FROM RESEARCH TO INDUSTRY





Solving inverse problems Olds and new

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What is an inverse problem ?



Retrieving the CMB From microwave observations



Mars express

Hyperspectral data in astrophysics Mars Express, Cassini, etc.



What is an inverse problem ?



Detection of a Massive Black Hole Binary signal from interferometric data



$$b = x + n$$
 $n \sim \mathcal{N}(0, \sigma^2)$

Formalism

More generally, we will focus on linear inverse problems where :



This models many inverse problems arising in physics :

- Denoising (A is the identity operator)
- Deconvolution (A is the convolution kernel)
- Inpainting/missing data interpolation (A is a binary mask)
- Tomographic reconstruction (A is the partial Radon transform)
- Radio-interferometric reconstruction (A is the partial Fourier transform)
- Compressed sensing
- Blind source separation

Where it started

There are many ways to tackle inverse problems (IP). So far, the vast majority of methods which have been proposed to solve (IP) boil down to finding some solution/estimator which minimizes some cost function:

$$\hat{x} = \operatorname{Argmin}_{x} \quad \mathcal{J}(x)$$

Probably the most popular estimator in Physics is the least-square estimator :

$$\hat{x} = \operatorname{Argmin}_{x} \quad \|b - Ax\|_{2}^{2}$$

which minimizes the Euclidean norm between the observations and the model.

In the previous example:

$$\hat{x}_{LS} = b$$



Remark: in case the noise is additive and Gaussian, the LS estimator is equivalent to the celebrated Maximum Likelihood estimator in statistics.

The least-square estimator does not assume any prior assumption about the signal to be retrieved. Including such kind of prior information can be done by penalizing/favoring certain desired signal properties in the estimate procedure. This is done by adding a prior/penalization term in the cost function:



Again, many penalization/penalty terms have been proposed in the literature (ex: energy, entropy, signal smoothness, positivity, etc). Probably the simplest penalty is the one that penalizes high-energy solutions:

$$\hat{x} = \operatorname{Argmin}_{x} \quad \lambda \|x\|_{2}^{2} + \|b - x\|_{2}^{2}$$

Remark: in statistics, the use of prior knowledge arises naturally in the Bayesian inference framework. The aforementioned estimator is then better known as the maximum a posteriori estimator (MAP).

A simple application

The least-square estimator does not assume any prior assumption about the signal to be retrieved. Including such kind of prior information can be done by penalizing/favoring certain desired signal properties in the estimate procedure. This is done by adding a prior/penalization term in the cost function:

$$\hat{x} = \operatorname{Argmin}_{x} \mathcal{P}(x) + \mathcal{J}(x)$$

penalty term (penalizes/favors certain signal properties)

data fidelity term (measures how well the model fits the data)

Again, many penalization/penalty terms have been proposed in the literature (ex: energy, entropy, signal smoothness, positivity, etc). Probably the simplest penalty is the one that penalizes high-energy solutions:

$$\hat{x} = \operatorname{Argmin}_{x} \quad \lambda \|x\|_{2}^{2} + \|b - x\|_{2}^{2}$$

$$\hat{x} = \frac{1}{\lambda + 1}b$$

1

Remark: this is best known as the Wiener filter

Remark: in statistics, the use of prior knowledge arises naturally in the Bayesian inference framework. The aforementioned estimator is then better known as the maximum a posteriori estimator (MAP).

In the last two decades, the most dramatic advances in signal estimation have focused on using prior information enforcing signal properties based on desired geometrical/morphological properties.

Gist of the sparsity : signals can be sparsely represented in representations (basis, etc.) that efficiently encode their geometrical/morphological properties.



