Generative Plug-and-Play: The Saga Continues†

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Outline*

- Historical perspective
  - PnP original recipe
  - Some cool PnP results

- Generative PnP Theory:
  - Proximal generators
  - GPnP Theorem

- Generative PnP Implementation:
  - Proximal generators and score matching
  - Pseudo-code algorithm

- Results

*For details see:
https://github.com/gbuzzard/generative-pnp-allerton
MBIR - Model Based Iterative Reconstruction

- Regularized inversion
- Variable Splitting and proximal maps
- The ADMM Algorithm
Computed Tomographic (CT) Imaging

Parallel Beam CT: synchrotrons, electron microscopy, nano-X-ray sources

Fan Beam CT: Industrial CT

Cone Beam CT: Industrial CT, C-arm Scanners

Multi-Slice Helical CT: Medical, transportation security
CT Forward Model

\[ y = Ax + w \]

- **Problems:**
  - Not enough measurements: sparse or missing views, etc.
  - Low quality data: high noise, low dosage, short exposure, etc.
  - Model mismatch: metal, beam-hardening, scatter, poly-energetic, etc.
  - Resolution loss: detector blur, motion blur, X-ray spot size, etc.

- **Applications:**
  - Medical, scientific, industrial, and security

- **Q:** How do we resolve these problems for **quantitative** imaging?
Model-Based Iterative Reconstruction (MBIR)

\[ \hat{x} = \arg \min_x \{- \log p(y|x) - \log p(x)\} \]

\[ = \arg \min_x \left\{ \frac{1}{2} \|y - Ax\|^2 - \log p(x) \right\} \]
**MBIR: Regularized Image Reconstruction**

- **Sensor model:**
  \[ u_1(x) = -\log p(y|x) = \frac{1}{2} \| y - Ax \|_\Lambda^2 \]

- **Prior model:**
  \[ u_0(x) = -\log p(x) \]

- **MBIR Reconstruction**
  \[ \hat{x} = \arg \min_x \{ u_1(x) + u_0(x) \} \]
MBIR: “Thin Manifold” View

Sensor manifold – Based on physical sensor model

Prior manifold – Based on empirical or assumed information

Sensor manifold minimizes $u_1(x)$

Prior manifold minimizes $u_0(x)$

Forward model likelihood

$f(x)$

Negative log likelihood

$\hat{x}$

Measurements

$y$

Unknown

$\hat{x} = \arg \min_x \{ u_1(x) + u_0(x) \}$

Prior model probability

$h(x)$

Unknown

Prior negative log likelihood

MBIR Reconstruction:
PnP Original Recipe*

- Motivation
- Variable Splitting and proximal maps
- The ADMM Algorithm
- PnP-ADMM

*Singanallur V. Venkatakrishanan, Charles A. Bouman, and Brendt Wohlberg, “Plug-and-Play Priors for Model Based Reconstruction,” IEEE Global Conference on Signal and Information Processing (GlobalSIP), Austin, Texas, USA, December 3-5, 2013.
PnP Motivation

- **Uncomfortable facts circa 2013:**
  - MBIR is great, but it wasn’t close to the best algorithm for the most basic MBIR problem: **denoising** (MBIR with the identity forward model).
  - Algorithms such as non-local means, BM3D, wavelet shrinkage, bilateral filters, were all much better at denoising than MBIR.

- **But denoising is the most basic inverse problem:**

  \[
  \hat{x} = \arg \min_x \left\{ \frac{1}{2\sigma^2} \|y - x\|^2 - \log p(x) \right\} = \text{denoise}(y; \sigma)
  \]

- **Questions:**
  - Is there a way to improve on MBIR?
  - Can a denoiser be used as a prior model? There’s nothing to minimize!
Fresh Look at MBIR (circa 2013)

- Forward model: \( u_1(x) = -\log p(y|x) \)
- Prior model: \( u_0(x) = -\log p(x) \)

- MAP or regularized inverse

\[ \hat{x} = \arg \min_x \{ u_1(x) + u_0(x) \} \]

Can we minimize these two terms separately?

Proximal maps
Proximal Maps

Minimize a function subject to a quadratic penalty on the distance (proximity) to a given base point.

