# Plug-and-Play: Algorithms, Parameters Tuning and Interpretation

Zhonglin Xie

Peking University

February 28, 2022

## Linear Inverse Problem

#### • Formulation:

$$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{w}, \quad \boldsymbol{w} \sim \mathcal{N}\left(\boldsymbol{0}, \sigma^{2}\boldsymbol{I}\right),$$

where A is a known block-diagonal matrix, and w denotes Gaussian random vector with mean **0** and covariance  $\sigma^2 I$ .

- Aim: Recovery  $\boldsymbol{x}$  from  $\boldsymbol{y}$ .
- Application: Magnetic Resonance Imaging (MRI).

### Signal Recovery and Denoising

• The maximum likelihood (ML) estimate:

$$\widehat{\boldsymbol{x}}_{\mathrm{ml}} \triangleq \operatorname*{argmax}_{x} p(\boldsymbol{y} \mid \boldsymbol{x}),$$

where  $p(\boldsymbol{y} \mid \boldsymbol{x})$ , the probability density of  $\boldsymbol{y}$  conditioned on  $\boldsymbol{x}$ , is known as the likelihood function.

• The equivalent form:

$$\widehat{\boldsymbol{x}}_{\mathrm{ml}} = \operatorname*{argmin}_{x} \{-\ln p(\boldsymbol{y} \mid \boldsymbol{x})\}.$$

• In the case of additive white Gaussian noise (AWGN)  $\mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$ , we have

$$-\ln p(\boldsymbol{y} \mid \boldsymbol{x}) = \frac{1}{2\sigma^2} \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|_2^2 + \text{const.}$$

## Maximum A Posteriori (MAP)

- $\blacksquare$  Since  $\boldsymbol{A}$  is fat, we can not perform least-squares estimation.
- Use a regularization term  $\phi(\boldsymbol{x})$  to encode priori knowledge:

$$\widehat{\boldsymbol{x}} = \operatorname*{argmin}_{\boldsymbol{x}} \left\{ \frac{1}{2\sigma^2} \| \boldsymbol{y} - \boldsymbol{A} \boldsymbol{x} \|_2^2 + \phi(\boldsymbol{x}) 
ight\}.$$

Bayes rule implies

$$\ln p(\boldsymbol{x} \mid \boldsymbol{y}) = \ln p(\boldsymbol{y} \mid \boldsymbol{x}) + \ln p(\boldsymbol{x}) - \ln p(\boldsymbol{y}).$$

• The maximum a posteriori (MAP) estimate:

$$\widehat{\boldsymbol{x}}_{\max} = \underset{\boldsymbol{x}}{\operatorname{argmin}} \{ -\ln p(\boldsymbol{y} \mid \boldsymbol{x}) - \ln p(\boldsymbol{x}) \}.$$

•  $\widehat{x}$  can be recognized as  $\widehat{x}_{map}$  with  $p(x) \propto \exp(-\phi(x))$ .

# More on $\phi(\boldsymbol{x})$

- $\phi(\boldsymbol{x})$  should mimic the negative log of the prior density.
- $\phi(\mathbf{x})$  must enable tractable optimization.
- Common choice:  $\phi(\boldsymbol{x}) = \lambda \| \Psi \boldsymbol{x} \|_1$ , where  $\Psi^{\dagger} \Psi = \boldsymbol{I}, \lambda > 0$ .
- Advantages: The problem remains convex. The transform output Ψx is sparse.

### Denoising

• When A = I, the linear inverse problem reduces to

$$oldsymbol{z} = oldsymbol{x} + oldsymbol{w}, \quad oldsymbol{w} \sim \mathcal{N}\left(oldsymbol{0}, \sigma^2 oldsymbol{I}
ight).$$

Recovering  $\boldsymbol{x}$  from noisy  $\boldsymbol{z}$  is known as **denoising**.

- State-of-the-art approaches are either algorithmic or neural.
- Can these state-of-the-art denoisers be leveraged for MRI?

## PnP-ADMM

 $\blacksquare \ \widehat{x}$  can be derived from an equivalent optimization

$$(\widehat{\boldsymbol{x}}, \widehat{\boldsymbol{v}}) = \operatorname*{arg\,min}_{\boldsymbol{x}, \boldsymbol{v} \in \mathbb{R}^n} \frac{1}{2\sigma^2} \| \boldsymbol{y} - \boldsymbol{A} \boldsymbol{x} \|_2^2 + \phi(\boldsymbol{v}), \quad \text{s.t. } \boldsymbol{x} = \boldsymbol{v}.$$

• The augmented Lagrangian:

$$\begin{split} L(\boldsymbol{x}, \boldsymbol{v}; \boldsymbol{\lambda}) &= \frac{1}{2\sigma^2} \| \boldsymbol{y} - \boldsymbol{A} \boldsymbol{x} \|_2^2 + \phi(\boldsymbol{v}) - \boldsymbol{\lambda}^{\mathsf{T}} (\boldsymbol{x} - \boldsymbol{v}) + \frac{1}{2\eta} \| \boldsymbol{x} - \boldsymbol{v} \|_2^2 \\ &= \frac{1}{2\sigma^2} \| \boldsymbol{y} - \boldsymbol{A} \boldsymbol{x} \|_2^2 + \phi(\boldsymbol{v}) + \frac{1}{2\eta} \| \boldsymbol{x} - \boldsymbol{v} + \boldsymbol{u} \|_2^2, \end{split}$$

where  $\boldsymbol{u} = \eta \boldsymbol{\lambda}$ .

