REGULARIZING (STABILIZING) DEEP LEARNING BASED RECONSTRUCTION ALGORITHMS

ABINASH NAYAK

Abstract. It’s well-known that inverse problems are ill-posed and to solve them meaningfully one has to employ regularization methods. Traditionally, popular regularization methods have been the penalized Variational approaches, also known as Tikhonov-type regularization. In recent years, the classical regularized-reconstruction approaches have been outclassed by the (deep-learning based) learned reconstruction algorithms. However, unlike the traditional regularization methods, the theoretical underpinnings, such as stability and regularization convergence, have been insufficient for such learned reconstruction algorithms. Hence, the results obtained from such algorithms, though empirically outstanding, can’t always be completely trusted, as they may contain certain instabilities or (hallucinated) features arising from the learned process. In fact, it has been shown that such learned algorithms are very susceptible to small (adversarial) noises in the data and can lead to severe instabilities in the recovered solution, which can be quite different from the inherent instabilities of the ill-posed (inverse) problem. Where as, the classical regularization methods can handle such (adversarial) noises very well and can produce stable recoveries. Here, we try to present certain regularization methods to stabilize such (unstable) learned reconstruction methods and recover a regularized solution, even in the presence of (adversarial) noises. For this, we need to extend the classical notion of regularization and incorporate it in the learned reconstruction algorithms. We also present some regularization techniques to regularize two of the most popular learned reconstruction algorithms, the Learned Post-Processing Reconstruction and the Learned Unrolling Reconstruction. We conclude with numerical examples validating the developed theories, i.e., showing instabilities in the learned reconstruction algorithms and providing regularization/stabilizing techniques to subdue them.

1. Classical Regularization

If the inverse problem, corresponding to the following forward equation

\[ Tx = y, \]  (1.1)

is ill-posed (in the sense of violating any of the Hadamard’s conditions for well-posedness: 1. Existence, 2. Uniqueness, and 3. Continuity), then one has to invoke certain regularization methods to recover a meaningful solution of (1.1).

As stated in [1], “a (convergent) regularization method” is defined as

\[ Date: September 1, 2021. 
2020 Mathematics Subject Classification. Primary 65K05, 65K10; Secondary 65R30, 65R32.
Key words and phrases. Inverse problems, Ill-posed problems, Regularization, Deep Learning Reconstruction, Instabilities, Post-Processing, Hallucinated features, Unrolling.

1

arXiv:2108.13551v1 [cs.LG] 21 Aug 2021
Definition 1.1. Let $T : \mathcal{X} \to \mathcal{Y}$ be a bounded linear operator between Hilbert spaces $\mathcal{X}$ and $\mathcal{Y}$, $\alpha_0 \in (0, +\infty]$. For every $\alpha \in (0, \alpha_0)$, let

$$R_\alpha : \mathcal{Y} \to \mathcal{X}$$

be a continuous (not necessarily linear) operator. The family $\{R_\alpha\}$ is called a regularization or a regularization operator (for $T^\dagger$, the pseudo-inverse of $T$), if, for all $y \in \mathcal{D}(T^\dagger)$, there exists a parameter choice rule $\alpha = \alpha(\delta, y_\delta)$ such that

$$\limsup_{\delta \to 0} \{||R_\alpha(\delta, y_\delta)y_\delta - T^\dagger y|| : y_\delta \in \mathcal{Y}, ||y_\delta - y|| \leq \delta\} = 0$$

holds. In addition,

$$\alpha : \mathbb{R}^+ \times \mathcal{Y} \to (0, \alpha_0)$$

is such that

$$\limsup_{\delta \to 0} \{\alpha(\delta, y_\delta) : y_\delta \in \mathcal{Y}, ||y_\delta - y|| \leq \delta\} = 0.$$ 

For a specific $y \in \mathcal{D}(T^\dagger)$, a pair $(R_\alpha, \alpha)$ is called a (convergent) regularization method (for solving $Tx = y$) if (1.3) and (1.5) hold.

The most popular way to formulate such a regularization method is known as

1.1. Variational/Penalized/Tikhonov- Regularization:

Here, one can define the regularization operator $R_\alpha$ as follows:

$$R_\alpha(y_\delta) := \arg\min_x D(Tx, y_\delta) + \alpha R(x),$$

where $D(Tx, y_\delta)$ is a discrepancy term (such as $||Tx - y_\delta||_Y$), $R(x)$ is a regularization term (like $||Lx - y_0||_Y$, for some smoothing operator $L : \mathcal{X} \to \mathcal{Y}$, or something else), and $\alpha \geq 0$ (the regularization parameter) balances between the data consistency term and the regularization term. Hence, a regularized solution, in this case, is given by $R_\alpha(\delta, y_\delta)(y_\delta)$, where $\alpha(\delta, y_\delta)$ is determined via a parameter choice rule, which satisfies (1.5), see [1] for details.

2. Learned Reconstruction and Regularization

With the advent of deep learning, the focus of solving an inverse problem has shifted from the traditional fashion towards the data-driven methods. That is, one can train a (deep) neural network $\mathcal{N}\mathcal{N}_\theta$, for a given set of training examples, so as to formulate a “reconstruction method” that enables to recover a solution of (1.1), for a given new data $y_\delta$ (that is outside of the training example set). In other words, given $\theta \in \mathbb{R}^d$, for some (high) dimension $d$, and neural-network structures $\mathcal{N}\mathcal{N}_\theta$ (depending on $\theta$), one has “a family of reconstruction methods”:

$$R(\mathcal{N}\mathcal{N}, \theta) := \mathcal{N}\mathcal{N}_\theta : \mathcal{Y} \to \mathcal{X}.$$ 

Now, fixing the structure of the neural network, one still gets “a family of reconstruction methods”, for $\theta \in \mathbb{R}^d$, for some $d$ (usually $>> 1$),

$$R_\theta := \mathcal{N}\mathcal{N}_\theta : \mathcal{Y} \to \mathcal{X}.$$ 

However, after training the network, one only has “a fixed reconstruction method”

$$R_{\theta_0} := \mathcal{N}\mathcal{N}_{\theta_0} : \mathcal{Y} \to \mathcal{X}.$$ 