Discrete cosine transform











sorted wavelet coefficients











0.1%

JPEG VS JPEG 2000

Original BMP 300x300x24 270056 bytes

JPEG 1:68 3983 bytes



JPEG2000 1:70 3876 bytes



Based on an harmonic basis (Discrete Cosine Transform)



Based on the wavelet transform

In general, sparse representations should be chosen based on the desired morphology



Let's assume x is sparse is some orthogonal basis: $\alpha = \Phi x$

$$\hat{x} = \operatorname{Argmin}_{x = \Phi \alpha} \quad \mathcal{P}(\alpha) + \|b - \Phi \alpha\|_{2}^{2}$$

sparsity-enforcing penalty

data fidelity term (measures how well the model fits the data)

Examples of penalty terms:

$$\mathcal{P}(\alpha) = \|\alpha\|_{\ell_0}$$

The 0-norm counts the number of nonzero elements

$$\mathcal{P}(\alpha) = \|\alpha\|_{\ell_1}$$
$$\|\alpha\|_{\ell_1} = \sum_i |\alpha[i]|$$

Denoising as a linear inverse problem:

$$b = x + n$$

The observation matrix A is the identity matrix.

The noise is assumed to be additive, white and Gaussian: $n \sim \mathcal{N}(0, \sigma^2)$





SNR = 1dB

It can be recovered from the noisy data by solving the following linear inverse problem:

$$\hat{x} = \operatorname{Argmin}_{x} \quad \lambda \|x\|_{\ell_{p}} + \frac{1}{2}\|b - x\|_{2}^{2}$$
with:
$$\|x\|_{\ell_{p}} = \left(\sum_{i} |x[i]|^{p}\right)^{1/p}$$



The solution amounts to a thresholding or shrinkage of b :

$$\hat{x} = \mathcal{T}_{\lambda}^{(p)}(b)$$

The most common sparse regularizers are the L1 norm and the L0-"pseudo" norm:



In case sparsity in enforced in some signal representation, the problem to be solved is the following:

$$\hat{x} = \operatorname{Argmin}_{x} \quad \lambda \| \Phi^{T} x \|_{\ell_{p}} + \frac{1}{2} \| b - x \|_{2}^{2} \longrightarrow \hat{x} = \operatorname{Argmin}_{x = \Phi \alpha} \quad \lambda \| \alpha \|_{\ell_{p}} + \frac{1}{2} \| \Phi^{T} b - \alpha \|_{2}^{2}$$
orthogonal case
$$\hat{x} = \Phi \ \mathcal{T}_{\lambda}^{(p)} (\Phi^{T} b)$$

b = x + n**L0** $\hat{x} = \mathbf{\Phi} \mathcal{H}_{\lambda}(\mathbf{\Phi}^T b)$

 ${\mathcal X}$

L1

 $\hat{x} = \mathbf{\Phi} \mathcal{S}_{\lambda} (\mathbf{\Phi}^T b)$

 $b - \hat{x}_{\ell_0}$ $b - \hat{x}_{\ell_1}$ $x - \hat{x}_{\ell_0}$ $x - \hat{x}_{\ell_1}$



Simulations of image from the *Hubble Space Telescope*

 ${\mathcal X}$



In imaging science, the (spatial) resolution of the images/signals is limited by the instrument/ sensor/... etc.

The loss of resolution is mathematically described by the convolution of the signal with the pointspread-function (PSF) of the optical device:

$$b = h \star x + n$$

$$b = Hx + n$$





GOOD NEWS: Toeplitz-circulant matrices are diagonalized by the Fourier transform:



Let's turn to the classical maximum likelihood estimator. In case of additive Gaussian noise, it is fully equivalent to a least-square estimator:

$$\hat{x}_{\text{ML}} = \operatorname{Argmin}_{x} \|b - Hx\|_{\ell_{2}}^{2}$$

which can be recast in the Fourier domain as follows:

$$\hat{x}_{\mathrm{ML}} = \mathcal{F}^{-1} \mathrm{Argmin}_u \|\mathcal{F}b - Du\|_{\ell_2}^2$$

which now fully separable in u:



600

One of the most common Bayesian estimator is the Wiener filter, which obtained when the signal x is assumed to be a Gaussian random field (GRF) that is described by its power spectrum P:

$$\hat{x}_{\text{Wiener}} = \operatorname{Argmin}_{x} \frac{1}{2} x^{T} \mathcal{F}^{T} W^{-1} \mathcal{F} x + \frac{1}{2\sigma_{n}^{2}} \|b - Hx\|_{\ell_{2}}^{2}$$
Inverse covariance matrix of x in the Fourier domain GRF: diagonal matrix W[k,k] = P[k]