### ADMM

Alternating the optimization of x, v with gradient ascent of u:

$$egin{aligned} oldsymbol{x}_k &= oldsymbol{h} \left(oldsymbol{v}_{k-1} - oldsymbol{u}_{k-1}; \sigma^2/\eta
ight) \ oldsymbol{v}_k &= \mathrm{prox}_\phi \left(oldsymbol{x}_k + oldsymbol{u}_{k-1}; \eta
ight) \ oldsymbol{u}_k &= oldsymbol{u}_{k-1} + \left(oldsymbol{x}_k - oldsymbol{v}_k
ight) \end{aligned}$$

where

$$\begin{aligned} \operatorname{prox}_{\phi}(\boldsymbol{z};\eta) &\triangleq \operatorname*{arg\,min}_{\boldsymbol{x} \in \mathbb{R}^{n}} \phi(\boldsymbol{x}) + \frac{1}{2\eta} \|\boldsymbol{x} - \boldsymbol{z}\|^{2}, \\ \boldsymbol{h}(\boldsymbol{z};\sigma^{2}/\eta) &\triangleq \operatorname*{arg\,min}_{\boldsymbol{x} \in \mathbb{R}^{n}} \frac{1}{2\sigma^{2}} \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|^{2} + \frac{1}{2\eta} \|\boldsymbol{x} - \boldsymbol{z}\|^{2} \\ &= \left(\boldsymbol{A}^{\mathsf{T}}\boldsymbol{A} + \frac{\sigma^{2}}{\eta}\boldsymbol{I}\right)^{-1} \left(\boldsymbol{A}^{\mathsf{T}}\boldsymbol{y} + \frac{\sigma^{2}}{\eta}\boldsymbol{z}\right). \end{aligned}$$

## PnP-ADMM

- $\operatorname{prox}_{\phi}(\boldsymbol{z};\eta)$  can be **recognized** as the MAP **denoiser** of  $\boldsymbol{z}$ .
- PnP plug in a image denoiser in place of the  $\text{prox}_{\phi}(\boldsymbol{z}; \eta)$ .
- Denoting the denoiser as  $f(\cdot; \eta)$ , PnP-ADMM writes:

$$egin{aligned} oldsymbol{x}_k &= oldsymbol{h} \left(oldsymbol{v}_{k-1} - oldsymbol{u}_{k-1}; \sigma^2/\eta
ight) \ oldsymbol{v}_k &= oldsymbol{f} \left(oldsymbol{x}_k + oldsymbol{u}_{k-1}; \eta
ight) \ oldsymbol{u}_k &= oldsymbol{u}_{k-1} + \left(oldsymbol{x}_k - oldsymbol{v}_k
ight) \end{aligned}$$

- The fixed point of the ADMM is independent of  $\eta$ , while  $\eta$  affects the fixed-point of the PnP-ADMM.
- To promote the PnP-ADMM, we until the parameters:

$$egin{aligned} oldsymbol{x}_k &= oldsymbol{h} \left(oldsymbol{v}_{k-1} - oldsymbol{u}_{k-1}; \mu_k 
ight) \ oldsymbol{v}_k &= oldsymbol{f} \left(oldsymbol{x}_k + oldsymbol{u}_{k-1}; \eta_k 
ight) \ oldsymbol{u}_k &= oldsymbol{u}_{k-1} + \left(oldsymbol{x}_k - oldsymbol{v}_k 
ight) \end{aligned}$$

## Discussion: The Effects of the Denoising Strength $\eta$

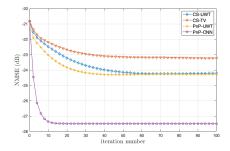
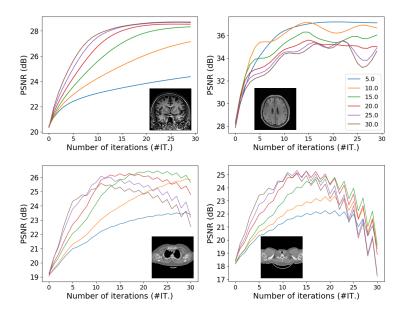


Figure: The normalized mean-squared error (NMSE) versus iteration.

ADMMPnP-ADMM

### The Effects of the Denoising Strength $\eta_k$



## **RL** Formulation for Automated Parameter Selection

- Motivation:  $\eta, \mu$  affect the result of the PnP-ADMM.
- Manually tuned parameters are time-cost.
- Aim: automatically select

 $\tau$  and  $(\eta_0, \mu_0, \eta_1, \mu_1, \cdots, \eta_{\tau-1}, \mu_{\tau-1})$ 

to recover  $\boldsymbol{x}_{\tau}$  that close to  $\boldsymbol{x}$ .

■ Tool: Reinforcement Learning (RL).