Now, to connect the above reconstruction algorithms (which depends on high-dimensional parameters $\theta$) to the classical regularization methods (depending on a single dimensional parameter $\alpha$), one needs to first generalize the definition of
a convergent regularization method, Definition 1.1. Note that, from the definition 1.1, one would like to approximate (in some sense) the (discontinuous) operator $T$ via a family of continuous (not necessarily linear) operators $\{R_\alpha\}_{\alpha \geq 0}$ such that, for all $y \in \mathcal{D}(T)$ and $y_\delta \in \mathcal{Y}$, with $||y_\delta - y||_\mathcal{Y} \leq \delta$, we have
\[
\limsup_{\delta \to 0} ||R_\alpha(y_\delta) - T^\dagger y||_\mathcal{X} = 0 \quad (2.4)
\]
\[
\limsup_{\delta \to 0} \alpha(y_\delta) = 0. \quad (2.5)
\]

Now, by extending the condition (2.5), one can generalize the idea of the single-parameter regularization methods $\{R_\alpha\}_\alpha$, to multi-parameters reconstruction methods $\{R_\theta\}_\theta$, for $\theta \in \mathbb{R}^d$. Here, we can define a convergent regularization method as a collection of “continuous operator (not necessarily linear)” such that, for a parameter choice rule $\theta(\delta, y_\delta) : \mathbb{R}_+ \times \mathcal{Y} \to \mathbb{R}^d$, we have
\[
\limsup_{\delta \to 0} ||R_\theta(y_\delta) - T^\dagger y||_\mathcal{X} = 0 \quad (2.6)
\]
\[
\limsup_{\delta \to 0} ||\theta(y_\delta)||_{\mathbb{R}^d} = 0. \quad (2.7)
\]

However, the above extended definition (2.6) + (2.7) would not always work for a reconstruction method based on a neural network $\mathcal{NN}_\theta$, especially for those $\mathcal{NN}_\theta$ which collapses when $\theta$ satisfies (2.7). Hence, one can try to further generalize the concept of a convergent regularization method as, when $\delta \to 0$, we need to have (in some sense of convergence)
\[
R_\theta(\delta) \to T^\dagger, \quad (2.8)
\]
where $R_\theta(\delta)$ is a reconstruction method based on a training example set $\mathcal{E}_\delta := \{(x^i, y^i, y_{i\delta}^{ij})\}_{i,j=1}^{n,m}$, such that $Tx^i = y^i \in \mathcal{D}(T^\dagger)$ and $y_{i\delta}^{ij} \in \mathcal{Y}$, such that $||y_{i\delta}^{ij} - y^i||_\mathcal{Y} \leq \delta$, and $R_\theta(\delta)y_{i\delta}^{ij} = x^i$, for all $1 \leq i \leq n$ and $1 \leq j \leq m$.

The problem with this formulation is that, the reconstruction method $R_\theta(\delta)$ may not be continuous, i.e., if in the set of examples $\mathcal{E}_\delta$, there exists two points $x^{i_1}$ and $x^{i_2}$, such that $||x^{i_1} - x^{i_2}||_\mathcal{X} >> \delta$ but $||y^{i_1} - y^{i_2}||_\mathcal{Y} \leq \delta$, then the reconstruction method $R_\theta(\delta)$ is discontinuous, as $||R_\theta(\delta)y^{i_1} - R_\theta(\delta)y^{i_2}||_\mathcal{Y} >> \delta$. Consequently, although for the training examples, we have $R_\theta(\delta)y_{i\delta}^{i_1} = x^{i_1}$ and $R_\theta(\delta)y_{i\delta}^{i_2} = x^{i_2}$, for all $1 \leq j \leq m$, but, for a new $y_\delta = y^{i_1} + \epsilon_\delta \in \mathcal{Y}$ (outside of the training examples set) such that $||y^{i_1} - y_\delta||_\mathcal{Y} \leq \delta$, it is possible to have $||R_\theta(\delta)y_\delta - x^{i_1}||_\mathcal{X} >> \delta$ and $||R_\theta(\delta)y_\delta - x^{i_2}||_\mathcal{X} \leq C(\delta)$, i.e., closer to $x^{i_2}$ and farther from $x^{i_1}$ (true solution). Now, the same is also true even when the training set $\mathcal{E}_\delta$ does not have such pairs of $x^{i_1}$’s, but the operator behaves in that manner, i.e., if for a $x^{i_1} \in \mathcal{E}_\delta$, there exist a $x^{i_2} \in \mathcal{X}\setminus\mathcal{E}_\delta$ such that $||x^{i_1} - x^{i_2}||_\mathcal{X} >> \delta$ but $||Tx^{i_1} - Tx^{i_2}||_\mathcal{Y} \leq \delta$, then for a $y_\delta = Tx^{i_2} + \epsilon_\delta$, such that $||Tx^{i_1} - y_\delta||_\mathcal{Y} \leq \delta$, we can have $||R_\theta(\delta)y_\delta - x^{i_2}||_\mathcal{X} >> \delta$ and $||R_\theta(\delta)y_\delta - x^{i_1}||_\mathcal{X} \leq C(\delta)$. But, for an injective $T$ one can circumvent the above issue, as for any two $x^{i_1}, x^{i_2} \in \mathcal{X}$, there exist a $\delta_0 > 0$ such that $||Tx^{i_1} - Tx^{i_2}||_\mathcal{Y} > 2\delta_0$, and hence, $R_\theta(\delta)$ is continuous for all $\delta \leq \delta_0$, at least on the training example set $\mathcal{E}_\delta$. Thus, in such scenarios, if (2.8) holds and $R_\theta(\delta)$ generalize properly (i.e., $R_\theta(\delta)$ is also continuous on $\mathcal{X}\setminus\mathcal{E}_\delta$), then $(R_\theta, \theta(\delta))$ can be considered as a convergent regularization method. However, for a non-injective $T$ (i.e., non empty null space, $\mathcal{N}(T) \neq \emptyset$), this is not possible (following the above procedure), as there does not exist any $\delta_0 > 0$ for which $\forall x^{i_1}, x^{i_2} \in \mathcal{X}$, $||Tx^{i_1} - Tx^{i_2}||_\mathcal{Y} > 2\delta_0$. The instabilities arising in such scenarios are illustrated in [2].
Moreover, one (usually) doesn’t construct a family of trained neural networks \( \{ R_\theta(\delta) := \mathcal{N}_\theta(\delta) \}_\delta \geq 0 \), based on a family of training examples sets \( \{ \mathcal{E}_\delta \}_\delta \geq 0 \), depending on different noise levels \( \delta \), rather, one trains a neural network \( R_\theta := \mathcal{N}_\theta \) for various noise levels and hopes to obtain a regularized method for solving the inverse problem (1.1), for all noise levels. Therefore, this defies the very essence of a (classical) convergent regularization method, which depends on a family of continuous operators designed to converge (in some sense) to the pseudo-inverse, when the noise level in the data goes to zero.

