Structure exploiting hierarchical optimization methods

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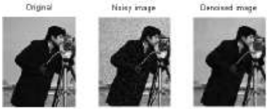
The context

The problem: large scale optimization problems

$$\min_{x \in \mathbb{R}^n} f(x), \quad n \text{ large}$$

- Image restoration

$$\min_x \|Ax - b\|^2 + \lambda \|Dx\|^2$$

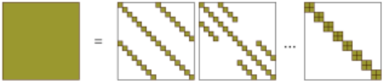


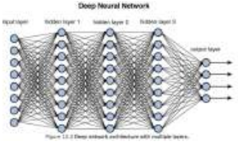
- Neural networks training

$$\min_\theta \sum_{i=1}^{N} \ell(NN(\theta; x_i), y_i)$$

- Matrix factorization

$$\min_{X_1, \dots, X_L} \|A - X_1 \dots X_L\|_F^2$$





Dimensionality reduction

AIM? Reduce the computational cost of the solution process
HOW? Exploit the structure to build approximated subproblems

Dimensionality reduction

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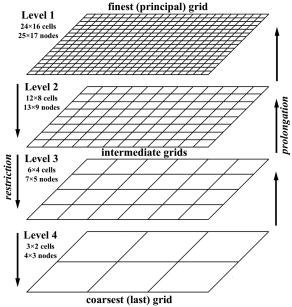
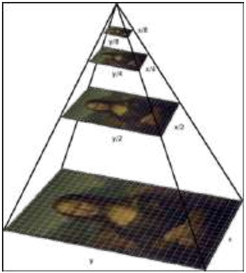
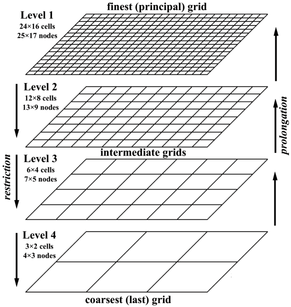
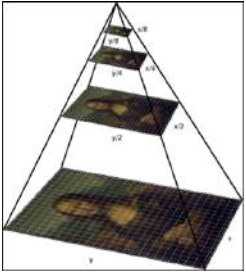




Dimensionality reduction

AIM? Reduce the computational cost of the solution process
HOW? Exploit the structure to build approximated subproblems





Multilevel methods (ML)

Outline

Origins of multilevel methods: multigrid (MG)

A block coordinate descent perspective on MG methods

Application domains of the ML framework

- Physics informed neural networks (distributed)
- Image restoration (hierarchical)

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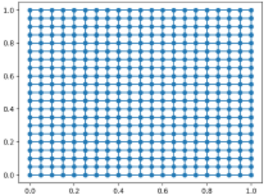
The numerical solution of PDEs

- Classically PDEs are discretized on a grid
- The resulting linear system $Au = f$ is solved using a fixed point method
- The size of the grids impacts the size of the system and the accuracy of the solution approximation



Fixed point: reduction of the error

Fixed point scheme :

$$u^{(m+1)} = Bu^{(m)} + g$$

After M iterations:

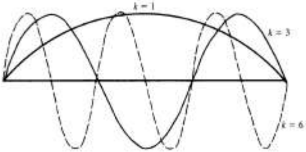
$$e^{(M)} = u^{(M)} - u^* = \sum_{k=1}^{n-1} c_k \lambda_k^M(B) v_k$$

Fourier modes:

$$v_k(j) = \sin\left(\frac{kj\pi}{n}\right), \ k \text{ frequency component}$$

On a n-point grid:

- $1 \leq k < \frac{n}{2}$ low
- $\frac{n}{2} \leq k < n-1$ high

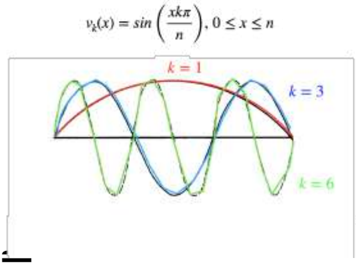


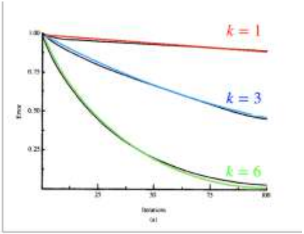
Limitation of iterative schemes: the smoothing property

$$e^{(M)} = u^{(M)} - u^* = \sum_{k=1}^{n-1} c_k \lambda_k^M(B) v_k$$

- $\lambda_1(B) \approx 1$
- $|\lambda_k(B)| < 1/3$ for $n/2 \leq k \leq n-1$

Hard to reduce the low frequency components of the error



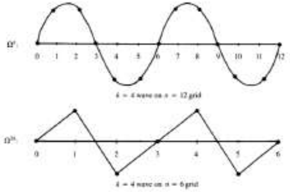


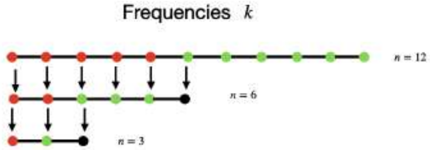
How to make the methods efficient on all frequencies?

Frequency shift!