## Markov decision process (MDP) $(\mathcal{S}, \mathcal{A}, p, r)$

- State space S: any feasible value of  $(\boldsymbol{x}_k, \boldsymbol{v}_k, \boldsymbol{u}_k)$ .
- Action space  $\mathcal{A}$ : any feasible value of  $\tau$  and  $(\mu_k, \eta_k)$ .
- Transition function  $p: \mathcal{S} \times \mathcal{A} \to \mathcal{S}$

several iterations of the PnP-ADMM.

• Reward function  $r: \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ 

$$r(s_t, a_t) = [\zeta(p(s_t, a_t)) - \zeta(s_t)] - \eta.$$

 $\zeta(s_t)$ : the PSNR of the recovered image at step t.  $\eta$ : penalizing the policy as it does not terminate at step t.

## Workflow of TFPnP

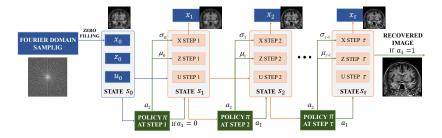


Figure: Workflow of the TFPnP instantiated by the PnP-ADMM.

### Formal Definition of the Goal

• 
$$s_k = (x_k, v_k, u_k), a_k = (a_{k,1}, a_{k,2}), r_k = r(s_k, a_k).$$

•  $a_{k,2} = (\mu_k, \eta_k)$ .  $a_{k,1}$  is a boolean that terminates the iterate at step k when  $a_{k,1} = 0$  and versus verse.

- Trajectory:  $T = \{s_0, a_0, r_0, \cdots, s_N, a_N, r_N\}.$
- Given T and  $\rho \in [0, 1]$ , define the return as

$$R_t = \sum_{t'=0}^{N-t} \rho^{t'} r\left(s_{t+t'}, a_{t+t'}\right).$$

• Goal: learn a policy  $\pi$  to maximize

$$J(\pi) = \mathbb{E}_{s_0,\pi} \left[ R_0 \right], \quad \pi(a \mid s) : \mathcal{S} \times \mathcal{A} \to [0, 1].$$

**RL-based** Policy Learning

■ State-value function:

$$V^{\pi}(s) = \mathbb{E}_{\pi} \left[ R_0 \mid s_0 = s \right]$$

• Action-value function:

$$Q^{\pi}(s,a) = \mathbb{E}_{\pi} [R_0 \mid s_0 = s, a_0 = a]$$

• Policy:  $\pi = (\pi_1, \pi_2)$ .

 $\pi_1$ : a **stochastic** policy that generate  $a_{t,1}$  to decide whether to terminate.

 $\pi_2$ : a **deterministic** policy that generate  $a_{t,2}$ .

### Actor-critic Framework

- Policy network (actor):  $\pi_{\theta} = (\pi_1, \pi_2)$  with  $\theta = (\theta_1, \theta_2)$ .  $\pi_1(\cdot \mid s)$ :  $\mathcal{S} \times \{0, 1\} \rightarrow [0, 1]$ , controlled by  $\theta_1$ .  $\pi_2(s)$ :  $\mathcal{S} \rightarrow \mathcal{A}$ , controlled by  $\theta_2$ .
- Value network (critic):  $V_{\phi}^{\pi}(s_t)$ .
- Train the value network:

$$L_{\phi} = \mathbb{E}_{s \sim B, a \sim \pi_{\theta}(s)} \left[ \frac{1}{2} \left( r(s, a) + \gamma V_{\hat{\phi}}^{\pi}(p(s, a)) - V_{\phi}^{\pi}(s) \right)^2 \right]$$

• Model-free training of  $\pi_1$ :

$$\nabla_{\theta_{1}} J(\pi_{\theta}) = \mathbb{E}_{s \sim B, a \sim \pi_{\theta}(s)} \left[ \nabla_{\theta_{1}} \log \pi_{1} \left( a_{1} \mid s \right) A^{\pi}(s, a) \right]$$

• Model-based training of  $\pi_2$ :

$$\nabla_{\theta_2} J(\pi_{\theta}) = \mathbb{E}_{s \sim B, a \sim \pi_{\theta}(s)} \left[ \nabla_{a_2} Q^{\pi}(s, a) \nabla_{\theta_2} \pi_2(s) \right]$$

## Training Scheme

#### Algorithm 1 Training Scheme

**Require:** Image dataset D, degradation operator  $g(\cdot)$ , learning rates  $l_{\theta}$ ,  $l_{\phi}$ , weight parameter  $\beta$ . 1: Initialize network parameters  $\theta$ ,  $\phi$ ,  $\hat{\phi}$  and state buffer B. for each training iteration do 2: 3: sample initial state  $s_0$  from D via  $q(\cdot)$ for environment step  $t \in [0, N)$  do 4: 5:  $a_t \sim \pi_{\theta}(a_t|s_t)$  $s_{t+1} \sim p(s_{t+1}|s_t, a_t)$ 6:  $B \leftarrow B \cup \{s_{t+1}\}$ 7: 8: break if the boolean outcome of  $a_t$  equals to 1 end for 9: for each gradient step do  $10 \cdot$ 11: sample states from the state buffer B $\theta_1 \leftarrow \theta_1 + l_\theta \nabla_{\theta_1} J(\pi_\theta)$ 12:  $\theta_2 \leftarrow \theta_2 + l_\theta \bigtriangledown_{\theta_2} J(\pi_\theta)$ 13: $\phi \leftarrow \phi - l_{\phi} \nabla_{\phi} L_{\phi}$ 14:  $\hat{\phi} \leftarrow \beta \phi + (1 - \beta) \hat{\phi}$ 15:16:end for 17: end for

