去噪器组合的尝试。即插即用优化重建对深度正则去噪网络具有较高的要求,深度正则网络应具有低计算复杂度和强鲁棒性。低计算复杂度保证了大规模计算重建的效率,深度正则网络可以从深度神经网络结构的发展中获取灵感,建立轻量级高精度的去噪网络。强鲁棒性使深度网络可以应用于多种成像系统与目标场景,一般去噪网络使用大规模数据集训练,保证网络的泛化性与鲁棒性。

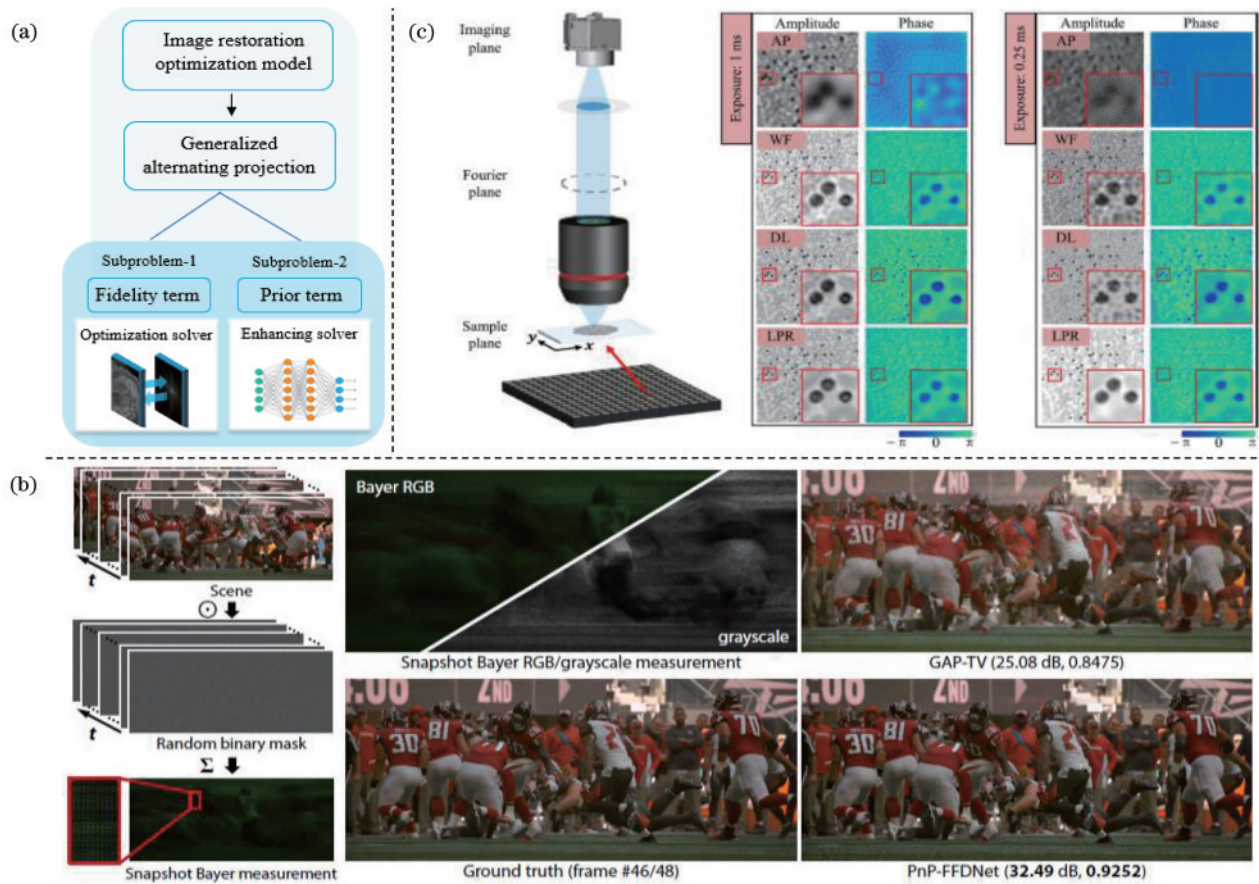


图 8 基于 GAP 框架的即插即用优化架构与应用。(a) 基于 GAP 的即插即用优化框架；(b)(c) 即插即用优化与其他算法在大规模快照压缩成像与傅里叶叠层显微成像上的对比^[6,90]