- Proximal map of $f$ with base point $x$:

$$\bar{F}_0(v) = \arg\min_x \left\{ u_0(x) + \frac{1}{2\gamma^2} \|x - v\|^2 \right\}$$

- Important: $\bar{F}_0(v)$ is an agent that updates solution
\[ \overline{F}_0(v) = \arg\min_x \left\{ u_0(x) + \frac{1}{2\gamma^2} \|x - v\|^2 \right\} \]

**Gradient Step:** For \( \gamma \) small, the proximal map is a gradient step

\[ \overline{F}_0(v) \approx v - \gamma \nabla u_0(v) \]
**Proximal Map Fact: Denoiser**

\[
\bar{F}_0(v) = \arg \min_x \left\{ u_0(x) + \frac{1}{2\gamma^2} \| x - v \|^2 \right\}
\]

- **Denoiser:** When \( u_0(x) = -\log p(x) \), the proximal map is a denoiser

\[
\bar{F}_0(v) = \arg \min_x \left\{ \frac{1}{2\gamma^2} \| v - x \|^2 - \log p(x) \right\}
\]

- Log likelihood for AWGN with variance \( \gamma^2 \)

\[
= \text{Denoise}(v; \gamma)
\]

MAP denoiser for AWGN
Denoisers are Gradient Steps!

- Prior distribution
  \[ p(\nu) = \frac{1}{Z} \exp\{-u_0(\nu)\} \]

- Then for small \( \gamma \),
  \[ \nu - \gamma \nabla u_0(\nu) = \text{Denoise}(\nu; \gamma) \]

- Denoisers are gradient steps for log priors

MAP denoiser for AWGN
Prior Model Proximal Map

\[ \bar{F}_0(v) = \arg \min_x \left\{ \frac{1}{2\gamma^2} \|v - x\|^2 + u_0(x) \right\} \]

- Interpretation
  - "Projection" of \(v\) onto prior manifold
  - Denoising operator for white additive Gaussian noise
Forward Model Proximal Map

\[ \bar{F}_1(v) = \arg \min_x \left\{ u_1(x) + \frac{1}{2\gamma^2} \|x - v\|^2 \right\} \]

- Interpretations
  - "Projection" of \( v \) onto sensor manifold
  - MAP estimate with additive white Gaussian noise prior
ADMM for MBIR Reconstruction

- Initialize $v, u = 0$
- Repeat {
  - $x \leftarrow \bar{F}_1(v - u)$  \hspace{1cm} // Project onto sensor manifold
  - $v \leftarrow \bar{F}_0(x + u)$  \hspace{1cm} // Projection onto prior manifold
  - $u \leftarrow u + (x - v)$  \hspace{1cm} // Augmented Lagrangian update
}

**ADMM:**
- Iteratively reproject on sensor/prior manifolds
- Minimizes $u(x) = u_1(x) + u_0(x)$
PnP for MBIR Reconstruction

Initialize $v, u = 0$
Repeat {
    $x \leftarrow \bar{F}_1(v - u)$ \hspace{1cm} // Project onto sensor manifold
    $v \leftarrow \text{Denoise}(x + u)$ \hspace{1cm} // Denoise
    $u \leftarrow u + (x - v)$ \hspace{1cm} // Augmented Lagrangian update
}

- Big Idea:
  - Replace $F_0$ with any denoiser!
  - Does it still converge? Does it minimize anything?
PnP circa 2013

Forward model: sparse subsampling

\[ u_1(x) = \sum_{s \in \{\text{sampled}\}} \frac{1}{2} \| x_s - y_s \|^2 \]

Noise std. dev.: 5% of max signal

Ground Truth

Subsamples

Prior model: denoising algorithm

K-SVD: RMSE : 14.11
BM3D: RMSE : 12.56

PLOW: RMSE : 14.54
TV: RMSE : 15.50
q-GGGMRF: RMSE : 15.72

\[ u(x) \in \mathbb{N} \]
Plug-and-Play Intuition

Question: Does PnP converge?
Answer: Yes, if $F_1$ and $F_0$ are nonexpansive.*

*Or more precisely, $T = (2F_1 - I)(2F_0 - I)$ nonexpansive ensures convergence.

Initialize $v = x$, $u = 0$
Repeat {
  $x \leftarrow F_1(v - u)$
  $v \leftarrow F_0(x + u)$
  $u \leftarrow u + (x - v)$
}
What’s great about PnP

- It produces great results

- It’s modular
  - You only need to train the prior distribution once
  - You can adapt different forward models with the same prior
  - The software is modular too!