3. Generating regularization methods from \( R_\theta \)

Here, we suggest certain techniques to formulate a convergent regularization method, for solving the inverse problem (1.1), when given a pre-trained/learned reconstruction method \( R_\theta := Y \mapsto X \). First, note that, the keys to a convergent regularization method are the following three conditions:

1. **Continuity**: The regularization method \( R_\alpha, \alpha \geq 0 \), (or \( R_\theta, \theta \in \mathbb{R}^d \)) needs to be continuous, as a function of \( y \).
2. **Parameter Choice Rule**: There needs to be a parameter choice rule \( \alpha(\delta, y_\delta) \) (or \( \theta(\delta, y_\delta) \)) such that for \( y \in \mathcal{D}(T^\dagger) \) and \( y_\delta \in \mathcal{Y} \), with \( ||y_\delta - y||_\mathcal{Y} \leq \delta \),

\[
\limsup_{\delta \to 0} \alpha(\delta, y_\delta) = 0 \quad \text{(or, \quad \limsup_{\delta \to 0} ||\theta(\delta, y_\delta)||_\mathcal{Y} = 0)} \quad (3.1)
\]

3. **Convergence**: Again, for \( y \in \mathcal{D}(T^\dagger) \) and \( y_\delta \in \mathcal{Y} \), such that \( ||y_\delta - y||_\mathcal{Y} \leq \delta \), we must have

\[
\limsup_{\delta \to 0} ||R_\alpha(\delta, y_\delta)y_\delta - T^\dagger y||_X = 0 \quad (3.2)
\]

\[
\left( \text{or, \quad \limsup_{\delta \to 0} ||R_\theta(\delta, y_\delta)y_\delta - T^\dagger y||_X = 0} \right) \quad (3.3)
\]

Hence, for a given learned \( R_\theta \), one can attempt to define a family of regularization operator as follows, for \( \alpha \geq 0 \),

\[
R_\alpha = T^\dagger + \alpha R_\theta, \quad (3.4)
\]

where \( T^\dagger \) is the pseudo-inverse of the forward operator \( T \). However, the problem with this formulation is that, the operator \( R_\alpha \) (as defined in (3.4)) might not be continuous, since \( T^\dagger \) is usually discontinuous for ill-posed inverse problems, and thus, \( R_\alpha \) is also discontinuous (even when \( R_\theta \) is continuous).

Therefore, one can circumvent the discontinuity issue by making use of a convergent family of regularized operators \( \{ R_\alpha \} \), such as, for all \( y \in \mathcal{Y} \), define

\[
R_\alpha^\theta(y) = R_\alpha(y) + \beta(\alpha, y)R_\theta(y), \quad (3.5)
\]

where \( \beta : [0, \infty) \times \mathcal{Y} \mapsto [0, \infty] \), with \( \beta(\alpha, y) = \infty \) implying \( R_\alpha^\theta(y) = R_\theta(y) \), is such that, for all \( \alpha \geq 0 \),

- the product \( \beta(\alpha, \cdot)R_\theta(\cdot) \) is continuous, \quad (3.6)

and \( \beta(\alpha, y) \) also satisfies, for all \( y \in \mathcal{Y} \),

\[
\limsup_{\alpha \to 0} \beta(\alpha, y) ||R_\theta(y)||_X = 0. \quad (3.7)
\]

Hence, the new family of operator \( \{ R_\alpha^\theta \} \) is also a convergent regularization method.
Typically, one can alter $\beta(\alpha, y)$ in (3.5) to a weighted average, such as,
\[
R_{\alpha}^{\delta, \beta}(y) = (1 - \beta(\alpha, y))R_{\alpha}(y) + \beta(\alpha, y)R_{\beta}(y),
\tag{3.8}
\]
where (now) $\beta : [0, \infty) \times \mathcal{Y} \rightarrow [0, 1]$. That is, for a given $\delta \in \mathcal{Y}$, such that $||y_\delta - y||_Y \leq \delta$, a regularized solution of the new regularization method, corresponding to a parameter choice $\alpha(\delta, y_\delta)$, is given by
\[
R_{\alpha(\delta, y_\delta)}^{\delta}(y_\delta) = (1 - \beta(\alpha(\delta, y_\delta), y_\delta))R_{\alpha(\delta, y_\delta)}(y_\delta) + \beta(\alpha(\delta, y_\delta), y_\delta)R_{\beta}(y_\delta),
\tag{3.9}
\]
Hence, even when the learned reconstruction $R_{\beta}(y_\delta)$ is unstable, by choosing an appropriate $\beta(\alpha(\delta, y_\delta), y_\delta)$, one can still recover a regularized (stable) solution $R_{\alpha(\delta, y_\delta)}^{\delta}(y_\delta)$, for the inverse problem (1.1).

Now, one can further generalize the regularization operator defined in (3.5) or (3.8), when having a family of classical regularization methods $\{R_{\alpha_i}\}_{i=1}^N$ and a collection of learned reconstruction algorithms $\{R_{\beta_i}\}_{i=1}^N$, in the following manner
\[
R(y; \{\alpha_i\}, \{\beta_i\}) = \sum_{i=1}^N \beta_i^1(\alpha_i, y)R_{\alpha_i}(y) + \sum_{i=1}^N \beta_i^2(\alpha_i, y)R_{\beta_i}(y),
\tag{3.10}
\]
such that, for all $y \in \mathcal{Y},$
\[
\sum_{j=1}^2 \sum_{i=1}^N \beta_i^j(\alpha_i, y) = 1 \tag{3.11}
\]
and $\beta_i^j(\alpha_i, y)$ satisfies conditions (3.6) and (3.7), for all $1 \leq i \leq N$ and $j = 1, 2$. This extended definition will be helpful when regularizing a learned unrolled reconstruction algorithm, which is defined in the next section.