Fig. 8 Framework and applications of the PnP-GAP optimization. (a) Diagram of plug-and-play optimization framework based on GAP; (b) (c) comparison of large-scale snapshot compressive imaging and Fourier ptychographic microscopy between plug-and-play optimization and other methods, respectively^[6,90]

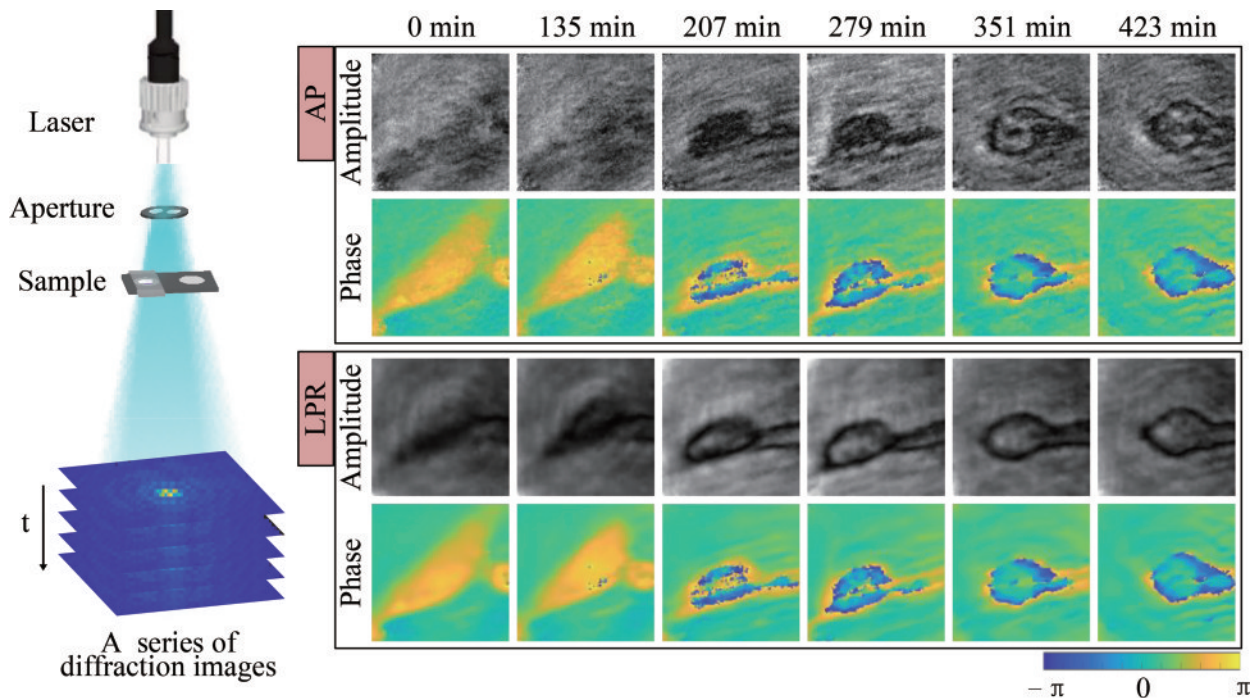


图 9 基于 GAP 的即插即用优化框架观测活的胶质母细胞融合过程^[6]

Fig. 9 Fusion process of living glioblastoma observed by using plug-and-play optimization framework based on GAP^[6]

表 3 即插即用优化框架及应用场景

Table 3 Plug-and-play optimization frameworks and their applications

Algorithm	Framework	Denoiser	Application
Algorithm in Ref. [75]	ADMM	BM3D	Tomography
Algorithm in Ref. [71]	FISTA(FASTA)	DnCNN	CDI & CDP
Algorithm in Ref. [74]	SGD & FISTA	TV & BM3D	FPM
Algorithm in Ref. [77]	ADMM	DnCNN	Tomography
Algorithm in Ref. [73]	ADMM & FISTA	DnCNN & MemNet & Residual Unet	MRI & CDP
Algorithm in Ref. [113]	GD	BM3D & FFDNET	CDP
Algorithm in Ref. [114]	RED	NLM & BM3D	Denoising & SR & Deblurring
Algorithm in Ref. [68]	HQS	SRResNet	SR
Algorithm in Ref. [90]	GAP	FFDNET	SCI
Algorithm in Ref. [115]	ADMM	DnCNN	CDI
Algorithm in Ref. [77]	GD	DnCNN	Tomography
Algorithm in Ref. [88]	ISTA	NLM	Inpainting & Deblurring
Algorithm in Ref. [116]	ADMM	BM3D	Hyperspectral PR
Algorithm in Ref. [6,117]	GAP	FFDNET	CDI & CDP & FPM & Pixel SR
Algorithm in Ref. [118]	GEC	Modified DnCNN	MRI