- **Fine** grid Ω^h with n points: $1 \leq k \leq n-1$
- **Coarse** grid Ω^{2h} with $n/2$ points: $1 \leq k \leq n/2$

Property: $v_k^h(2j) = v_k^{2h}(j)$
Frequency $1 \leq k \leq n/2$ in Ω^h $\rightarrow$ Frequency k in Ω^{2h}





Two-level multigrid methods

Consider a PDE:

$$\mathcal{A}(u) = f.$$

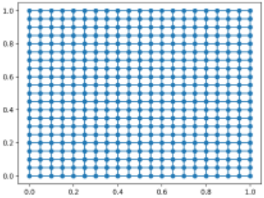
Consider two discretizations:

- Fine grid: $\mathcal{A}_h(u_h) = f_h$
- Coarse grid: $\mathcal{A}_H(u_H) = f_H$

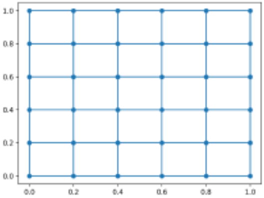
Idea: write the solution u as the sum of a fine and a coarse term:

$$u \sim \underbrace{v_h}_{\in \mathbb{R}^h} + P(\underbrace{e_H}_{\in \mathbb{R}^H}), \; H < h.$$

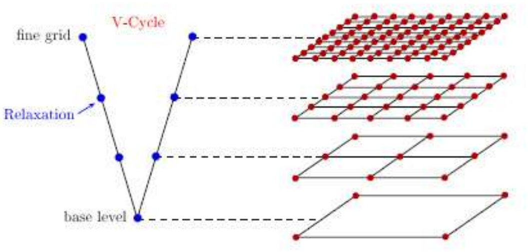
and update the two components in an alternate fashion.



$R \Downarrow$ $\qquad$ $P \Uparrow$



General multigrid methods



W. Briggs, V. Henson, S. McCormick. A Multigrid Tutorial, SIAM, 2000.

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ML methods: abstraction from the PDE context

Problem: $\mathcal{F}$ space of continuous functions parametrized by x

$$\min_{y \in \mathcal{F}} f(y)$$

Approach: we look for y as the sum of two terms

$$y(x) = y_1(x_1) + y_2(x_2).$$

This yields the optimization problem

$$\min_{(x_1, x_2) \in \mathbb{R}^n} f(y_1(x_1) + y_2(x_2)),$$

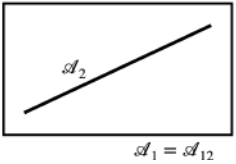
where $n = n_1 + n_2$.

ML methods: approximation spaces

$$\mathcal{A}_{12} = \left\{ y \in \mathcal{F} \mid y(x) = y_1(x_1) + y_2(x_2) \ \text{ for some } \ (x_1, x_2) \in \mathbb{R}^n \right\}$$
$$\mathcal{A}_i = \left\{ y \in \mathcal{F} \mid y(x) = y_i(x_i) \ \text{ for some } \ x_i \in \mathbb{R}^{n_i} \right\} \quad (i = 1, 2).$$

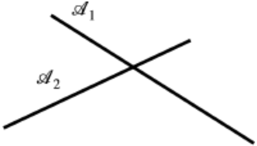
Hierarchical context

$\mathcal{A}_2 \subset \mathcal{A}_1 = \mathcal{A}_{12}$



Distributed context

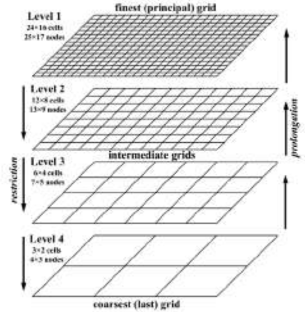
$\mathcal{A}_1, \mathcal{A}_2 \subset \mathcal{A}_{12}$



The hierarchical context

Example: classical MG

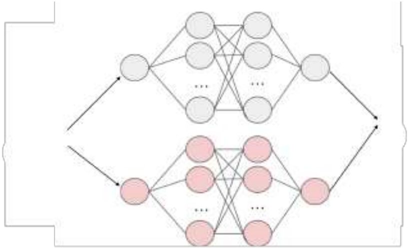
$$f(x) = \frac{1}{2}x^T A x + x^T b$$



The distributed context

Example: neural networks

$$f(x) = \text{loss}$$
$$y_1(x_1) = NN_1(x_1)$$
$$y_2(x_2) = NN_2(x_2)$$



A block coordinate descent (BCD) perspective on ML

The hierarchical context

Alternate:

$$\min_{(x_1, x_2) \in \mathbb{R}^{n_1+n_2}} f(y_1(x_1)+y_2(x_2))$$

and

$$\min_{\substack{x_2 \in \mathbb{R}^{n_2} \\ x_1 \text{ fixed}}} f(y_1(x_1)+y_2(x_2))$$

The distributed context

Alternate:

$$\min_{\substack{x_2 \in \mathbb{R}^{n_1} \\ x_1 \text{ fixed}}} f(y_1(x_1)+y_2(x_2))$$

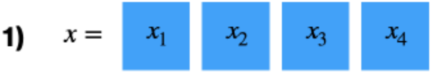
and

$$\min_{\substack{x_1 \in \mathbb{R}^{n_1} \\ x_2 \text{ fixed}}} f(y_1(x_1)+y_2(x_2)).$$

A BCD-ML algorithm: an iteration

How to update x?

1 Partition x in blocks: $(x_1, \ldots, x_n)$



A BCD-ML algorithm: an iteration

How to update x?

2 Select a block i $(x_1, \ldots, x_i, \ldots, x_n)$
- Criterion: $\|\nabla_i f(x)\| \geq \tau \|\nabla f(x)\|$, $\tau \in (0, 1)$

2)

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A BCD-ML algorithm: an iteration

How to update x?