**Ensure:** Learned policy network  $\pi_{\theta}$ 

## Experiment Results: CS-MRI

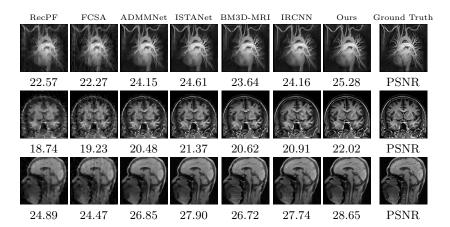


Figure: Visual and numerical CS-MRI reconstruction comparison against the state-of-the-art techniques on medical images. The numerical values denote the PSNR obtained by each technique.

## Rethinking of the PnP-ADMM: On Derivation

- **f** is not the proximal map of any regularizer  $\phi$ .
- f coincides with  $prox_{\phi}(\boldsymbol{z}; \eta)$  only when

$$p(\boldsymbol{x}) \propto \exp(-\phi(\boldsymbol{x})), \quad \boldsymbol{z} - \boldsymbol{z}_{\text{true}} \sim \mathcal{N}(\boldsymbol{0}, \eta^2 \boldsymbol{I}).$$

■ However, p(x) may **not** prompt to  $\exp(-\phi(x))$  and the distribution of

$$(\boldsymbol{x}_k + \boldsymbol{u}_{k-1}) - (\boldsymbol{x}_k + \boldsymbol{u}_{k-1})_{ ext{true}}$$

#### is **unknown**!

• PnP-ADMM is a result of the similarity of the formulation.

## Rethinking of the PnP-ADMM: On Convergence

- PnP-ADMM may not be an implementation of ADMM.
- If the PnP-ADMM converges?
- If it does converge, what it converges to?

### PnP FISTA

$$\begin{split} \min_{\boldsymbol{x}} \ \frac{1}{2\sigma^2} \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|_2^2 + \phi(\boldsymbol{x}) \\ \boldsymbol{z}_k &= \boldsymbol{s}_{k-1} - \frac{\eta}{\sigma^2} \boldsymbol{A}^{\mathsf{T}} \left( \boldsymbol{A} \boldsymbol{s}_{k-1} - \boldsymbol{y} \right) \quad \boldsymbol{z}_k = \boldsymbol{s}_{k-1} - \frac{\eta}{\sigma^2} \boldsymbol{A}^{\mathsf{T}} \left( \boldsymbol{A} \boldsymbol{s}_{k-1} - \boldsymbol{y} \right) \\ \boldsymbol{x}_k &= \operatorname{prox}_{\phi}(\boldsymbol{z}_k; \eta) \quad \boldsymbol{x}_k = \boldsymbol{f} \left( \boldsymbol{z}_k \right) \\ \boldsymbol{s}_k &= \boldsymbol{x}_k + \frac{q_{k-1} - 1}{q_k} \left( \boldsymbol{x}_k - \boldsymbol{x}_{k-1} \right) \quad \boldsymbol{s}_k = \boldsymbol{x}_k + \frac{q_{k-1} - 1}{q_k} \left( \boldsymbol{x}_k - \boldsymbol{x}_{k-1} \right) \\ \end{split}$$
FISTA PnP FISTA

where it is typical to use  $q_k = \left(1 + \sqrt{1 + 4q_{k-1}^2}\right)/2$  and  $q_0 = 1$  with step-size  $\eta \in \left(0, \sigma^2 \|A\|_2^{-2}\right)$ .

Regularization by Denoising (RED)

Recover x from measurements y by solving

$$\mathbf{0} = \frac{1}{\sigma^2} \mathbf{A}^{\mathsf{T}} (\mathbf{A} \widehat{\mathbf{x}} - \mathbf{y}) + \frac{1}{\eta} (\widehat{\mathbf{x}} - \mathbf{f}(\widehat{\mathbf{x}})).$$

- f is an arbitrary image denoiser.
- When f is a sophisticated denoiser and  $\eta$  is well tuned, the solutions  $\hat{x}$  are state-of-the-art.

## **RED**: Assumptions

Define

$$ho_{ ext{RED}}(oldsymbol{x}) riangleq rac{1}{2} \langle oldsymbol{x}, oldsymbol{x} - oldsymbol{f}(oldsymbol{x}) 
angle, \quad \ell(oldsymbol{x};oldsymbol{y}) = rac{1}{2\sigma^2} \|oldsymbol{y} - oldsymbol{A}oldsymbol{x}\|_2^2.$$

We get

$$\widehat{oldsymbol{x}}_{ ext{RED}} = rgmin_{oldsymbol{x} \in \mathbb{R}^n} \ \ell(oldsymbol{x};oldsymbol{y}) + 
ho_{ ext{RED}}(oldsymbol{x}).$$

The denoiser f(x) obeys the following assumption:

**1** Local Homogeneity:

$$\boldsymbol{f}((1+\varepsilon)\boldsymbol{x}) = (1+\varepsilon)\boldsymbol{f}(\boldsymbol{x}), \quad \forall \boldsymbol{x} \in \mathbb{R}^n, 0 < \varepsilon \ll 1.$$

2 f(·) is differentiable where Jf ∈ ℝ<sup>n×n</sup> denotes its Jacobian.
3 Jacobian Symmetry: Jf(x)<sup>T</sup> = Jf(x), ∀x ∈ ℝ<sup>n</sup>.