After some basic calculation, we can show that in the Fourier domain:

$$\forall k; \ \hat{u}_{\text{Wiener}}[k] = \frac{P[k]}{P[k] + \frac{\sigma_n^2}{D[k,k]^2}} \ \frac{v[k]}{D[k,k]}$$

ML estimator

Similarly to the case of denoising, the state-of-art deconvolution methods are based on sparsityconstrained least-square solution.

It allows to better account for the sparsity of the signal x in some sparse representation (*e.g.* wavelet, ... X-let) as well as noise through the data fidelity term and a choice of the regularization parameter.

$$\hat{x} = \operatorname{Argmin}_{x} \quad \lambda \| \boldsymbol{\Phi}^T x \|_{\ell_p} + \frac{1}{2} \| b - H x \|_2^2$$

No explicit solution !

This can be solved using an iterative thresholded Landweber scheme (Bertero 98):













b





 \hat{x}

Sparsity-based deconvolution

Input





Observation

Richardson-Lucy





Wavelets

Beyond denoising: inpainting









Beyond denoising: inpainting

mask recast as a diagonal matrix

Inpainting has been tackled by solving a L1-penalized least-square problem of the form:

$$\hat{x} = \operatorname{Argmin}_{x = \Phi \alpha} \lambda \|\alpha\|_{\ell_1} + \frac{1}{2} \|b - \mathbf{M} \Phi \alpha\|_{\ell_2}^2$$

$$(x = \operatorname{Convex} \text{ but not differentiable})$$

$$(x = \operatorname{Convex} \text{ and differentiable})$$

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$$(x = \operatorname{Convex} \text{ and differentiable})$$

The forward-backward algorithm then reads:

$$\alpha^{(t+1)} = \operatorname{prox}_{\gamma f} \left(\alpha^{(t)} + \gamma \Phi^T (b - \mathbf{M} \Phi \alpha)) \right)$$









Blind source separation

Analysing multispectral data



Courtesy of M. Lennon Hyperspectral data remote sensing, aerial data, etc.





Hyperspectral data in astrophysics Mars Express, Cassini, etc.





Multispectral data in astrophysics Planck, Fermi, radio-interferometry (Lofar/SKA/...), etc.

Analysing multispectral data



Different scientific fields but ...

common problems: mixtures of elementary signals or sources

The underlying mixture model



Unsupervised matrix factorisation



Blind Source Separation: Estimation both A and S from X only

This is an ill-posed matrix factorization problem

Non-negative Matrix Factorization, Dictionary Learning, ...

A complex problem to be tackled

$$\min_{A,S} \mathscr{R}(A) + \mathscr{J}(S) + \mathscr{D}(X, AS)$$
Regularization
Terms
Data fidelity term
Terms

Data fidelity term: - measures a discrepancy between the data and the model

- allows to account for the noise statistics
- general formulation for various mixture models

Instantaneous mixture, non-stationary mixture (e.g. Planck), Joint convolution/mixing (radio), non-linear mixtures, ...

Regularization terms: - make "better"-posed an ill-posed problem

- favour solution properties for increased interpretability

Sparse BSS - a building block



This is an ill-posed matrix factorization problem

Regularization terms: - sparsity of the sources in some signal representation

- scaling of the mixing matrix is constrained

Sparse source separation

Changing the way the sources are represented to get a sparse/compressed representation



Wavelet transform for spherical data

Sparse source separation





Wavelet coefficients



Morphological diversity

Sparse source separation



Generalized Morphological Component Analysis (GMCA):

- S-BSS with redundant sparse representations
- Iterative soft/hard thresholding algorithm
- Thresholding strategy, robustness to Gaussian noise/local stationary points
- No parameters to tune

Bobin, Starck, Fadili, and Moudden, Sparsity, Morphological Diversity and Blind Source Separation, IEEE Trans. on Image Processing, Vol 16, No 11, pp 2662 - 2674, 2007. Bobin, Starck, Fadili, and Moudden, Blind Source Separation: The Sparsity Revolution, Advances in Imaging and Electron Physics, Vol 152, pp 221 -- 306, 2008.