3 Update the block:

- p_k iterations of a first-order method (possibly *stochastic*)

$$\min_{x_i} f(x_1, \ldots, x_i, \ldots, x_n) \to x_i^{new}$$

- $x_i \leftarrow x_i^{new}$

3)

$$\min_{x_3} f(x_1, x_2, x_3, x_4)$$

$$x_3 \leftarrow x_3^{new}$$

BCD theory for nonconvex problems

- Powell (1973): cyclic BCD may fail on nonconvex continuously differentiable functions.
- Bertsekas (1999): convergence of cyclic BCD if minimizer along any coordinate direction from any point is unique
- Attouch et all. (2010) + Bolte et all (2014), proximal alternating methods under Kurdyka-Lojasiewicz (KL) property convergence of sequence to stationary points
- Amaral et all. (2022) high (p)-order BCD smooth nonconvex for Lipschitz continuous $\nabla f(x_k)$ + regularized models $\rightarrow O(\epsilon^{-(p+1)})$

A BCD-ML algorithm: convergence theory

Theorem (Gratton, Mercier, R., Toint, 2023)

If f has L-Lipschitz continuos gradient and step-size $\alpha_k = \alpha < 1/L$

- **Deterministic**

$$\|\nabla f(x^{(K)})\| \leq \epsilon \to K = O\left(\frac{1}{\epsilon^2 p}\right)$$

- **Stochastic**

$$\mathbb{E}\left(\sum_{k=1}^{K} \|\nabla f(x^{(k)})\|^2\right) \leq C_1(\sigma^2) + O\left(\frac{1}{K}\right) - C_2(\sigma^2) p$$

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Physics informed neural networks

Approximate the solution of a PDE by a neural network

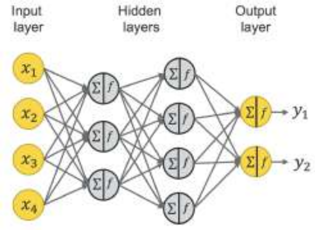
M. Raissi, P. Perdikaris, G. Karniadakis, Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, 2019.

Why this approach ?

- Natural approach for nonlinear equations
- Provides analytic and continuously differentiable expression of the approximate solution
- The solution is meshless, well suited for problems with complex geometries
- The training is highly parallelizable on GPU
- Allows to alleviate the effect of the curse of dimensionality

General neural network strategy for learning problems

Neural network



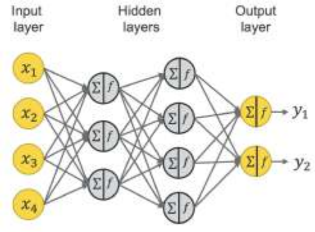
Training data

Training problem:

$$\min_{\theta \in \Theta} L(\theta) = \frac{1}{m} \sum_{i=1}^{m} (NN(\theta, x_i) - y_i)^2$$

General neural network strategy for learning problems

Neural network



Training data

Training problem:

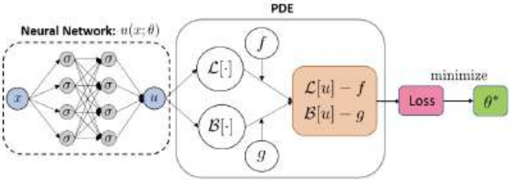
$$\min_{\theta \in \Theta} L(\theta) = \frac{1}{m} \sum_{i=1}^{m} (NN(\theta, x_i) - y_i)^2$$

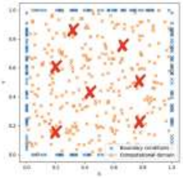
How to integrate the physical knowledge in the model?

Physics Informed Neural Networks (PINNs)

Neural network

Training data





Training problem: $\underset{\theta\in\Theta}{min} L(\theta) = L_{OBS}(\theta) + L_{PDE}(\theta)$

$$L_{OBS}(\theta) = \frac{1}{m_1} \sum_{x_i\in\Omega\cup\partial\Omega} (NN(\theta,x_i) - y_i)^2,$$

$$L_{PDE}(\theta) = \frac{1}{m_{2,i}} \sum_{x_i\in\Omega} (\mathcal{L}(NN(\theta,x_i)) - f(x_i))^2) + \frac{1}{m_{2,b}} \sum_{x_i\in\partial\Omega} (\mathcal{B}(NN(\theta,x_i)) - g(x_i))$$

How to fit the training of PINNs in the ML framework?

An important ingredient: the F-principle

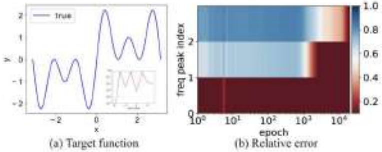
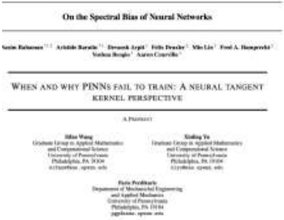


Figure 1: 1d input. (a) $f(x)$. Inset : $|\hat{f}(k)|$. (b) $\Delta_F(k)$ of three important frequencies (indicated by black dots in the inset of (a)) against different training epochs. The parameters of the DNN is initialized by a Gaussian distribution with mean 0 and standard deviation 0.1. We use a tanh-DNN with widths 1-8000-1 with full batch training. The learning rate is 0.0002. The DNN is trained by Adam optimizer [20] with the MSE loss function.