**4** The spectral radius the Jacobian satisfies  $\eta(Jf(x)) \leq 1$ .

### **RED:** Proof

• From the multivariate calculus:

$$abla 
ho_{\text{RED}}(\boldsymbol{x}) = \boldsymbol{x} - \frac{1}{2}\boldsymbol{f}(\boldsymbol{x}) - \frac{1}{2}[J\boldsymbol{f}(\boldsymbol{x})]^{\mathsf{T}}\boldsymbol{x}.$$

• Local homogeneity implies [Jf(x)]x = f(x):

$$0 = \lim_{\varepsilon \to 0} \frac{\|\boldsymbol{f}(\boldsymbol{x} + \varepsilon \boldsymbol{x}) - \boldsymbol{f}(\boldsymbol{x}) - [J\boldsymbol{f}(\boldsymbol{x})]\boldsymbol{x}\varepsilon\|}{\|\varepsilon \boldsymbol{x}\|}$$
$$= \lim_{\varepsilon \to 0} \frac{\|(1 + \varepsilon)\boldsymbol{f}(\boldsymbol{x}) - \boldsymbol{f}(\boldsymbol{x}) - [J\boldsymbol{f}(\boldsymbol{x})]\boldsymbol{x}\varepsilon|}{\|\varepsilon \boldsymbol{x}\|}$$
$$= \lim_{\varepsilon \to 0} \frac{\|\boldsymbol{f}(\boldsymbol{x}) - [J\boldsymbol{f}(\boldsymbol{x})]\boldsymbol{x}\|}{\|\boldsymbol{x}\|}.$$

Jacobian symmetry gives ∇ρ<sub>RED</sub>(x) = x − f(x).
η(Jf(x)) ≤ 1 guarantees the convexity.

• When the denoiser  $\boldsymbol{f}(\cdot)$  is locally homogeneous, then

$$abla 
ho_{ ext{RED}}(oldsymbol{x}) = oldsymbol{x} - oldsymbol{f}(oldsymbol{x}) \quad \Leftrightarrow \quad Joldsymbol{f}(oldsymbol{x}) = [Joldsymbol{f}(oldsymbol{x})]^\intercal.$$

- When  $J \boldsymbol{f}(\cdot) \neq J \boldsymbol{f}(\cdot)^{\intercal}$ , there exists no regularizer  $\rho(\cdot)$  for which  $\nabla \rho(\boldsymbol{x}) = \boldsymbol{x} f(\boldsymbol{x})$ .
- Many popular denoisers lack symmetric Jacobian, making the gradient expression invalid.

### Proximal-based PnP v.s. RED: a Toy Example

• f(z) = Wz with  $W = W^{\top}$ .

*f* is the proximal map of φ(*x*) = (1/2η)*x*<sup>T</sup> (*W*<sup>-1</sup> − *I*) *x*.
Proximal-based PnP:

$$\widehat{oldsymbol{x}}_{ ext{pnp}} = \operatorname*{argmin}_{oldsymbol{x}} \left\{ rac{1}{2\sigma^2} \|oldsymbol{y} - oldsymbol{A}oldsymbol{x}\|^2 + rac{1}{2\eta}oldsymbol{x}^{ op} \left(oldsymbol{W}^{-1} - oldsymbol{I}
ight)oldsymbol{x} 
ight\}$$

RED:

$$\widehat{\boldsymbol{x}}_{\mathrm{red}} = \operatorname*{argmin}_{\boldsymbol{x}} \left\{ \frac{1}{2\sigma^2} \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|^2 + \frac{1}{2\eta} \boldsymbol{x}^\top (\boldsymbol{I} - \boldsymbol{W}) \boldsymbol{x} \right\}$$

## Algorithms for RED

- GD, inexact ADMM, and a "fixed-point" heuristic that was later recognized as a special case of the proximal gradient (PG) algorithm.
- Accelerated proximal gradient (fastest):

$$\begin{split} \boldsymbol{x}_{k} &= \boldsymbol{h} \left( \boldsymbol{v}_{k-1} ; \eta/L \right) \\ \boldsymbol{z}_{k} &= \boldsymbol{x}_{k} + \frac{q_{k-1}-1}{q_{k}} \left( \boldsymbol{x}_{k} - \boldsymbol{x}_{k-1} \right) \\ \boldsymbol{v}_{k} &= \frac{1}{L} \boldsymbol{f} \left( \boldsymbol{z}_{k} \right) + \left( 1 - \frac{1}{L} \right) \boldsymbol{z}_{k} \end{split}$$

where L > 0 is a design parameter that can be related to the Lipschitz constant of  $\phi_{\text{red}}$  (·).

