How to Implement Physics-based Learning

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1. Introduction

Computational imaging systems (*e.g.* tomographic systems, computational optics, magnetic resonance imaging) jointly design software and hardware to retrieve information which is not traditionally accessible. Generally, such systems are characterized by how the information is encoded (forward process) and decoded (inverse problem) from the measurements. Critical aspects of computational imaging systems, such as experimental design and image priors, can be optimized through deep networks formed by *unrolling* the iterations of classical model-based reconstructions (Gregor & LeCun, 2010; Sun et al., 2016; Kellman et al., 2019). Termed physics-based learning, this paradigm is able to incorporate knowledge we understand, such as the physics-based forward model and optimization methods, while relying on data-driven learning for parameters that we do not.

The goal of this note is to explain practically how to implement physics-based learning for the rapid prototyping of an imaging system. Specifically, we advocate exploiting the auto-differentiation functionality (Griewank & Walther, 2008) twice, once to build ones physics-based network and again to perform physics-based learning. This will allow the user to only have to implement the forward model process for their system, whereby speeding up prototyping time. In this note, we provide a basic overview of physics-based learning, the construction of a physics-based network, and review its reduction to practice with a snippet of code. Finally, We provide an open-source implementation of physics-based learning with the physics-based network in Sec. 3 and training procedure using Pytorch (Paszke et al., 2017) for a sparse recovery problem.

2. Background

Computational imaging systems are described by how sought information is encoded to and decoded from a set of measurements. The encoding of information, $\mathbf{x}$ into measurements, $\mathbf{y}$, is given by

$$\mathbf{y} = \mathcal{A}(\mathbf{x}) + \mathbf{n}, \tag{1}$$

where $\mathcal{A}$ is the forward model process that characterizes the formation of measurements and $\mathbf{n}$ is random system noise. The retrieval of information from a set of measurements, *i.e.* decoding, is commonly structured using an inverse problem formulation,

$$\mathbf{x}^\star = \arg\min_{\mathbf{x}} \underbrace{\|\mathcal{A}(\mathbf{x}) - \mathbf{y}\|^2}_{\mathcal{D}(\mathbf{x};\mathbf{y})} + \mathcal{P}(\mathbf{x}) \tag{2}$$

where $\mathbf{x}$ is the sought information, $\mathcal{D}(\cdot)$ is the data consistency penalty (commonly ℓ_2 distance between the measurements and the estimated measurements), and $\mathcal{P}(\cdot)$ is the signal prior (*e.g.* sparsity, total variation). The solver to this optimization is often non-linear and iterative in nature. Proximal gradient descent (also referred to as iterative soft thresholding algorithm) can efficiently solve the optimization problem in the case of non-linear signal prior (Parikh & Boyd, 2014). Methods such as Alternating direction method of multipliers (Boyd et al., 2011) and half-quadratic splitting can be efficient solvers when multiple constraints are placed on the image reconstruction.

The physics-based network is then formed by unrolling K iterations of one of these optimization algorithms into the layers of a network. The input to the network will be the measurements and initialization and the output will be an estimate of the information or signal after K iterations of the optimizer.

3. Implementation

For the purposes of demonstration, we will perform physics-based learning for an under-determined sparse recovery problem from linear Gaussian random measurements (*i.e.* compressed sensing). The sparse signals have uniform random support and has amplitude that is normally distributed. The learnable parameters in the physics-based network will be the measurement matrix, the sparsity prior penalty, and the step size of the optimizer. Specifically, we solve the ℓ_1 relaxation of the sparse recovery problem,

$$\mathbf{x}^\star = \arg\min_{\mathbf{x}} \|\mathbf{A}\mathbf{x} - \mathbf{y}\|^2 + \lambda\|\mathbf{x}\|_1, \tag{3}$$

where λ is the sparsity prior penalty that trades off the penalty of the prior with the data consistency term, $\mathbf{A} \in \mathbb{R}^{M\times N}$ is the measurement matrix.

We consider proximal gradient descent algorithm (Alg. 1) to solve the optimization problem (Eq. 3) and to form the architecture of the physics-based network.