On the Spectral Bias of Neural Networks

When and why PINNs fail to train: A neural tangent kernel perspective

$\Rightarrow$ PINNs are not effective in approximating highly oscillatory solutions

How to transpose the ingredients of success of MG

Basic idea of MG: Exploiting "complementarity" between problems involved

Classical MG vs Neural networks

- Consider a minimization method and a class of problems for which this method is efficient

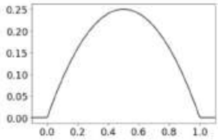
Classical MG	Neural networks
smoothing (GS orJ)	first-order (GD, SGD)
high-frequency	low-frequency

- Split the problem depending of its frequency content
- Shift the frequencies

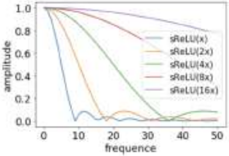
Classical MG	Neural networks
Coarser discretizations	Specialized architectures (Mscale networks)

Specialized architectures

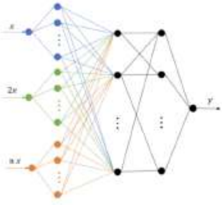
- **Mscale networks**: [Liu, Cai and Xu, (2020)] frequency-selective subnetworks + wavelet-inspired and frequency-located activation functions



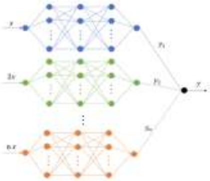
(b) sReLU



(a) sReLU



(a) MscaleDNN-1



(b) MscaleDNN-2

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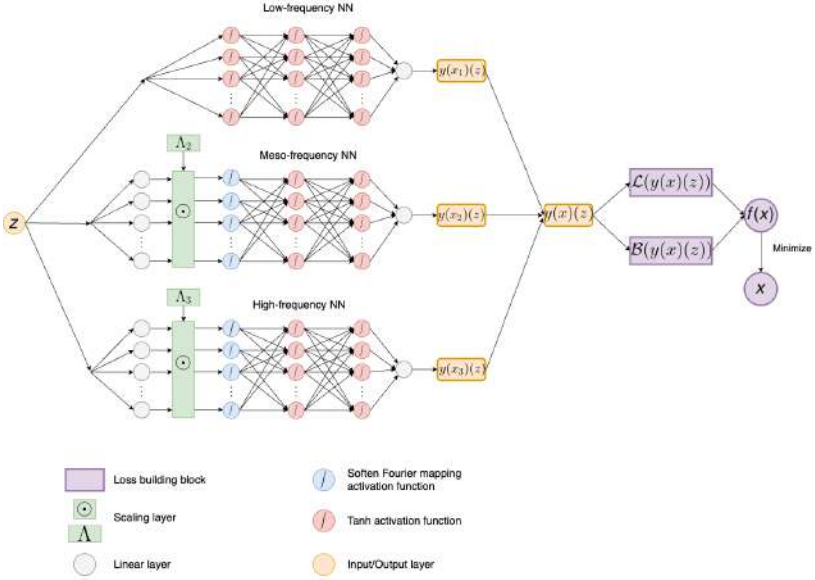
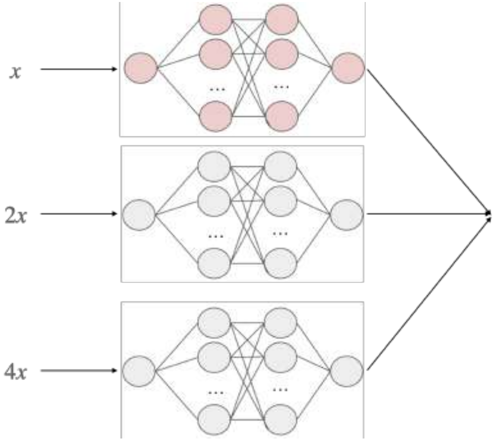
Our architecture



Multilevel PINNs: the training

From simultaneous training to BCD training!



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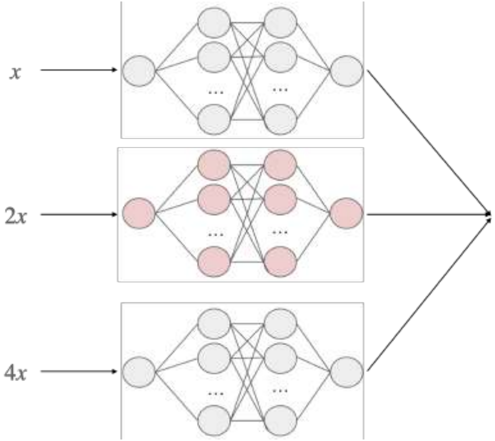

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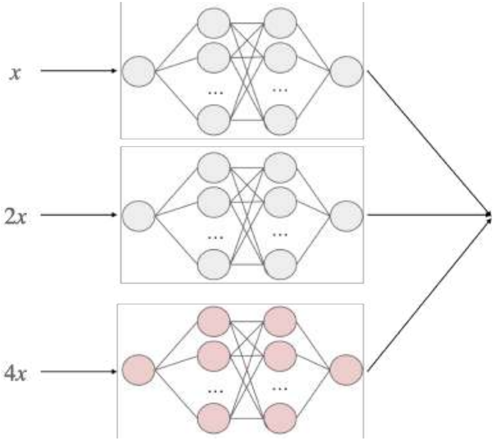
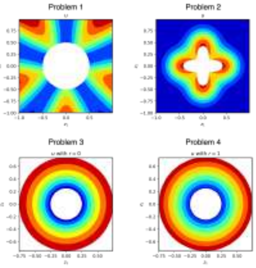
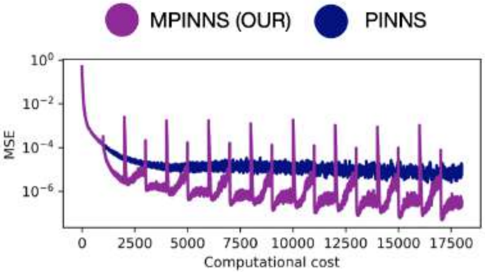