5 总结与展望

大规模计算重建需同时满足高精度、低复杂度以及适用不同系统的灵活性的要求。总结梳理了 3 类具有高精度大规模重建潜力的方法:交替投影算法、深度图像先验算法与即插即用算法。交替投影算法作为一种简单高效的方法在宽视场高分辨率相位成像领域已经获得广泛的应用,然而噪声鲁棒性较差,易陷于局部最优解;深度图像先验算法和即插即用算法得益于近年来深度学习理论与技术的发展,将深层神经网络与传统优化方法有机地结合起来,规避了端到端深度学习面临的大规模训练数据获取与模型训练耗时的问题,但由于神经网络“黑盒子”的特性,其可解释性相比传统优化方法较差。3 类算法在一定程度上实现了大规模计算重建,但由于模型项与先验项均存在建模精度与计算解耦效率的固有矛盾,难以同时满足大规模数据重建的快速和高精度要求。综合考虑当下技术瓶颈以及研究热点,本文总结分析了未来大规模计算重建的潜在发展方向。

1) 提高大规模计算重建的灵活性

高灵活性的大规模重建算法应具有“举一反三”的能力,能快速适配不同的系统以及系统参数。提高大规模重建算法的灵活性可诉诸机器学习领域的研究方向:一是借鉴深度学习理论中的迁移学习策略,利用已有问题的模型求解其他不同但相关的问题,例如深度域适应技术^[119]等,提高重建算法对不同参数域的适应能力;二是重建-增强模式,将计算重建算法分为两部分,重建部分依赖对物理模型的求解,增强部分是基于人工设计或统计的图像先验继续提升重建效果的,可适用于不同成像系统。重建-增强模式已应用在全息

成像^[120]、低光相位恢复^[121]等领域,但其增强部分仍依赖于特定模型下的统计特性。未来能够处理复杂降质过程的通用增强算法可以显著提高重建-增强式计算重建的灵活性。

2) 提高大规模计算重建的效率

大规模计算重建可以从自适应重建、架构精简和工程优化等三个角度提升重建效率。生物视觉系统往往更加关注语义或细节丰富的区域,从而大幅度地降低了功耗。受此启发,可以针对性地发展智能化大规模重建技术,集中主要计算资源,处理感兴趣区域或语义信息丰富区域,实现自适应重建,如傅里叶域^[122]与小波域^[123]自适应重建等。未来上述自适应策略亦可与深度学习技术相结合,借鉴 Nonlocal network^[124]或 Transformer^[125]等的注意力机制,直接或间接地利用神经网络中的注意力模型处理重点区域。在重建架构精简方面,可以针对特定的场景或样本,利用剪枝、低秩分解、量化、知识蒸馏^[126]等模型压缩技术设计专用轻量化模型,减小计算负担。在工程实现阶段,利用边缘计算^[127]或分布式架构^[128]分解复杂任务,充分利用计算资源,结合嵌入式、并行计算技术等进一步优化底层架构,精简指令集,能够在部署应用端大幅提升大规模重建的效率。

3) 提高大规模计算重建的精度

提高大规模重建算法的精度需要充分挖掘潜在的高维先验信息。现有重建算法大多基于通用的图像先验,如全变分^[129]、域稀疏先验^[122]、非局部先验^[130]或数据驱动的统计先验^[21,88],较少考虑成像系统的物理特性。未来可将通用图像先验与物理模型深度融合,设计符合成像系统特性的专用先验正则,从而进一步提升重建精度。对于常规物理模型有较大误差或者难以

显式建模的场景,需纠正简化模型带来的误差,或以全参数建模的形式^[131]准确表征成像过程中存在的干扰与噪声,有效避免系统误差引起的精度退化。此外,借鉴神经结构搜索(NAS)^[132]或强化学习^[133]的思想,智能化、自动化地构建最适合特定成像任务的模型架构与模型参数,也是提升大规模计算重建精度的可行研究方向。

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