4. Practical Applications

Here, we provide two instances where one can use the above formulation to regularize two popular deep-learning based reconstruction algorithms:

4.1. Regularizing Learned Post-Processing Reconstruction Methods:

Here, for a given $y_\delta$, one recovers a solution of (1.1) via the following two steps

- Step 1: A classical recovery method, as defined in (1.6), i.e., $R_{\alpha(\delta, y_\delta)}(y_\delta) := \text{arg min}_x D(Tx, y_\delta) + \alpha(\delta, y_\delta)\mathcal{R}(x)$, typically, $\mathcal{R}(x) = ||x||_X$.
- Step 2: A learned recovery method ($R_{\beta_0}$) applied to $R_{\alpha(\delta, y_\delta)}(y_\delta)$, usually, $R_{\beta_0} = \mathcal{NN}_{\theta_0}$, where $\mathcal{NN}_{\theta_0}$ is a pre-trained neural network.

That is, the final recovered solution is given by a composition of the above two methods:
\[
R_{\alpha(\delta, y_\delta)}^{\beta_0}(y_\delta) := R_{\beta_0}(R_{\alpha(\delta, y_\delta)}(y_\delta)).
\tag{4.1}
\]

Note that, the recovery method (as defined in (4.1)) may not be continuous for a discontinuous $R_{\beta_0}$, and hence, the recovered solution might not be a “regularized” solution for the inverse problem (1.1). Now, as defined in (3.9), one can recover a regularized solution, for an appropriate $\beta(\alpha(\delta, y_\delta), y_\delta)$, as follows
\[
R_{\alpha(\delta, y_\delta)}^{\beta_0}(y_\delta) = (1 - \beta(\alpha(\delta, y_\delta), y_\delta))R_{\alpha(\delta, y_\delta)}(y_\delta) + \beta(\alpha(\delta, y_\delta), y_\delta)R_{\beta_0}(y_\delta).
\tag{4.2}
\]
In other words, starting from the classical regularized solution $R_{\alpha(\delta, y_\delta)}(y_\delta)$, one moves along the direction of the learned reconstruction,
\[
d_{\alpha, \beta_0}(y_\delta) := R_{\alpha(\delta, y_\delta)}^{\beta_0}(y_\delta) - R_{\alpha(\delta, y_\delta)}(y_\delta),
\tag{4.3}
\]
upto a certain extent, i.e.,

\[ R^\delta_{\alpha(\delta,y_b)}(y_b) = R_{\alpha(\delta,y_b)}(y_b) + \beta(\alpha(\delta,y_b),y_b) \ d^{\delta}_{\alpha,\theta_0}(y_b). \]  \hspace{1cm} (4.4)

Hence, for a continuous \( R_{\alpha}(\cdot) \), the expression in (4.4) is continuous when \( \beta(\alpha, \cdot) d_{\alpha,\theta_0}(\cdot) \) is continuous.

4.2. Regularizing Learned Unrolled Reconstruction Methods:

In this case, for a given \( y_b \), instead of a single classical recovery \( (R_{\alpha(\delta,y_b)}(y_b)) \) which is then followed by a single learned recovery \( (R^\delta_{\alpha(\delta,y_b)}(y_b)) \), there is a series or sequence of classical recovery methods \( \{R_{\alpha_i(\delta,y_b)}\}_{i=0}^N \) and learned recovery methods \( \{R_{\theta_i}\}_{i=0}^N \) which are stacked alternatively (in certain fashion) to produce a final solution of the inverse problem (1.1), i.e., for \( 1 \leq i \leq N \), we have either (the composition structure)

\[ f_i(R_{\alpha_1}, R_{\theta_1}; y_b) = R_{\theta_1}(R_{\alpha_1}(y)_b, R_{\theta_1-1}; y_b)), \]

or (the addition structure)

\[ f_i(R_{\alpha_1}, R_{\theta_1}; y_b) = R_{\alpha_1}(f_{i-1}(R_{\alpha_{i-1}}, R_{\theta_{i-1}}; y_b)) + R_{\theta_1}(f_{i-1}(R_{\alpha_{i-1}}, R_{\theta_{i-1}}; y_b)), \]

and the final recovered solution is given by

\[ R(y_b; \{\alpha_i\}, \{\theta_i\}) = f_N(R_{\alpha_N}, R_{\theta_N}; y_b). \hspace{1cm} (4.7) \]

Here, \( R_{\alpha}(\cdot) \) are also referred as the data-consistency steps, that generate solutions (in a regularized manner) to fit the noisy data \( y_b \), and \( R_{\theta}(\cdot) \) as the data-denoising steps, which denoise (further smoothing) the generated \( R_{\alpha}(\cdot) \)-solutions. The inspiration behind such algorithms are derived from optimization architectures such as ADMM (Alternating Direction of Methods of Multipliers) or PGM (Proximal-Gradient Methods). Again, the above recovery method may not end up being a continuous process, and hence, the final recovered solution might not be “regularized”. Now, similar to the previous regularizing technique, one can regularize such unrolled methods, by defining a regularized solution as

\[ R(y_b; \{\alpha_i\}, \{\theta_i\}, \beta(\{\alpha_i\}, y_b)) = R_{\alpha_0}(y_b) + \beta(\{\alpha_i\}, y_b) \ d^{\delta_0}(y_b; \{\alpha_i\}, \{\theta_i\}), \hspace{1cm} (4.8) \]

where the direction \( d^{\delta_0}(y_b; \{\alpha_i\}, \{\theta_i\}) \) can be defined as follows

\[ d^{\delta_0}(y_b; \{\alpha_i\}, \{\theta_i\}) := f_N(R_{\alpha_N}, R_{\theta_N}; y_b) - R_{\alpha_0}(y_b). \hspace{1cm} (4.9) \]