### **RED** as Score Matching

Given a training set  $\{\boldsymbol{x}_t\}_{t=1}^T$ , the empirical prior model is

$$\widehat{p}(oldsymbol{x}) riangleq rac{1}{T} \sum_{t=1}^{T} \delta\left(oldsymbol{x} - oldsymbol{x}_{t}
ight)$$

Build a prior model using kernel density estimation (KDE):

$$\tilde{p}(\boldsymbol{x};\eta) \triangleq rac{1}{T} \sum_{t=1}^{T} \mathcal{N}\left(\boldsymbol{x}; \boldsymbol{x}_t, \eta \boldsymbol{I}\right)$$

• Adopting  $\tilde{p}$  as the prior, MAP becomes

$$\widehat{\boldsymbol{x}} = \operatorname*{argmin}_{\boldsymbol{x}} \frac{1}{2\sigma^2} \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|^2 - \ln \widetilde{p}(\boldsymbol{x};\eta)$$

### **RED** as Score Matching

**Because**  $\ln \tilde{p}$  is differentiable,  $\hat{x}$  must obey

$$\mathbf{0} = \frac{1}{\sigma^2} \mathbf{A}^{\top} (\mathbf{A} \widehat{\mathbf{x}} - \mathbf{y}) - \nabla \ln \widetilde{p}(\widehat{\mathbf{x}}; \eta)$$

•  $f_{\text{mmse}}(z; \eta) = \mathbb{E}[x|z]$ , where  $z = x + \mathcal{N}(0, \eta I), x \sim \hat{p}$ • Tweedie's formula says that

$$abla \ln \tilde{p}(oldsymbol{z};\eta) = rac{1}{\eta} \left( oldsymbol{f}_{ ext{mmse}}(oldsymbol{z};\eta) - oldsymbol{z} 
ight)$$

• The MAP estimate  $\hat{x}$  under the KDE prior  $\tilde{p}$  obeys

$$\mathbf{0} = \frac{1}{\sigma^2} \boldsymbol{A}^\top (\boldsymbol{A} \widehat{\boldsymbol{x}} - \boldsymbol{y}) + \frac{1}{\eta} \left( \widehat{\boldsymbol{x}} - \boldsymbol{f}_{\text{mmse}}(\widehat{\boldsymbol{x}}; \eta) \right)$$

which matches the RED condition when  $\boldsymbol{f} = \boldsymbol{f}_{\text{mmse}}(\cdot; \eta)$ 

# RED as Score Matching: $\boldsymbol{f} \neq \boldsymbol{f}_{\text{mmse}}(\cdot; \eta)$

- **f\_{\theta}**: neural denoiser parameterized by  $\theta$
- Training strategy:

 $\min_{\theta} \ \mathbb{E} \| \boldsymbol{x} - \boldsymbol{f}_{\theta}(\boldsymbol{z}) \|^2, \quad \text{where} \quad \boldsymbol{x} \sim \widehat{p}, \quad \boldsymbol{z} = \boldsymbol{x} + \mathcal{N}(\boldsymbol{0}, \eta \boldsymbol{I})$ 

MMSE orthogonality principle:

$$\begin{split} \mathbb{E} \| \boldsymbol{x} - \boldsymbol{f}_{\boldsymbol{\theta}}(\boldsymbol{z}) \|^2 = & \mathbb{E} \| \boldsymbol{x} - \boldsymbol{f}_{\text{mmse}}(\boldsymbol{z}; \boldsymbol{\eta}) \|^2 \\ & + \mathbb{E} \| \boldsymbol{f}_{\text{mmse}}(\boldsymbol{z}; \boldsymbol{\eta}) - \boldsymbol{f}_{\boldsymbol{\theta}}(\boldsymbol{z}) \|^2 \end{split}$$

■ Using Tweedie's formula, we get

$$\begin{split} \widehat{\boldsymbol{\theta}} &= \operatorname*{argmin}_{\boldsymbol{\theta}} \mathbb{E} \| \boldsymbol{x} - \boldsymbol{f}_{\boldsymbol{\theta}}(\boldsymbol{z}) \|^{2} \\ &= \operatorname*{argmin}_{\boldsymbol{\theta}} \mathbb{E} \| \boldsymbol{f}_{\mathrm{mmse}}(\boldsymbol{z}; \boldsymbol{\eta}) - \boldsymbol{f}_{\boldsymbol{\theta}}(\boldsymbol{z}) \|^{2} \\ &= \operatorname*{argmin}_{\boldsymbol{\theta}} \mathbb{E} \| \nabla \ln \widetilde{p}(\boldsymbol{z}; \boldsymbol{\eta}) - \frac{1}{\eta} \left( f_{\boldsymbol{\theta}}(\boldsymbol{z}) - \boldsymbol{z} \right) \|^{2} \end{split}$$

Choose  $\boldsymbol{\theta}$  so that  $(f_{\theta}(z) - z)/\eta$  matches the "score"  $\nabla \ln \tilde{p}$ 