Numerical results: MSE vs iterations

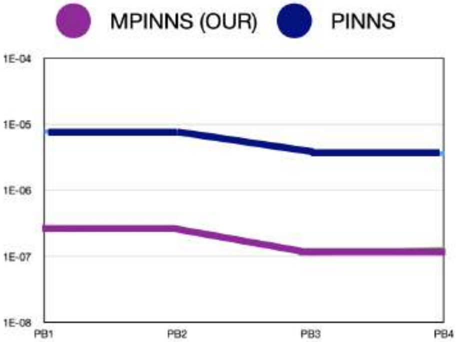
Problem: $\Delta u = f$ on Ω



Ω

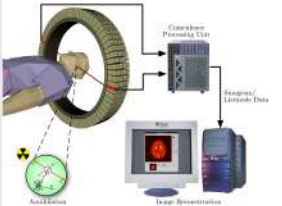


Numerical results: final MSE on average (10 runs)

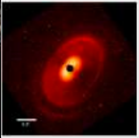


Inverse problems in imaging: various applications

Medical imaging



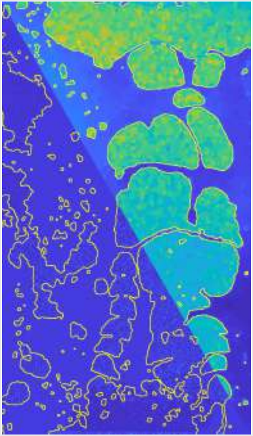
Astronomy



@ L. Denneulin

SPHERE/IRDIS

Physics



@ B. Pascal

Thanks to Nelly and Guillaume for the pictures !

Problem formulation

$$\widehat{x} \in \arg\min_{x} \frac{1}{2}\|Ax - z\|_2^2 + \lambda\|Lx\|_\star$$

with $\|Lx\|_\star$ usually sparsity inducing norm.

$\overline{x}$

z

$\widehat{x}$

Problem formulation

More generally

$$\min_x \; f(x) + g(x)$$

- f differentiable with Lipschitz gradient
- g possibly non-smooth but proximable

Classical solution methods:

- require prox computation (usually not available in closed form)
- suitable for problems of reasonable size

ML to leverage large dimensions?

Multilevel methods in nonlinear optimization (NO)

ML approaches for nonlinear smooth problems

- S.G. Nash, MG/Opt (2000)
- S. Gratton, A. Sartenaer, and P. Toint, RMTR (2008)

Multilevel methods for imaging problems?

ML approaches on smoothed image problems

- A. Javaherian and S. Holman, (tomography, 2017)
- S. W. Fung and Z. Wendy, (phase retrieval, 2020)
- J. Plier, F. Savarino, M. Kocvara, and S. Petra, (tomography, 2021)

Multilevel methods for imaging problems?

ML approaches on smoothed image problems

- A. Javaherian and S. Holman, (tomography, 2017)
- S. W. Fung and Z. Wendy, (phase retrieval, 2020)
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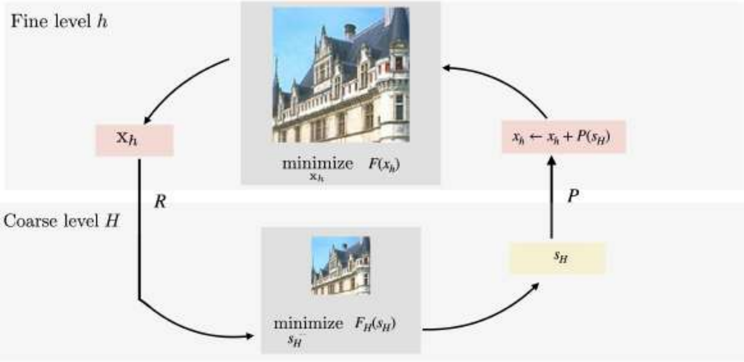
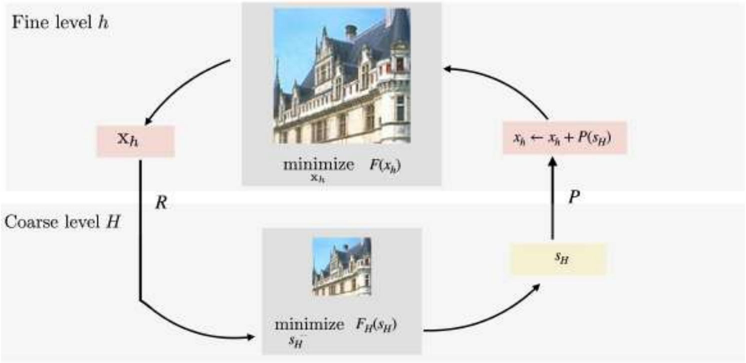
Extension of ML to a non-smooth setting?

An iteration of a multilevel procedure



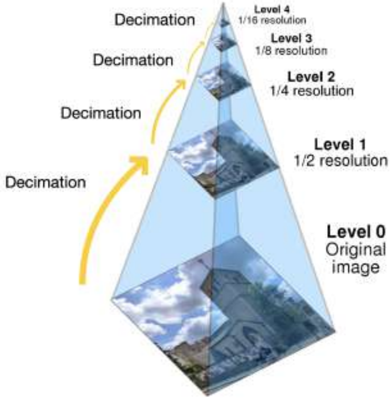
An iteration of a multilevel procedure

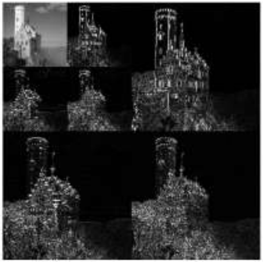


R, P?