However, in this case, instead of the starting point \( R_{\alpha_0}(y_b) \), one can choose any intermediate iterate (of course, assuming the recovery upto that point is regularized) as the initial point for the direction \( d^{\delta_0} \), as defined in (4.9), and can (even) recover a sequence of regularized solutions. In other words, similar to (3.10), one can generalize the definition (4.8), of a regularized solution, to a weighted regularized-solution, defined as follows

\[ R(y_b; \{\alpha_i\}, \{\theta_i\}, \{\beta_i(\alpha_i, y_b)\}) = \sum_{i=1}^{N} \beta^1_i(\alpha_i, y_b) R_{\alpha_i}(y_b) + \sum_{i=1}^{N} \beta^2_i(\alpha_i, y_b) R_{\theta_i}(y_b) + \sum_{i=1}^{N} \beta^3_i(\alpha_i, y_b) f_i(R_{\alpha_i}, R_{\theta_i}; y_b), \hspace{1cm} (4.10) \]
such that
\[ \sum_{j=1}^{3} \sum_{i=1}^{N} \beta_i^j (\alpha_i, y_\delta) = 1. \]  \hspace{1cm} (4.11)

Note that, with the definition (4.10), the regularization parameter \((\beta(\{\alpha_i\}, y_\delta) \geq 0)\) is not a single dimensional anymore, instead \(\Theta = (\beta_i^j (\alpha_i, y_\delta)) \in \mathbb{R}^{3N}\), and can be cumbersome to estimate an appropriate value for it.

Another approach to regularize such unrolled scheme is to introduce a regularization parameter at every unrolled steps, i.e.,
\[ f_i(\beta, R_{\alpha_i}, R_{\theta}; y_\delta) = (1 - \beta_i) R_{\alpha_i}(f_{i-1}(R_{\alpha_{i-1}}, R_{\theta_{i-1}}; y_\delta)) + \beta_i R_{\theta_i}(f_{i-1}(R_{\alpha_{i-1}}, R_{\theta_{i-1}}; y_\delta)) \]  \hspace{1cm} (4.12)
or
\[ f_i(\beta, R_{\alpha_i}, R_{\theta}; y_\delta) = (1 - \beta_i) R_{\alpha_i}(f_{i-1}(R_{\alpha_{i-1}}, R_{\theta_{i-1}}; y_\delta)) + \beta_i R_{\theta_i}(f_{i-1}(R_{\alpha_{i-1}}, R_{\theta_{i-1}}; y_\delta)), \]  \hspace{1cm} (4.13)
to encounter instabilities arising (if any) at each and every steps.

In the next section we present examples illustrating the instabilities that can arise in such learned reconstruction algorithms, if not regularized properly. We also show that, by using the techniques presented above, one can recover a regularize (stable) solution. This is explained in details in [3], where it’s showed that the Plug-and-Play algorithms (which is a special case of the unrolled scheme) can also suffer instabilities, arising from a learned denoiser \((R_{\theta_0})\) in its denoising step and, by using regularization techniques, such as (4.12) or (4.13), one can stabilize the recovery process, and thus, can obtain excellent (stable) solutions.

5. Numerical Results

In this section, we consider \(\mathcal{X} = \mathbb{R}^n\), \(\mathcal{Y} = \mathbb{R}^m\) and \(T \in \mathbb{R}^{m \times n}\), and solve the following linear (matrix) equation
\[ T \hat{x} = y_\delta, \]  \hspace{1cm} (5.1)
for a given noisy \(y_\delta \in \mathbb{R}^m\), such that \(||y_\delta - y||_2 \leq \delta\), and known \(T \in \mathbb{R}^{m \times n}\). In the following example, the forward equation (5.1) corresponds to a discretization of the radon transformation, which is associated with a (parallel-beam) X-ray computed tomography (CT) image reconstruction problem. Here, we generate the matrix \(T\) from the MATLAB codes presented in [4]. The dimension \(n = n_1 \times n_2\) corresponds to the size of a \(n_1 \times n_2\) (phantom) image, and the dimension \(m = m_1 \times m_2\) corresponds to a \(m_1 \times m_2\) (sinogram) image, where \(m_1\) implies the number of rays per angle and \(m_2\) implies the number of angles. We consider a 128 \(\times\) 128 chest CT-image \((\hat{x})\) (obtained from MATLAB’s “chestVolume” dataset) and generate a noiseless sparse view data \((y = A\hat{x})\), with only 90 views and 181 rays/angle (181 \(\times\) 90 sinogram image). To avoid inverse-crime we add Poisson noise of intensity \(I_0 = 10^6\), i.e., first normalize the intensities of \(y\) to \(y_0^\text{ol} := \frac{y - \min(y)}{\max(y) - \min(y)} \in [0, 1]\) and add Poisson noise
\[ y_\delta^0 = -\log \left( \frac{\text{poissrnd}(I_0 \exp(-y_0^0))}{I_0} \right), \]  \hspace{1cm} (5.2)
where \(\log()\), \(\text{poissrnd}()\) and \(\exp()\) are MATLAB’s inbuilt routines. Finally, \(y_\delta^0\) is scaled back up via \(y_\delta := y_\delta^0 (\max(y) - \min(y)) + \min(y)\).
Note that, the experiments presented here is to illustrate the instabilities arising in a reconstruction algorithm which is based on a learned component and different (regularization) techniques to subdue these instabilities, so as to produce an effective and stable recovery. Hence, we won’t be proposing a new $\mathcal{NN}_0$ structure and train it for a set of examples, and claim it to outperform some existing structures. Instead, we use a pre-trained $\mathcal{NN}_{\theta_0}$ (which can also be a deep-learning denoiser) in our learned modules and show that, if used naively, it can produce strange instabilities (hallucinated features/structures or complete breakdown of the recovery process), which are quite different from the inherent instabilities of an ill-posed (inverse) problem. Furthermore, to show that the $\mathcal{NN}_{\theta_0}$ is not completely unfeasible, we use the same $\mathcal{NN}_{\theta_0}$, but in a regularized fashion, to recover excellent (stable) regularized solutions. Therefore, validating that, the instabilities issues not only arise from the (training) learning process, but also the manner in which it is used/implemented, i.e., the instabilities can be inherent to the reconstruction structure (including the trained components), and with a proper (regularization) technique, one can subdue these instabilities and recover stable solutions.