- There are lots of denoisers to choose from
Some Cool Results

- Transmission electron microscopy
- 3D reconstruction from sparse views
- 4D reconstruction from sparse views
Bright Field Electron Microscopy
Suhas Shreehari, Purdue/Oak Ridge National Laboratory
Singanallur V Venkatakrishnan, Purdue/Oak Ridge National Laboratory
Greg Buzzard, Purdue
Jeff Simmons, Larry Drummy, AFRL
Charles Bouman, Purdue
3D Bright Field Tomography: Aluminum Spheres (Real) Dataset

67 equi-spaced views from -65° to +65°

Slice 307
Aluminum Spheres (Real) Dataset: Reconstructions

- FBP
- qGGMRF prior
- PnP prior
Cone-Beam CT for Imaging AM Parts
Thilo Balke, Soumend Majee, Greg Buzzard, Purdue
Pat Howard, GE Healthcare
Scott Poveromo, Northrop Grumman
**Cone-Beam CT**

- **Cone-Beam Geometry**
  - Source
  - Rotation axis
  - Detector
  - X-rays

- **Image**
  - X - reconstructed image
  - Y - measured sinogram

- **Beer’s Law attenuation**
  \[
  \int \mu(r)dr = -\log \left( \frac{I_0(u,v)}{I_1(u,v)} \right)
  \]

- **Discretized model**
  \[
  y = Ax + w
  \]
Reconstructions

- FBP
  - 2160 Views

- MBIR
  - q-GGMRF
  - 270 Views

- MBIR
  - Plug-and-Play
  - BM4D
  - 270 Views

mm⁻¹
4D Recon using PnP/MACE

Soumendu Majee, Purdue
Thilo Balke, Purdue
Craig A. J. Kemp, Eli Lilly
Gregery T. Buzzard, Purdue
Charles A. Bouman, Purdue
4D MBIR Reconstruction

TIMBIR:
- Showed 16x increase in temporal resolution
- Based on simple 4D MRF prior

4D MBIR reconstruction:
\[ \hat{x} \leftarrow \arg \min_x \{- \log p(y|x) - \log p(x)\} \]

Can we do better with 4D PnP prior?
### Experimental Setup

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Scanner Model</strong></td>
<td>North Star Imaging X50</td>
</tr>
<tr>
<td><strong>Source-Detector Distance</strong></td>
<td>839 mm</td>
</tr>
<tr>
<td><strong>Magnification</strong></td>
<td>5.57</td>
</tr>
<tr>
<td><strong>Cropped Detector Array</strong></td>
<td>$731 \times 91$, $(0.254 \text{ mm})^2$</td>
</tr>
<tr>
<td><strong>Detector resolution at ISO</strong></td>
<td>45.7 $\mu$m</td>
</tr>
<tr>
<td><strong>Number of Views per Rotation</strong></td>
<td>150</td>
</tr>
<tr>
<td><strong>Voxel Size</strong></td>
<td>$(45.7 \mu$m)$^3$</td>
</tr>
<tr>
<td><strong>Reconstruction Size ($x, y, z, t$)</strong></td>
<td>$731 \times 731 \times 91 \times 16$</td>
</tr>
</tbody>
</table>

Other details:

- Object held in place by fixtures: artifacts
- All 4D results undergo preprocessing to correct for jig artifacts
Multi-Slice Fusion: Qualitative Comparison

FBP (3D)  MBIR with 4D prior  PnP:Multi-Slice Fusion
Vial Scan with Force-Curve

- Scanner parameters:
  - 758 × 290 pixels, 3750 views, 25 full rotations
  - Detector spacing: 0.254 × 0.254 mm
  - Source-object distance: 152 mm
  - Object-detector distance: 695 mm
  - Magnification: ≈ 5.57

- Image Parameters (ROR)(rotations 5-8):
  - 758 × 758 × 290 × 4 voxels
  - Voxel size: (0.05 mm)
  - Field of view: 38 mm (758 voxels)
Reconstruction (180° per time-point)

FBP

Multi-Slice Fusion
Generative PnP (GPnP):

- Proximal generators
- Markov chains
- Intuition behind GPnP
Can PnP be Generative?