F_H?

A hierarchy of images: R, P





Coarse model definition F_H

$$F(x) = \frac{1}{2}\|Ax - z\|_2^2 + \lambda\|Lx\|_1$$
$$F_H(x) = \frac{1}{2}\|A_H x_H - z\|_2^2 + \lambda\|L_H x_H\|_1$$

Coarse model definition F_H

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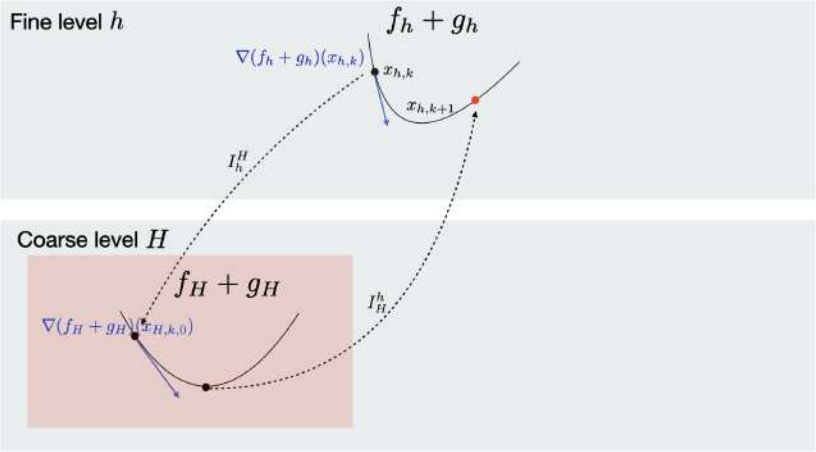
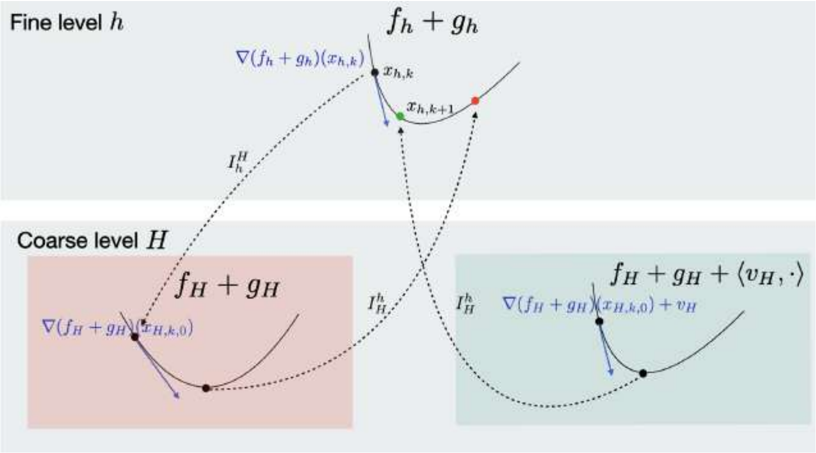
Is this model useful in minimizing F?

Design of F_H in smooth context: First order coherence



Design of F_H in smooth context: First order coherence



Coarse model definition F_H

$$F(x) = \frac{1}{2}\|Ax - z\|_2^2 + \lambda\|Lx\|_1$$

$$F_H(x_H) = \frac{1}{2}\|A_H x_H - z\|_2^2 + \lambda\|L_H x_H\|_1 + < v_H, x_H >$$

$$v_H = R\nabla F(x) - \nabla F_H(Rx)$$

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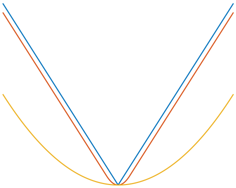
$$v_H = R\nabla F(x) - \nabla F_H(Rx)$$

[Parpas 2017] Nonsmooth case $\rightarrow$ smoothing!



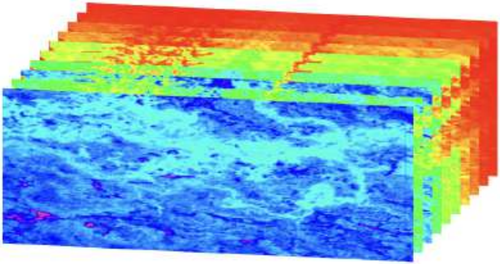
Our contributions

- Specify the method for the context of image restoration: $g(x) = \varphi(Lx)$
- Inexact proximal steps to handle state-of-the-art regularization: TV, NLTV

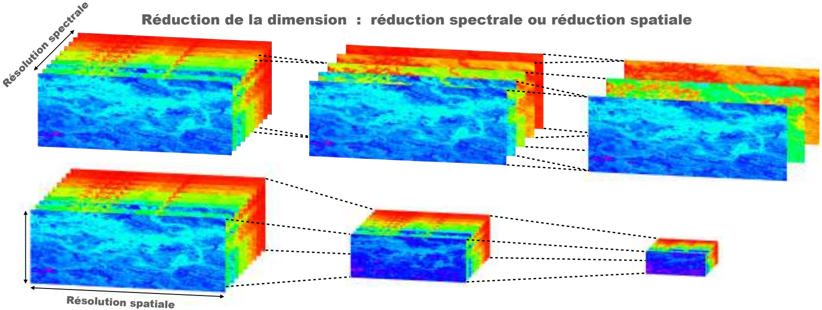
$$x_{k+1} = \tilde{\text{prox}}_{\tau\varphi\circ\mathrm{L}}\left(\bar{y}_k - \tau\nabla f(\bar{y}_k)\right)$$
$$y_{k+1} = x_{k+1} + \alpha_k(x_{k+1} - x_k)$$