**Example 5.1. [Breakdown of the recovery process]**

The unrolled scheme followed here is as follows, for $1 \leq i \leq N$,

$$R_{\alpha_i}(y) := x^\delta_{N_i}(x^0_0),$$

(5.3)

where, starting from an initial point $x^0_0 = x^0_0$, for $1 \leq k \leq N_i$,

$$x^\delta_i = x^\delta_{i-1} - \tau_i^k \delta x^\delta_{i-1} - y_0,$$

(5.4)

for appropriate (step-sizes) $\tau_i^k \geq 0$. For simplicity, we choose a fixed number of inner iterations ($N_i = N_0$) and a constant step-size $\tau_i^k = \tau$ for all $1 \leq i \leq N$ and $1 \leq k \leq N_i$, where the values of these parameters are stated below. However, the starting points $(x^0_0)$ for each inner iterative processes are layer dependent (i.e., $x^0_0 = x^0_0(i)$ in (5.4)), and the nature of dependence is also defined below. Also, note that, the regularization parameter for each of these classical regularization components (data-consistency steps) is the iteration index, $\alpha_i(\delta, y_0) = N_i(\delta, y_0)$, i.e., here $R_{\alpha_i}$ is the traditional (semi-) iterative regularization method.

As for the learned components (data-denoising steps), we use MATLAB’s pre-trained DnCNN denoising network ($R_{\theta_0} = \mathcal{NN}_{\theta_0}$), which is a substantially effective denoiser. That is, for all $1 \leq i \leq N$,

$$R_{\alpha_i}(y) := R_{\theta_0}(R_{\alpha_i}(y_0))$$

(5.5)

Now, the initial point $(x^0_0)$ for each data-consistency step is given by, starting from a user defined $x_0^0 = x_0$ (typically, $x_0 \equiv 0$), for $1 \leq i \leq N$,

$$x_0^i = R_{\alpha_i}(R_{\alpha_i}(y_0)), \quad x_0^i = x_0^i + \gamma_i(x_0^i - x_0^i-1),$$

(5.6)

(5.7)

where the parameters in the momentum step (5.7) are defined as $\gamma_i = \frac{t_{k-1}}{t_k}$, $t_k = 1 + \sqrt{1 + 2t_{k-1}}$, and $t_0 = 1$. Note that, for $N_0 = 1$ and $N \rightarrow \infty$ we have the FISTA-PnP algorithm and for some additional tweaks in (5.4) (or to (5.3)) one can get the ADMM-PnP algorithm. However, with the above formulation, it’s neither of them, rather, it’s a superposition of both these algorithms. Nevertheless, one can still have a meaningful interpretation of the recovery process and the recovered solution, according to some class (family) of regularized solutions, as defined in [5].
For all the simulations, we consider (the total unrolling steps) \( N = 100 \), the constant step-size \( \tau = 10^{-5} \) and repeated the experiment for \( N_0 = \{1, 10, 50, 100\} \), the total number of inner iterations. Here, we choose the parameter choice criterion \((S_0)\) as the Cross-Validation errors, for a fixed leave out set \( y_{\delta,s} \subset y_\delta \), where \( s \subset \{1, 2, \cdots, m\} \) and \( |s| = 0.01m \). That is, when performing regularization at each unrolled step, the values of \( \beta_i \) in (4.12) is determined by the selection criterion \( S_0 \), i.e., \( \beta_i = \beta_i(S_0) \), such that

\[
\beta_i(S_0) := \arg \min_{\beta} ||Tf_i(\beta, R_{\alpha}, R_\theta; y_\delta) - y_{\delta,s}||_2, \tag{5.8}
\]

where \( f_i(\cdot) \) is as defined in (4.12). Note that, the minimization problem (5.8) may not be convex, and hence, can be difficult to find the global minimum. Still, even for a local minimizer, the regularized iterate \( f_i(\beta_i(S_0), R_{\alpha}, R_\theta; y_\delta) \) can be much better (in the sense of satisfying the selection criterion \( S_0 \)) than the unregularized iterate \( R_\theta(y_\delta) \), in addition to regularizing \( R_\theta s \), when \( R_\theta(y_\delta) \) suffers from instabilities. This can be seen in the presented examples. Furthermore, (5.8) is a single variable optimization problem, and hence, not much computationally expensive to solve.

Now, although one can also perform further regularization in the data-consistency steps by defining a regularized solution as

\[
R_{\alpha_i}(y_\delta) := x^\delta_{\beta_i(S_0)}(x^i_0), \tag{5.9}
\]

instead of \( x^\delta_{N_i}(x^i_0) \), we opted out of it, as it does not make much difference here.

Figure 1 shows the final recovered solutions \( x^{N_0}_N \), where \( N = 100 \) for various values of \( N_0 \) and Figure 2 shows the iterates \( x^{N_0}_i \) which best satisfies the selection criterion \( S_0 \) during the unrolled iterative process, i.e.,

\[
x^{N_0}_i := \{x^{N_0}_{i_0} : x^{N_0}_{i_0} := R_\theta(y_s) \text{ and } i_0 = \arg \min_{1 \leq i \leq N} S_0(x^{N_0}_i)\} \tag{5.10}
\]

The performance metrics for each of these recoveries are stated at the top of the figures, where PSNR stands for the peak signal-to-noise ratio, SSIM stands for the structure similarity index measure and \( i(S_0) \) indicates the index for which \( x^{N_0}_{i(S_0)} \) best satisfies \( S_0 \) or the last iterate when \( i(S_0) = N \).

Figure 1 reflects that, the final reconstructed image \( x^{N_0}_N \) in an unrolled scheme may not always be stable, without regularizing \( R_\theta \) (i.e., \( \beta_i = 1 \) in (4.13)), however, it can improve when the classical (regularized) components \( (R_{\alpha}, s) \) are improved \( (N_0 \) increases). In other words, in this case, the learned components \( (R_\theta s) \) are very strong, and hence, dominate the reconstruction algorithm for weaker classical components, leading to an unstable recovery process. Note that, the instability in the solution (for weaker \( R_{\alpha}, s \) and \( \beta_i = 1 \)) is quite different than the instabilities of the ill-posed inverse problem, which are noisy features and streaky artifacts, as can be seen when \( R_{\alpha}, s \) get stronger. Where as, for the same classical regularization components \( R_{\alpha}, s \), the final solution corresponding to regularized \( R_\theta s \) is quite stable and well denoised, where the quality improves when \( R_{\alpha}, s \) improve.