- Problem: PnP only generates a single “best” result

- Question:
  - Can PnP be modified to generate samples from the posterior distribution?
  - What is the posterior distribution?

\[
\hat{X} \sim p_{x|y}(x|y) = \frac{1}{Z} p(y|x)p(x)
\]
The posterior distribution is given by

\[ p(x|y) = \frac{1}{Z} \exp\{-u_1(x) - u_0(x)\} \]

where

\[ u_1(x) = -\log p(y|x) \]
\[ u_0(x) = -\log p(x) \]

Strategy:
- Create Markov chain
- Proximal generators: create sequential random samples
- Modular implementation
Proximal Generators

- **Proximal Map**
  \[
  \bar{F}_0(x) = \arg\min_v \left\{ u_0(v) + \frac{1}{2\gamma^2} \|v - x\|^2 \right\}
  \]

- **Proximal distribution**
  \[
  q_0(v|x) = \frac{1}{Z} \exp \left\{ -u_0(v) - \frac{1}{2\gamma^2} \|v - x\|^2 \right\}
  \]

- **Proximal Generator**
  \[
  V = F_0(x) \sim q_0(v|x)
  \]

Generates a sample from the proximal distribution
Interpretation of Proximal Generator

**Intuition:**
- Locally samples from the prior distribution
- Expected change approximates score

\[ V = F_0(x) \sim q_0(v|x) \]

\[ p(x) = \frac{1}{Z} \exp\{-u(x)\} \]
Generative PnP

Initialize \( X = \text{Random}(0, I) + \frac{1}{2} \)

Repeat {
    \( X \leftarrow F_0(X) \)  // Prior Model Proximal Generator
    \( X \leftarrow F_1(X) \)  // Forward Model Proximal Generator
}

Return(\( x \))

- Observations/questions:
  - This is a Markov chain
  - Does it converge to a stationary distribution?
  - If so, then what is the stationary distribution?
Theorem: Consider $X_n = F_1(F_0(X_{n-1}))$, then

- $X_n$ is a reversible Markov chain
- $X_n$ has a stationary distribution given by

$$\tilde{p}(x|y) = \frac{1}{Z} \exp\{-u_1(x) - \tilde{u}_0(x; \gamma^2)\}$$

  - where $\tilde{u}_0(x; \gamma^2)$ is $u_0(x)$ blurred with a Gaussian noise of variance $\gamma^2$.

**Bottom line:**

- Repeated sequential application of $F_0$ and $F_1$ converges to “desired” distribution.
- But GPnP introduces AWGN with variance $\gamma^2$ to the prior distribution!
Generative Plug-and-Play Intuition

Repeat {
  \( X \leftarrow F_0(X) \)
  \( X \leftarrow F_1(X) \)
}
Implementing Proximal Generators:

- Generic implementation
- Prior model proximal generator
- GPnP Pseudo-code
How to implement the Proximal Generator?

- For $\gamma$ small, just add white noise!

$$F(x) \approx \bar{F}(x) + \gamma W$$

- Proximal generator
- Ordinary proximal map
- Proximal map parameter
- White Gaussian noise
For small $\gamma$ …

$$\bar{F}_1(v) = \arg\min_x \left\{ W(x) + \frac{1}{2\gamma^2} \text{Proximal Generator} \right\}$$

"projection" onto "sensor manifold"
For the prior, we know that

\[ F_0(v) = \bar{F}_0(v) + \gamma W \]

\approx \text{Denoise}(v, \gamma) + \gamma W

But we will use **score matching** for:

- More flexible/accurate form
- Easier training (closed form loss function)
- But there is a “catch”…
Denoising Score Matching (Vincent 2011)*

- **Amazing result:**
  - The AWGN denoiser provides an exact MMSE estimate of the score

\[
-\nabla \tilde{u}_0(x; \sigma^2) \approx \frac{1}{\sigma^2} \left[ \text{Denoise}(x; \sigma) - x \right]
\]
  - Exactly true for any \( \sigma \)

- **But….**
  - \( \tilde{u}_0(x; \sigma^2) \) is the energy function for the “noisy” prior
  - So we have the exact solution, but for a noisy prior