### CE for Prox-based PnP

■ View Prox-based PnP as seeking a solution to

$$egin{aligned} \widehat{m{x}}_{ ext{pnp}} &= m{h}\left(\widehat{m{x}}_{ ext{pnp}} - \widehat{m{u}}_{ ext{pnp}};\eta
ight) \ \widehat{m{x}}_{ ext{pnp}} &= m{f}\left(\widehat{m{x}}_{ ext{pnp}} + \widehat{m{u}}_{ ext{pnp}}
ight) \end{aligned}$$

■ It equals to find a fixed point of

$$\underline{z} = (2\boldsymbol{G} - \boldsymbol{I})(2\mathcal{F} - \boldsymbol{I})\underline{z}$$

$$\underline{z} = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}, \quad \mathcal{F}(\underline{z}) = \begin{bmatrix} \boldsymbol{h}(z_1; \eta) \\ \boldsymbol{f}(z_2) \end{bmatrix}, \quad \mathcal{G}(\underline{z}) = \begin{bmatrix} (z_1 + z_2)/2 \\ (z_1 + z_2)/2 \end{bmatrix}$$

Mann iteration writes:

$$\underline{\boldsymbol{z}}^{(k+1)} = (1-\gamma)\underline{\boldsymbol{z}}^k + \gamma(2\boldsymbol{G}-\boldsymbol{I})(2\boldsymbol{\mathcal{F}}-\boldsymbol{I})\underline{\boldsymbol{z}}^{(k)}$$

### CE for RED

• CE for ADMM-based RED:

$$egin{aligned} \widehat{m{x}}_{\mathrm{red}} &= m{h}\left(\widehat{m{x}}_{\mathrm{red}} - \widehat{m{u}}_{\mathrm{red}}; \eta
ight) \ \widehat{m{x}}_{\mathrm{red}} &= \left(\left(1 + rac{1}{L}
ight)m{I} - rac{1}{L}m{f}
ight)^{-1}\left(\widehat{m{x}}_{\mathrm{red}} + \widehat{m{u}}_{\mathrm{red}}
ight) \end{aligned}$$

• A more intuitive form:

$$egin{aligned} \widehat{m{x}}_{\mathrm{red}} &= m{h}\left(\widehat{m{x}}_{\mathrm{red}} - \widehat{m{u}}_{\mathrm{red}}; \eta
ight) \ \widehat{m{x}}_{\mathrm{red}} &= m{f}\left(\widehat{m{x}}_{\mathrm{red}}
ight) + L\widehat{m{u}}_{\mathrm{red}} \end{aligned}$$

• Solving the first equation gives:

$$\widehat{\boldsymbol{u}}_{\mathrm{red}} = rac{\eta}{\sigma^2} \boldsymbol{A}^{\mathsf{T}} \left( \boldsymbol{y} - \boldsymbol{A} \widehat{\boldsymbol{x}}_{\mathrm{red}} 
ight)$$

Plugging  $\widehat{u}_{red}$  back:

$$\frac{L\eta}{\sigma^2} A^{\mathsf{T}} \left( A \widehat{\boldsymbol{x}}_{\text{red}} - y \right) = f\left( \widehat{\boldsymbol{x}}_{\text{red}} \right) - \widehat{\boldsymbol{x}}_{\text{red}}$$

RED via Fixed-point Projection (RED-PRO)

**RED-PRO** problem writes:

$$\hat{oldsymbol{x}}_{ ext{RED-PRO}} = rgmin_{oldsymbol{x} \in \mathbb{R}^n} \ell(oldsymbol{x};oldsymbol{y}), \quad ext{ s.t. } oldsymbol{x} \in ext{Fix}(oldsymbol{f}).$$

- Interpretation: searching for a minimizer of  $\ell(x; y)$  over the set of "clean" images.
- The manifold of natural images  $\mathcal{M}$  is generally not well-defined, it is not easy accessible and it is not convex, making the search within this domain difficult. Therefore, as an alternative, we propose to use  $\operatorname{Fix}(f)$  which is well-behaved for demicontractive denoisers and should satisfy  $\mathcal{M} \subset \operatorname{Fix}(f)$  for a "perfect" denoiser.
- Common denoisers are far from being ideal, hence, the solution is sensitive to the choice of the denoiser and it may vary considerably for different choices.

## *d*-demicontractive Mapping

A mapping T is d-demicontractive  $(d \in [0, 1))$  if for any  $\boldsymbol{x} \in \mathbb{R}^n$ and  $\boldsymbol{z} \in \text{Fix}(T)$  it holds that

$$||T(x) - z||^2 \le ||x - z||^2 + d||T(x) - x||^2$$

or equivalently

$$\frac{1-d}{2} \|\boldsymbol{x} - T(\boldsymbol{x})\|^2 \leq \langle \boldsymbol{x} - T(\boldsymbol{x}), \boldsymbol{x} - \boldsymbol{z} \rangle$$

## RED-PRO

- Assume the denoiser  $f(\cdot)$  is a *d*-demicontractive mapping. Then, RED-PRO defines a convex minimization problem.
- Consider a demicontractive denoiser  $f(\cdot)$  and assume f(0) = 0. Then,

$$ho_{ ext{RED}}(oldsymbol{x}) = rac{1}{2} \langle oldsymbol{x}, oldsymbol{x} - oldsymbol{f}(oldsymbol{x}) 
angle = 0 ext{ iff } oldsymbol{x} \in ext{Fix}(oldsymbol{f}).$$