Figure 2 presents the iterates obtained during the recovery process which best satisfies the selection criterion \( S_0 \), i.e., \( x^{N_0}_{i(S_0)} \), as defined in (5.10), for various values of \( N_0 \). Here, one can observe that even without regularizing \( R_\theta s \), one can still recover fine solutions (much better than its final counterparts \( x^{N_0}_N \)), of course, the quality improves upon regularizing \( R_\theta s \). Note that, there is not much difference in \( x^{N_0}_{i(S_0)} \) over \( x^{N_0}_N \) when using regularized \( R_\theta s \), in fact, the later is even slightly
better than the former, in terms of the evaluation metrics. This suggests that one can consider $x^\mathcal{N}_i^0$ as the recovered solution, over $x^\mathcal{N}_i(S_0)$, when using regularized $R_{\theta_i}s$ and the converse, otherwise.

The natural question that one can ask is, when does the recovery fail? The answer to this question is not straightforward, otherwise, the ill-posed problem won’t be ill-posed anymore. However, one can have certain measuring/monitoring criteria to (at least) indicate when an algorithm might fail. Here, we present few of such criteria to indicate when an algorithm can break down. Note that, from (4.4), the recovery process $R^\theta_{\alpha_i}$ (at each unrolled step) is continuous if $\beta_i(\alpha_i(\delta, y_\delta), \ldots)d_{\alpha_i, \theta_i}(\cdot)$ is continuous, as a function of $y_\delta$. Again, this is not easy to verify for $\beta_i(\cdot, y_\delta) = \beta_i(S_0, y_\delta)$ and for a pre-trained $R_{\theta_i}$, which can be non-linear. Now, although we don’t have a theoretical proof, we empirically try to show that $\beta_i(S_0, \ldots)d_{\alpha_i, \theta_i}(\cdot)$ is “continuous” here. First, we show that (in Figure 3a) for $\beta_i = 1$ (unregularized $R_{\theta_i}s$), the function $g(i) = ||\beta_i(\cdot, y_\delta)d_{\alpha_i, \theta_i}(y_\delta)||_2$ tends to be unbounded ($g(i)$ increases exponentially) as $i$ increases, especially for smaller values of $\mathcal{N}_0$ (weaker $R_{\alpha_i}$), indicating an unstable recovery process. Where as, the function $g(i)$ does not blow up for $\beta_i = \beta_i(S_0, y_\delta)$ (regularized $R_{\theta_i}s$), see Figure 3b. However, this might not guarantee continuity or discontinuity, for $\beta_i = \beta_i(S_0, y_\delta)$ and $\beta_i = 1$, respectively, as $\beta_i(\cdot, \cdot) d_{\alpha_i, \theta_i}(\cdot)$ may be non-linear. Hence, in our second attempt we try to verify the continuity of $\beta_i(\cdot, y)d_{\alpha_i, \theta_i}(y)$ directly by computing

$$g(i) = ||\beta_i(\cdot, y)d_{\alpha_i, \theta_i}(y) - \beta_i(\cdot, y)d_{\alpha_i, \theta_i}(y')||_2,$$

for large values of $\delta_j$, $\delta_j'$. $\varepsilon_j$, $\varepsilon_j'$ is a Gaussian noise with mean zero and std. dev. equaling max(||$y_\delta||)/1000, and $d_{\alpha_i, \theta_i}(y'_{\delta})$ is computed according to the definition in (4.3).

Again, from Figure 3c, one can observe that, the values of $g(i)$ are (relatively) high for unstable recovery processes (when $\mathcal{N}_0$ is small and unregularized $R_{\theta_i}s$) and (relatively) low for stable recovery process, in Figure 3d, especially when $R_{\theta_i}s$ are regularized (irrespective of $R_{\alpha_i}s'$ strength), indicating that $\beta_i(\cdot, y)d_{\alpha_i, \theta_i}(y)$ might be continuous for $\beta_i(\cdot, y) = \beta_i(S_0, y)$.

Another indicator, for an unstable recovery process, can be the iterates’ norms during the iterative process, i.e., if $||x_i||_2$ blows up exponentially, then the recovery algorithm has become unstable. This can be seen in Figure 3e or in Figure 3g, which shows the relative norms $\left(r_i := \frac{||x_i^\mathcal{N}_i||_2}{||x_i^\mathcal{N}_i||_2} \right)$ of the iterates $x_i^\mathcal{N}_0$ for various values $\mathcal{N}_0$, i.e., for different $R_{\alpha_i}s'$ strength. As expected, the ratio $r_i$ saturates to one for stable recovery processes, Figure 3h, and explodes beyond one for unstable processes, Figure 3g. In addition, to understand how an unstable process becomes stable, upon regularizing it via the parameter $\beta_i(S_0, y_\delta)$, we plot the values of $\beta_i(S_0, y_\delta)$ over the iterations, see Figure 3f. Here, one should also expect that, for large values of $r_i$s (indicating instabilities in those iterates), the corresponding values of $\beta_i$s should be small, to compensate it. This counter balancing effect, small $\beta_i$ values for large $r_i$ values, can be seen by comparing Figure 3e ($r_i$ values) with Figure 3f ($\beta_i$ values).

To further validate our regularization method, we experimented on sparser views, higher noise levels and few other CT phantoms from MATLAB’s chestVolume dataset. For the unrolled network architecture, we stuck with $N = 100$ (total unrolled steps), $\mathcal{N}_0 = 100$ and $\tau = 10^{-5}$ for the total number of gradient steps and
step-size in each $R_\alpha_i$, respectively, and the recovered solution as the final output of the unrolled network, i.e., $x^N$.

1. Figures 4a and 4b show the recovered solutions, for 90-views with $I_0 = 10^5$ (higher noise level), corresponding to the unregularized and the regularized $R_\theta_i s$, respectively.

2. Figures 4c and 4d show the recovered solutions, for 60-views (even sparser) with $I_0 = 10^6$ (noise level unchanged), corresponding to the unregularized and the regularized $R_\theta_i s$, respectively. Note that, in this case, even with stronger classical regularization components ($R_\alpha_i s$), the final solution is unstable, unlike the previous examples. The reason might be, the ill-posedness of the problem for 60-views is stronger than that of 90-views.

3. Figures 4e, 4f, 4g and 4h show the recovered solutions, for 90-views (unchanged) with $I_0 = 10^6$ (unchanged), corresponding to the unregularized and the regularized $R_\theta_i s$, respectively, for different phantom images. Note that, the behavior of all the recovery processes corresponding to 90-views and $I_0 = 10^6$, for different phantom images, are very similar, as expected.