Interpretation of Denoising Score Matching

Intuition:
- Denoiser moves towards larger probability
- Expected change approximates score

\[-\sigma^2 \nabla \tilde{u}_0(x; \sigma^2) \approx (\text{Denoise}(x) - x)\]

white noise ball with radius $\sigma$

probability density blurred by $\sigma$

Denoise($x$)
Prior Proximal Generator

- Define

\[ \beta = \frac{\gamma^2}{\sigma^2} \]

- Using score matching, the prior proximal generator is:

\[ \tilde{F}_0(x; \beta, \sigma) \approx (1 - \beta)x + \beta \text{Denoise}(x; \sigma) + \sqrt{\beta} \sigma W \]

- Remember:
  - \( \tilde{F}_0 \) is based on “noisy” prior, but noise decreases as \( \sigma \to 0 \)
  - More accurate approximation for \( \beta \ll 1 \)
Prior Model Proximal Generator

\[ \tilde{F}_0(x; \beta, \sigma) \approx (1 - \beta)x + \beta \text{Denoise}(x; \sigma) + \sqrt{\beta} \sigma W \]

- Prior blurred by \( \sigma \)
- Step size scaled by \( \beta \)
GPnP Basic Algorithm

\[ \beta = \frac{1}{4}; \sigma_{\text{max}} = 2; \]

Initialize \( X = \text{Random}(0, I) + \frac{1}{2} \)

Repeat {

\[ X \leftarrow (1 - \beta)X + \beta \text{Denoise}(X; \sigma) + \sqrt{\beta} \sigma \text{RandN}(0, I) \]
\[ X \leftarrow \bar{F}_1(X) + \sqrt{\beta} \sigma \text{RandN}(0, I) \]
\[ \sigma \leftarrow \text{Reduce}(\sigma) \]

}

Return(\( x \))

- Prior is blurred by \((1 + \beta)\sigma^2\)
- But with time \(\sigma \to 0\)
\[ \beta = \frac{1}{4}; \sigma_{\text{max}} = 2; \alpha = 1.3; \]

Initialize \( X = \text{Random}(0, I) + \frac{1}{2} \)

Repeat {
\[
X \leftarrow (1 - \beta)X + \beta \text{Denoise}(X; \alpha \sigma) + \sqrt{\beta} \sigma \text{RandN}(0, I)
\]
\[
X \leftarrow \bar{F}_1(X) + \sqrt{\beta} \sigma \text{RandN}(0, I)
\]
\[
\sigma \leftarrow \text{Reduce}(\sigma)
\]
}

Return(\( x \))

- Prior is blurred by \((1 + \beta)\sigma^2\)
- But with time \( \sigma \to 0 \)
Experiments

- **Experiment:**
  - Prior proximal generator: BM3D, DRUNet*, DDPM denoiser trained on CelebAHQ-256**
  - Forward model: interpolation with sparse sampling of 10%, 5%, 2% and missing rectangle.

- **Parameters**
  - $N = 100; \sigma_{\text{max}} = 0.5 \text{ or } 2.0; \sigma_{\text{min}} = 0.005; \beta = \frac{1}{4}; \alpha = 1.3$;
  - Same parameters work for different problems (interpolation, tomography, …) and different denoisers (BM3D, DRUNet, …).


Sparse interpolation: 10% of pixels sampled, BM3D prior
(Std dev intensity window changes)
Sparse interpolation: 10% of pixels sampled, DRUNet prior (Std dev intensity window changes)
Sparse interpolation: 5% of pixels sampled, DRUNet prior
(Std dev intensity window changes)
Sparse interpolation: 2% of pixels sampled, DRUNet prior (Std dev intensity window changes)
Inpainting: Center rectangle omitted - 3 samples, DRUNet prior (Std dev intensity window changes)
Inpainting: Center rectangle omitted - 3 samples, **BM3D prior** (Std dev intensity window changes)
Inpainting: Center rectangle omitted - 3 samples, DDPM denoiser trained on CelebAHQ-256 prior (Std dev intensity window changes)

IT’S A FACE!!
Conclusions

- **Generative PnP: A natural generalization of PnP original recipe**
  - Denoiser for prior
  - Proximal map for forward model
  - Iterate and add noise

- **GPnP vs Langevin Dynamics***:
  - Discrete Markov Chain vs Stochastic Differential Equation
  - Proximal Maps vs Gradient Descent
  - New Approach vs Established Method