Algorithm 1 Proximal Gradient Descent

Inputs $\mathbf{x}^{(0)}$-initialization, α-step size, K-number of iterations, $\mathbf{y}$-measurements
Output $\mathbf{x}^{(N)}$-final estimate of image

```
1: $k \leftarrow 0$
2: for $k < K$ do
3:     $\mathbf{z}^{(k)} \leftarrow \mathbf{x}^{(k)} - \alpha \nabla_{\mathbf{x}} \mathcal{D}(\mathbf{x}^{(k)}; \mathbf{y})$
4:     $\mathbf{x}^{(k+1)} \leftarrow \texttt{soft thr}_{\alpha\lambda}(\mathbf{z}^{(k)})$
5:     $k \leftarrow k + 1$
6: end for
```

Physics-based network

With some extra Pytorch specific flags and functionalities, the physics-based network (Fig. 1 mirrors the basic structure of Alg. 1. In implementation, it requires all learnable parameters as input (measurement matrix, step size, and sparsity penalty), initialization, ground truth, and number of iterations (or depth of network). As output, the network returns the final estimate of the sparse recovery optimization.

```
 1 def pbnet(A, alpha, lamb, x0, xt, K, testFlag=True):
 2     # pbnet - Physics-based Network
 3     # args in -
 4     #   A - measurement matrix
 5     #   alpha - step size
 6     #   lamb - sparsity penalty
 7     #   x0 - initialization
 8     #   xt - ground truth sparse vector
 9     #   K - number of layers (i.e. iterations)
10     #   testFlag - disables training (default True)
11     # args out -
12     #   x - output of network (final estimate)
13
14     x = x0.detach().clone()
15     x.requires_grad = True
16
17     y_meas = Aop(A, xt)
18     if testFlag: y_meas = y_meas.detach()
19
20     for kk in range(K):
21         y_est = torch.matmul(A,x)
22         res = y_est - y_meas
23         loss_dc = torch.sum(res**2)
24         g = torch.autograd.grad(loss_dc,
25                                 x,
26                                 create_graph = not testFlag)
27
28         x = x - alpha*g[0]           # gradient update
29         x = softthr(x, lamb*alpha)   # proximal update
30     return x
```

Figure 1. Implementation of a physics-based network for compressed sensing sparse recovery using automatic differentiation to compute gradients with respect to $\mathbf{x}$. The network is setup to learn the measurement matrix, step size, and sparsity penalty. Soft thresholding is used as the proximal operator.

The specific Pytorch flags and functionalities that enable us to properly use the automatic differentiator for sparse recovery and for physics-based learning are contained in lines 14, 15, and 26. Lines 14 and 15 set up the initialization to the network, first in line 14 detaching it from any previous automatic differentiation graphs and second in line 15 setting its *requires_grad* field to be True. This will allow the automatic differentiation to track operations related to $\mathbf{x}$ for taking derivatives of $\mathcal{D}(\mathbf{x}; \mathbf{y})$ with respect to $\mathbf{x}$. Line 26 sets the *create_graph* flag of the automatic differentiator to True. This tells Pytorch to store these operations so that they can be traced through by a second automatic differentiator for computing derivatives with respect to learnable parameters.

While some physics-based networks take in measurements as input, this is often not possible when learning a system's experimental design. Here, in line 17, the measurements are synthesized using the learnable measurement matrix and ground truth sparse vector.

Physics-based Learning

The mechanics of training a physics-based network are similar to that of training any neural net or convolutional neural network in that it relies on a dataset, an optimizer, and automatic differentiation to compute gradients. In our particular application our dataset consists of sparse vectors with amplitudes that are normally distributed and support that is uniformly distributed. As for the optimizer, we use the Adam (Kingma & Ba, 2014) to perform the gradient updates.

4. Remarks

In this note we overview the basic principles of physics-based learning, as well as, how to implement a physics-based network in Pytorch. We provide a simple open-source implementation for physics-based learning should provide a minimum working example for those looking to optimize their own system. While this particular example demonstrates physics-based learning for 1D sparse recovery using proximal gradient descent to form the physics-based network, the concepts discussed here generalize to vast set of applications and optimization algorithms.

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