Unmixing X-ray images



NASA - Chandra

Unmixing X-ray images

CasA with Chandra 1 Ms observation ~1 billions counts !!

- Ejecta thermal emission gives insight on :
 - Individual elements distribution
 - Morphology, asymmetries
 - Velocities

Application to the Chandra data

Application to the Chandra data

Picquenot et al, A&A, 2019.

Blindly estimates red/blue-shifted atomic components !

Beyond sparse modelling

All along these courses, we have explored how signals representations can be built to obtain sparse representations.

All these representations are built on certain generic morphological/geometrical specificities of the signal to be modeled.

Main advantage: they are adapted to the content of a very large span of "natural" images, they come with fast transforms.

Main drawback: they are not specifically adapted to the content of individual signal/images/... which might typical of specific data/applications, etc.

All these signal representations can be combined to sparsely represent more complex images that combines morphologies of various nature; see Morphological Component Analysis (MCA), etc.

What about this very specific signals ?

Tissue observed through a confocal microscope

Simulation of the Cosmic Web (galaxy distribution)

Simulation of cosmic strings

Ideally, one would like to learn a dictionary/sparse representation that is adapted to the specific morphological component of a single image or a class of images.

The question of learning a "relevant" representation for natural images first was first raised in the field of neuroscience by Olshausen & Fields.

Their work focused on understanding the kind of patterns in natural images the primary visual cortex (V1) is sensitive to.

Learning experiment:

each image is divide into small patches and stored in some matrix **X**

 $\min_{\boldsymbol{\Phi},\mathbf{S}} \|\mathbf{X} - \mathbf{S}\boldsymbol{\Phi}\|_F^2 + \lambda \sum_i f(S_i)$ **Expansion coefficient Signal representation** of each data patch

Olshausen & Fields, Sparse Coding with an Overcomplete Basis Set: A Strategy Employed by V1 ?, 1997

In their experiment, they chose the penalization f so as to promote sparseness since it is believed that the primary visual cortex compresses information into a few significant features.

$$\min_{\mathbf{\Phi},\mathbf{S}} \|\mathbf{X} - \mathbf{S}\mathbf{\Phi}\|_F^2 + \lambda \sum_i f(S_i)$$

They found that the learnt dictionary contains oriented/elongated/oscillatory features which are reminiscent of Gabor-wavelets.

In the setting of imaging processing, the use of overcomplete representations has long been advocated as a mean to provide sparser and therefore more efficient signal representations.

Learning sparse overcomplete signal representation has been introduced by Elad and Aharon in 2006.

$$\min_{\Phi,\alpha} \sum_{j} \mu_{j} \|\alpha_{j}\|_{\ell_{0}} + \|x_{j} - \Phi \alpha_{j}\|_{2}^{2}$$

$$\sum_{j \in \mathbb{Z} \\ j \in$$

Images are modeled in a patch-based representation

Elad & Aharon, Image Denoising Via Sparse and Redundant Representations Over Learned Dictionaries, 2006

The K-SVD algorithm can be described as follows:

- Initialization, Φ is set to an overcomplete DCT
- Sparse coding:

Decompose each data patch in the current dictionary:

$$\min_{\alpha_j} \|\alpha_j\|_{\ell_0} \text{ s.t. } \|x_j - \Phi \alpha_j\|_2 \le \epsilon$$

- Dictionary update:

For each atom (element of the dictionary), build the residual:

$$\mathbf{R}_{k} = \mathbf{X} - \sum_{k' \neq k} \sum_{j} \alpha_{j} [k'] \phi_{k'}$$

part of the data "explained" the atoms except atom #k

The atom and the corresponding decomposing are updated via SVD:

$$\mathbf{R}_{k} = \mathbf{U}_{k} \boldsymbol{\Sigma}_{k} \mathbf{V}_{k} \implies \phi_{k} = \mathbf{U}_{k}^{1}$$
$$\alpha^{k} = \mathbf{V}_{k,1}$$

take the principal eigenvectors

Sample images

Overcomplete DCT dictionary

Learnt dictionary with K-SVD

Elad & Aharon, Image Denoising Via Sparse and Redundant Representations Over Learned Dictionaries, 2006

Denoised Image Using Global Trained Dictionary (28.8528 dB)

Noisy Image (22.1307 dB, σ=20)

Denoised Image Using Adaptive Dictionary (30.8295 dB)

Elad & Aharon, Image Denoising Via Sparse and Redundant Representations Over Learned Dictionaries, 2006

Created Adaptive Dictionary

$= \underset{\substack{D \in C_1\\A \in C_2}}{\operatorname{arg\,min}(Y = DA)} \text{Dictionary learning}$

From sparse modelling to learning-based representations

Let's go back to the basics,

$$\min_{\mathbf{X}} \lambda \|\mathbf{X}\|_1 + \frac{1}{2} \|\mathbf{Y} - \mathbf{X}\|_2^2$$

Classically gives

$$\mathbf{X} = \mathscr{S}_{\lambda}(\mathbf{Y})$$

Basically, the regularisation often boils down to a denoiser, or more generally to providing a low-dimensional approximation of the signal.

Gist of plug&play methods (in this context) is to learn denoisers Romano et al. 2016

$$\mathbf{X} = \mathscr{D}_{\theta}(\mathbf{Y})$$

and plug them in classical solvers:

$$\mathbf{S} \leftarrow \mathcal{D}_{\theta} \left(\mathbf{S} + \alpha \mathbf{A}^{T} (\mathbf{X} - \mathbf{A}\mathbf{S}) \right)$$

here in a forward-backward splitting algorithm

which could be interpreted as some regularization

$$\min_{\mathbf{S}} \mathscr{J}_{\theta}(\mathbf{S}) + \frac{1}{2} \|\mathbf{X} - \mathbf{A}\mathbf{S}\|_{2}^{2}$$

- Virtually any denoiser architecture can be used
- U-Net quite popular for image denoising (Though being highly over-parameterized)
- Applied to denoising, deconvolution, tomographic reconstruction, etc. but not to BSS

Sureau et al. 2019

U-Net architectures for galaxy image denoising

Sureau et al. 2019

U-Net architectures for galaxy image deconvolution

Sureau et al. 2019

April, 7th 2022

Learning non-linear signal representations

Physically relevant signals generally belong to a smooth low-dimensional manifold

Learning a signal representation \equiv learning to "navigate" on the manifold

Learning non-linear signal representations

Learning non-linear signal representations

Combining with unmixing

sGMCA : a semi-blind sparse unsupervised matrix factorization method

$$\begin{aligned} \operatorname{argmin}_{\mathbf{A},\mathbf{S}} \| \mathbf{\Lambda} \odot \mathbf{SW} \|_{1} + \sum_{j \neq \mathcal{F}} \iota_{\mathcal{S}_{m}} \left(\mathbf{A}^{j} \right) + \sum_{j \in \mathcal{F}} \iota_{\mathcal{B}_{\phi_{j}}(\{\varphi^{e}_{\mathcal{M}_{j}}\})} \left(\mathbf{A}^{j} \right) + \frac{1}{2} \| \mathbf{X} - \mathbf{AS} \|_{F}^{2} \\ & \uparrow & \uparrow & \uparrow \\ \\ \underbrace{Sparsity}_{regularization} & Oblique \\ constraint & c$$

- With the exception of the barycentric constraint, the problem is multi-convex

- In practice, the barycentric constraint seems to behave like a convex constraint
- For its robustness, the minoration scheme is based on an alternate least-squares

Carloni-Gertosio, Bobin, Acero, submitted to DSP, 2022

Unsupervised matrix factorisation