  - FISTA: $\bar{y}_k = y_k$
  - IML FISTA: $\bar{y}_k = ML(y_k) \longleftrightarrow \min F_H$
- Obtain state-of-the-art convergence guarantees
- Explore definition of R, P, F_H in different contexts

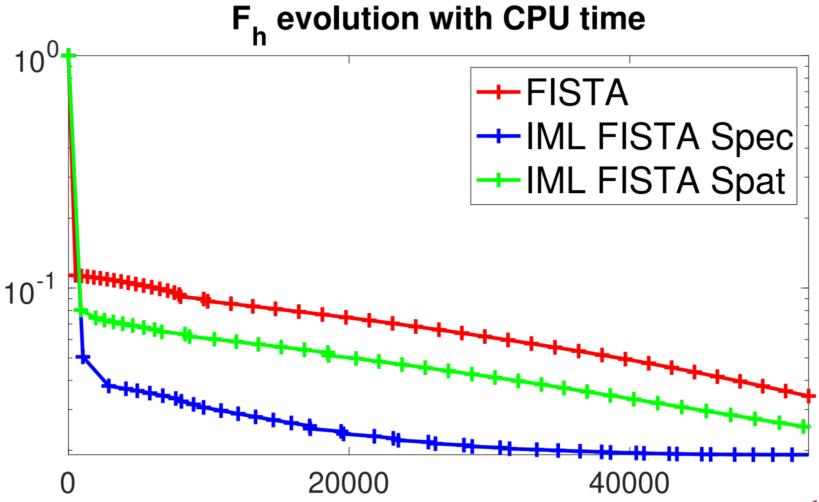
Hyperspectral images



How to build the coarse approximations?

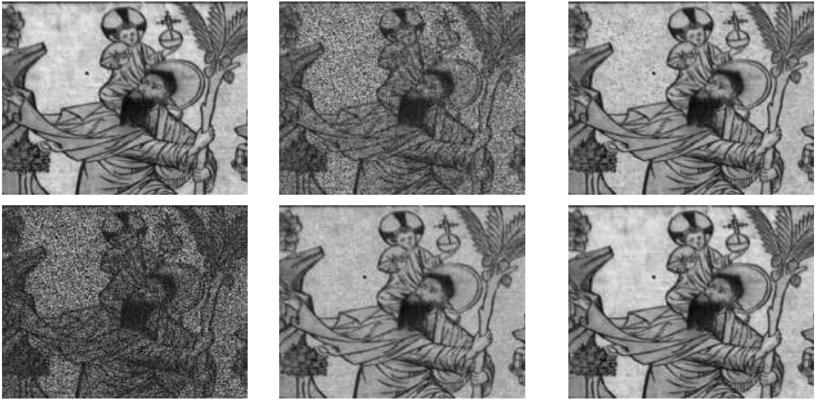


Objective function evolution



Results with Spectral IML FISTA

$\bar{x}$ (SNR) $\quad x_{2,\mathrm{FISTA}}$ (7 dB) $\quad x_{\mathrm{end,FISTA}}$ (21 dB)



z (3 dB) $\quad \mathrm{x}_{2,\mathrm{IML\ FISTA}}$ (19 dB) $\quad \mathrm{x}_{\mathrm{end,IML\ FISTA}}$ (35 dB)

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Conclusions

- We have presented a new BCD perspective on multilevel methods with unifying convergence analysis
- We have adapted the framework to two practical problems:
  - PINNs training
  - Image restoration
- We have demonstrated that exploiting multiple scales provides significant computational benefits (faster convergence).

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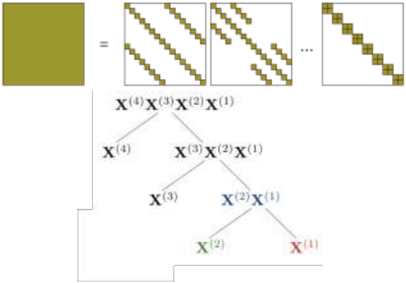
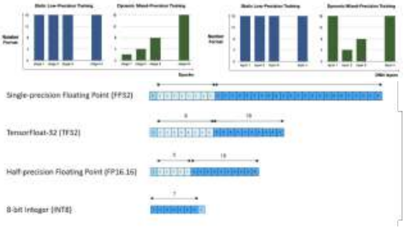
Study structure exploiting hierarchical techniques in other contexts

Sparse matrix factorization



- application to neural networks ?
- quantization?

Mixed precision training



...ongoing work with

Thank you for your attention!

A few references

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- G. Lauga, E. Riccietti, N. Pustelnik, P. Gonçalves, IML FISTA: A Multilevel Framework for Inexact and Inertial Forward-Backward. Application to Image Restoration, preprint, 2023.
- S. Gratton, V. Mercier, E. Riccietti, Ph.L. Toint, A Block-Coordinate Approach of Multi-level Optimization with an Application to Physics-Informed Neural Networks, arXiv preprint, 2023.