• Hybrid steepest descent method for RED-PRO:

$$\begin{aligned} \boldsymbol{v}_{k+1} &= \boldsymbol{x}_k - \mu_k \nabla \ell \left( \boldsymbol{x}_k; \boldsymbol{y} \right), \\ \boldsymbol{z}_{k+1} &= f \left( \boldsymbol{v}_{k+1} \right), \\ \boldsymbol{x}_{k+1} &= (1-\alpha) \boldsymbol{v}_{k+1} + \alpha \boldsymbol{z}_{k+1}, \end{aligned}$$

• which is equivalent to

$$\boldsymbol{x}_{k+1} = f_{\alpha}(\boldsymbol{x}_k - \mu_k \nabla \ell(\boldsymbol{x}_k; \boldsymbol{y})), \text{ where } f_{\alpha} = (1 - \alpha) \mathrm{Id} + \alpha f.$$

## Uniform Algorithm Framework

• accelerated-PG (proximal gradient) RED algorithm, which uses the iterative update:

$$\begin{aligned} \boldsymbol{v}_{k+1} &= \boldsymbol{x}_{k} - \mu_{k} \nabla \ell \left( \boldsymbol{x}_{k}; \boldsymbol{y} \right), \\ \boldsymbol{z}_{k+1} &= \boldsymbol{v}_{k+1} + q_{k} \left( \boldsymbol{v}_{k+1} - \boldsymbol{v}_{k} \right), \text{ (FISTA-like acceleration)} \\ \boldsymbol{x}_{k+1} &= (1 - \alpha) \boldsymbol{z}_{k+1} + \alpha f \left( \boldsymbol{z}_{k+1} \right), \text{ (SOR-like acceleration)} \end{aligned}$$

- Thus, when we set  $q_k \equiv 0$ , i.e. when we skip the acceleration step, the above RED variant reduces to the iterative update of the Hybrid steepest for RED-PRO.
- When we continue and set  $\alpha = 1$ , we obtain the PnP-PGD method (Proximal-based).

Projection Gradient Descent

Projected Gradient Descent writes

$$\boldsymbol{x}_{k+1} = P_{\mathrm{Fix}(f)} \left( \boldsymbol{x}_k - \mu_k \nabla \ell(\boldsymbol{x}; y) \right)$$

• Replacing the projection operator  $P_{\text{Fix}(f)}(\cdot)$  with denoiser (Plug and Play)  $f(\cdot)$  we get PnP-PGD:

$$\boldsymbol{x}_{k+1} = f\left(\boldsymbol{x}_k - \mu_k \nabla \ell(\boldsymbol{x}; y)\right)$$

### Convergence Theorem

Let  $f(\cdot)$  be a continuous *d*-demicontractive denoiser and  $\ell(\cdot; \boldsymbol{y})$  be a proper convex lower semicontinuous differentiable function with *L*-Lipschitz gradient  $\nabla \ell(\cdot; \boldsymbol{y})$ . Assume the following:

(A1) 
$$\alpha \in (0, \frac{1-d}{2}).$$
  
(A2)  $\{\mu_k\}_{k \in \mathbb{N}} \subset [0, \infty)$  where  $\mu_k \xrightarrow[k \to \infty]{} 0$  and  $\sum_{k \in \mathbb{N}} \mu_k = \infty.$ 

Then, the sequence  $\{x_k\}_{k\in\mathbb{N}}$  generated by

$$\boldsymbol{x}_{k+1} = f_{\alpha}(\boldsymbol{x}_k - \mu_k \nabla \ell(\boldsymbol{x}_k; \boldsymbol{y})), \text{ where } f_{\alpha} = (1 - \alpha) \mathrm{Id} + \alpha f_{\alpha}$$

converges to an optimal solution of the RED-PRO problem:

$$\hat{\boldsymbol{x}}_{ ext{RED-PRO}} = \operatorname*{arg\,min}_{\boldsymbol{x} \in \mathbb{R}^n} \ell(\boldsymbol{x}; \boldsymbol{y}), \quad ext{ s.t. } \boldsymbol{x} \in ext{Fix}(f).$$

## Conclusion

There are various ways to model the denoising problem:

- PnP: Inspired by ADMM, Proximal gradient, while lacking objective function.
- **2** RED: Regularization by Denoising, while many denoisers do not satisfy the assumptions.
- **3** RED-PRO: require the denoisers to be demicontractive.

However, as pointed by, when applying practical algorithms (e.g. PnP-ADMM and PnP primal-dual hybrid gradient method (PnP-PDHG), satisfy the same fixed-point equation as PnP-PGM (Proximal Gradient Method)) to solve these models, different models have the same aim:

$$\boldsymbol{x}_* = f_{\alpha}(\boldsymbol{x}_* - \mu_k \nabla \ell(\boldsymbol{x}_*; \boldsymbol{y})), \text{ where } f_{\alpha} = (1 - \alpha) \mathrm{Id} + \alpha f.$$

Thus, we only need to guarantee the convergence of the above formulation.

## Future Directions

- RL for general parameters tuning
- The convergence theory of the PnP with weaker assumptions
- PnP for general ADMM-based algorithms