Unlike the previous examples, where there is a complete breakdown of the recovery process (severe instabilities), in the next example, we show that the recovered solution may contain certain (hallucinated) features/structures that are not present in the true phantom, even for a “well recovered” solution (i.e., without severe instabilities). These recoveries are even more treacherous than the completely broken recoveries, as it can lead to an impression of a proper recovery with (hallucinated) features, that can be deceiving, and can lead to wrong interpretations/diagnoses.

Example 5.2. [Hallucinated features]

In this example, we consider a brain phantom from MATLAB’s “mri” dataset and generated the sinogram data, corresponding to 90-views and $I_0 = 10^6$, as discussed in the previous example. Here, we kept $N = 100$ (# unrolled steps), $\tau = 10^{-5}$, but $N_0 = 30$ (# inner iterations). In addition, here the intensities of true image is always non-negative ($\hat{x} \geq 0$), and hence, one can also restrict the iterates to be non-negative ($x_i \geq 0$, for all $i$), during the recovery process. Figure 5a shows the true phantom, Figure 5e shows the final solution $x^\beta_{+N} = 1$ (with the constraint $x \geq 0$) and Figure 5c shows the final solution $x^\beta_{+N} = 1$ (without the constraint), for the unrolled scheme without regularizing $R_\theta_i s$. Note that, although the constrained solution $x^\beta_{+N} = 1$ doesn’t completely break down like the unconstrained one ($x_N^\beta = 1$), it does contain certain (hallucinated) features (which are circled red) that are not present in the true image $\hat{x}$. However, if we notice the solutions corresponding to the selection criterion ($S_0$), they are neither unstable nor contaminated by the hallucinated features, but they are of not great qualities, i.e., see Figures 5f and 5d for $x^\beta_{+S_0} = 1$ (constrained) and $x^\beta_{+S_0} = 1$ (unconstrained), respectively. Of course, the recoveries ($x^\beta_{+S_0}$ and $x^\beta_{-S_0}$) significantly outperforms all other recoveries, irrespective of whether constrained or nor, and whether stopped early or not, see Figures 5b, 5g and 5h. This example validates that, even with additional constraints (like non-negativity etc.), the solutions of such learned reconstructive algorithms can not only be unstable, but can also contain (hallucinated) features/structures that are absent in the true solution, and by regularizing the learned components (together with the classical components), one can subdue these instabilities, and hence, can recover excellent stable solutions of the ill-posed inverse problems.
6. Conclusion and Future Research

In this paper, we showed that the recovery processes (or reconstruction algorithms) depending on a learned component can be very susceptible to strange instabilities, if not regularized properly. It’s shown that such learned algorithms, which depends on pre-trained denoisers or pre-learned reconstruction components, can be inherently unstable and can exhibit instabilities in the recovered solutions, even without the adversarial noises, i.e., simple additive noises (in this case, Poisson noises) can still break down the recovery process completely or can induce hallucinated features/structures that are not present in the true solution. We also presented certain regularization methods to stabilize these instabilities, leading to a much efficient and stable recoveries. We present the importance of continuity in a reconstruction algorithm, the failure of which, can lead to these wild instabilities. It is shown that, by parameterizing each step in an unrolled scheme one can stabilize/regularize an unstable recovery process. Furthermore, we also presented a technique to select the values of these (intermediate) regularization parameters, which is dependent on some selection criterion for the solution. Hence, the quality of the recovered solution, as well as, the stability of the reconstruction algorithm, is greatly dependent on the selection criterion, which is also the essence of a convergent regularization method.

In a future work we would to extend this idea of regularization to a proper (deep) unrolled reconstruction scheme, i.e., to train a deep neural network with classical regularization and learned regularization components and test the robustness of the algorithm by exposing it to adversarial noises.

References

[1] H. W. Engl, M. Hanke, and A. Neubauer, *Regularization of inverse problems*, vol. 375 of Mathematics and its Applications. Kluwer Academic Publishers Group, Dordrecht, 1996.
[2] V. Antun, F. Renna, C. Poon, B. Adcock, and A. C. Hansen, “On instabilities of deep learning in image reconstruction and the potential costs of ai,” *Proceedings of the National Academy of Sciences*, vol. 117, no. 48, pp. 30088–30095, 2020.
[3] A. Nayak, “Instabilities in Plug-and-Play (PnP) algorithms from a learned denoiser,” 2021.
[4] S. Gazzola, P. Hansen, and J. Nagy, “Ir tools - a matlab package of iterative regularization methods and large-scale test problems,” *Numerical Algorithms*, 2018.
[5] A. Nayak, “Interpretation of Plug-and-Play (PnP) algorithms from a different angle,” 2021.

Visiting Assistant Professor, Department of Mathematics, University of Alabama at Birmingham, University Hall, Room 4005, 1402 10th Avenue South, Birmingham AL 35294-1241, (p) 205.934.2154, (f) 205.934.9025

Email address: nash101@uab.edu; avinashnike01@gmail.com
Figure 1. Final solution of an unrolled reconstruction algorithm for various $R_{\alpha_i}$ strengths, with and without regularizing $R_{\theta_i}s$. 
Figure 2. Selection criterion solution of an unrolled scheme for various $R_{\alpha_i}'$ strength, with and without regularizing $R_{\theta_i}$s.
(a) $\|d_{\alpha_i}(y_\delta) \|_2$, No regularization

(b) $\|\beta_i(S_0, y_\delta) d_{\alpha_i}(y_\delta) \|_2$, Regularization

(c) Discontinuity, without regularization

(d) Continuity, with regularization

(e) Iterates norm $\|x_i^{N_j}\|_2$

(f) $R_{\beta_i}$ regularization parameter $\beta_i(S_0, y_\delta)$

(g) Relative norms $\|x_i^{N_j}\|_2 / \|F\|_2$, Unregularized

(h) Relative norms $\|x_i^{N_j}\|_2 / \|F\|_2$, Regularized
Figure 4. Final solutions of an unrolled reconstruction algorithm, for regularized and not regularized $R_{\theta_i}s$. 
Figure 5. Instabilities and hallucinations in the recovered solutions for constrained and unconstrained learned algorithms.