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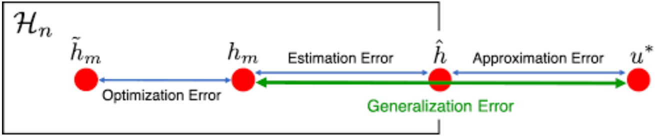
Convergence theory [Shin, Darbon, Karniadakis, 2020]

- the universality property of NN (approximation error)
- statistical sampling,
- ability of numerical optimizers (ADAM,SGD,...) to reach an approximate global optimum of nonconvex function



- $\tilde{h}_m$ our network,
- h_m a perfectly trained network on the dataset,
- $\hat{h}$ function minimizing the problem with infinitely many data,
- u^* the solution of the underlying PDE

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Convergence theory [Shin, Darbon, Karniadakis, 2020]

- L_{PINN} expected loss
- L_m empirical loss over m samples
- α Holder constant
- d dimension
- HP: the derivation is based on the probabilistic space filling arguments, assume that training data distributions cover the interior and the boundary

With high probability

$$L_{PINN}(h) \leqslant L_m(h) + C(m^{\alpha/d})$$

and

$$L_{PINN}(h_m) \leqslant C(m^{\alpha/d})$$

with $h_m \in H_n$ minimizer of L_m If PDE is linear (elliptic or parabolic)

$$\lim_{m\to\infty} h_m = u^*$$

(seq of minimizers conv uniformly to PDE sol in infinite data regime)

Inexact FISTA

$$\min_x f(x) + \varphi(\mathrm{L}x)$$

[Aujol, Dossal, 2015]:

$$\begin{aligned} x_{k+1} &\approx_{\epsilon_k} \operatorname{prox}_{\tau\varphi\circ\mathrm{L}}\left(y_k - \tau\nabla f(y_k) + e_k\right) \\ y_{k+1} &= x_{k+1} + \alpha_k(x_{k+1} - x_k) \end{aligned}$$

Contribution: update y_k through a multilevel step.

IML FISTA

$$\min_x \frac{1}{2}\|Ax - b\|^2 + \varphi(\mathrm{L}x)$$

$$x_{k+1} = \tilde{\text{prox}}_{\tau\varphi\circ\mathrm{L}}\left(\bar{y}_k - \tau\nabla f(\bar{y}_k)\right)$$
$$y_{k+1} = x_{k+1} + \alpha_k(x_{k+1} - x_k)$$

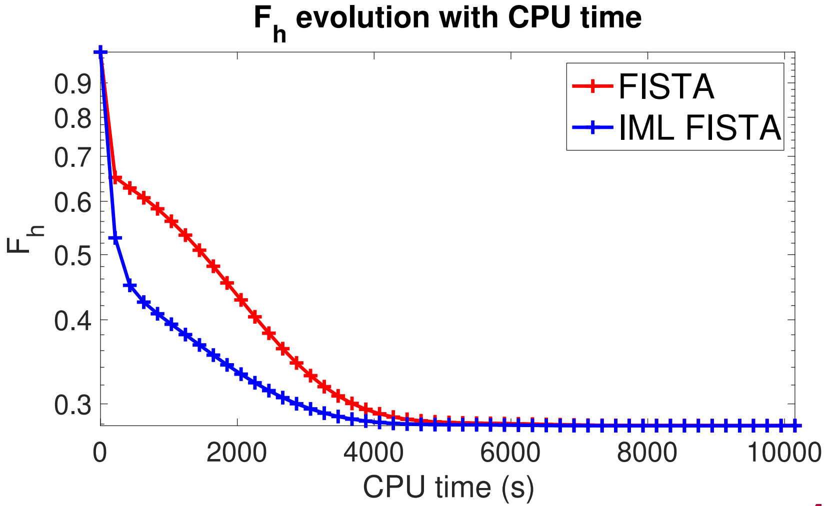
- FISTA: $\bar{y}_k = y_k$
- IML FISTA: $\bar{y}_k = ML(y_k) \longleftrightarrow \min F_H$

$$F_H(x) := \frac{1}{2}x^T(P^TAP)x - b^TPx + {}^{\gamma}\varphi_H \circ L_H + {v_H}^T x$$

$${}^{\gamma}\varphi, {}^{\gamma}\varphi_H \to v_H$$

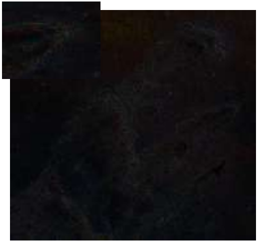
Image reconstruction with NLTV prior

Evolution of F_h for a $N_h = 2048 \times 2048 \times 3$ image

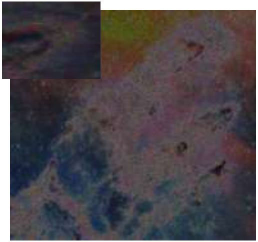


Reconstruction after 2 iterations with NLTV

z



x_2 FISTA



x_2 IML FISTA

The hierarchical context

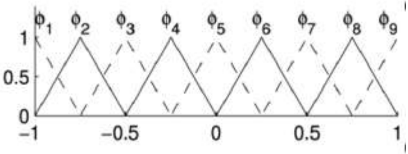
Example: classical MG

$$f(x) = \frac{1}{2}x^T A x + x^T b$$

$$y_1(x_1) = \sum_{j=1}^{n_1} x_{1,j} b_j$$

$$y_2(x_2) = \sum_{j=1}^{n_1} (Px_2)_j \, b_j$$

$$\mathcal{F} = \mathrm{span}\{b_j\}_{j=1}^{m}, \; m = n_1$$



In this context, we have that

$$\mathcal{A}_2 = \left\{ \sum_{j=1}^{m} (Px_2)_j \, b_j \right\} \subset \left\{ \sum_{j=1}^{m} (x_{1,j} + (Px_2)_j) \, b_j \right\} = \mathcal{A}_1 = \mathcal{A}_{12}.$$