

Review

Optimization-Based Data Analysis

http://www.cims.nyu.edu/~cfgranda/pages/OBDA_spring16

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How to deal with a data-analysis problem

- 1. Define the problem
- 2. Establish assumptions on signal structure
- 3. Design an efficient algorithm
- 4. Understand under what conditions the problem is well posed
- 5. Derive theoretical guarantees

Data-analysis problems

Signal structure

Methods

General techniques Denoising Signal recovery Signal separation Regression Compression / dimensionality reduction Clustering

When is the problem well posed?

Theoretical analysis

Aim: Extracting information (signal) from data in the presence of uninformative perturbations (noise)

Additive noise model

data = signal + noise y = x + z





Signal ñ H ü i I

Data









Signal recovery

- Compressed sensing
- Deconvolution / super-resolution
- Matrix completion

Aim: Estimate signal x from measurements y

$$y = Ax$$

Linear underdetermined system where dimension (y) < dimension(x)

Compressed sensing





Compressed sensing

Signal

Spectrum

Data

Super-resolution

The resolving power of lenses, however perfect, is limited (Lord Rayleigh)



Diffraction imposes a fundamental limit on the resolution of optical systems

Super-resolution



Spatial Super-resolution



Spectrum

Spectral Super-resolution



Spectrum

Seismology



Reflection seismology



Deconvolution



Data \approx convolution of pulse and reflection coefficients

Deconvolution



Matrix completion

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Matrix completion



Aim: Decompose the data into two (or more) signals

$$y = x_1 + x_2$$

Electrocardiogram



Electrocardiogram



Temperature data



Temperature data







Sines



Sines



 $\mathcal{F}_{c} x + s$



 $\mathcal{F}_{c} x$ s Collaborative filtering with outliers



Background subtraction


Regression

Aim: Predict the value of a response $y \in \mathbb{R}$ from p predictors $X_1, X_2, \ldots, X_p \in \mathbb{R}$

Methodology:

1. Fit a model with using *n* training examples y_1, y_2, \ldots, y_n

$$y_i \approx f(X_{i1}, X_{i2}, \dots, X_{ip}) \quad 1 \leq i \leq n$$

2. Use learned model f to predict from new data

Assumption: Response only depends on a subset S of $s \ll p$ predictors

Model-selection problem: Determine what predictors are relevant

Classification

Aim: Predict the value of a binary response $y \in \{0, 1\}$ from p predictors $X_1, X_2, \ldots, X_p \in \mathbb{R}$

Methodology:

1. Fit a model with using *n* training examples y_1, y_2, \ldots, y_n

$$y_i \approx f(X_{i1}, X_{i2}, \dots, X_{ip}) \quad 1 \leq i \leq n$$

2. Use learned model f to predict from new data

Arrhythmia prediction

Predict whether patient has arrhythmia from n = 271 examples and p = 182 predictors

- Age, sex, height, weight
- Features obtained from electrocardiogram recordings



Aim: Map a signal $x \in \mathbb{R}^n$ to a lower-dimensional space

 $y \approx f(x)$

such that we can recover x from y with minimal loss of information

Compression



Compression



Projection of data onto lower-dimensional space

- Decreases computational cost of processing the data
- Allows to visualize (2D, 3D)

Difference with compression: Not necessarily reversible

Dimensionality reduction

Seeds from three different varieties of wheat: Kama, Rosa and Canadian

Dimensions:

- Area
- Perimeter
- Compactness
- Length of kernel
- Width of kernel
- Asymmetry coefficient
- Length of kernel groove

Clustering

Aim: Separate signals $x_1, \ldots, x_n \in \mathbb{R}^d$ into different classes

Clustering



Collaborative filtering



Topic modeling



Data-analysis problems

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When is the problem well posed?

Theoretical analysis

Models

- Sparse models
- ► Group sparse models
- Low-rank models

Sparsity

$$x = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 2 \\ 0 \\ 0 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

Group sparsity

Entries are partitioned into m groups $\mathcal{G}_1, \mathcal{G}_2, \ldots, \mathcal{G}_m$

$$x = \begin{bmatrix} x_{\mathcal{G}_1} \\ x_{\mathcal{G}_2} \\ \dots \\ x_{\mathcal{G}_m} \end{bmatrix}$$

Assumption: Most groups are zero

Sparse models

Let D be a dictionary of atoms

1. Synthesis sparse model

x = Dc where c is sparse

2. Analysis sparse model:

 $D^T x$ is sparse

Low-rank model

Signal is structured as a matrix that presents significant correlations

Collaborative filtering



 SVD

$$A - \bar{A} = U \Sigma V^{T} = U \begin{bmatrix} 7.79 & 0 & 0 & 0 \\ 0 & 1.62 & 0 & 0 \\ 0 & 0 & 1.55 & 0 \\ 0 & 0 & 0 & 0.62 \end{bmatrix} V^{T}$$

Topic modeling



 SVD

$$A = U \Sigma V^{T} = U \begin{bmatrix} 23.64 & 0 & 0 & 0 & \\ 0 & 18.82 & 0 & 0 & 0 & 0 \\ 0 & 0 & 14.23 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3.63 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2.03 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.36 \end{bmatrix} V^{T}$$

Designing signal representations

- Frequency representation
- Short-time Fourier transform
- Wavelets
- Finite differences

Frequency representation



Discrete cosine transform



Electrocardiogram



Electrocardiogram (spectrum)



Electrocardiogram (spectrum)



Short-time Fourier transform



Speech signal



Spectrogram (log magnitude of STFT coefficients)



Frequency

Wavelets

Scaling function Mother wavelet

Electrocardiogram

Signal Haar transform



Contribution









Contribution






Scale 2^7

Contribution







Contribution





Scale 2^5

Contribution





Scale 2^4

÷

Contribution







Contribution







Contribution







Scale 2^1

Contribution Approximation



Contribution







2D wavelet transform



2D wavelet transform



Finite differences



Learning signal representations

Aim: Learn representation from a set of n signals

$$X := \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix}$$

For each signal

$$x_j pprox \sum_{i=1}^k \Phi_i \ A_{ij}, \quad 1 \le j \le n, \quad ext{for } k \ll n$$

• $\Phi_1, \ldots, \Phi_k \in \mathbb{R}^d$ are atoms

• $A_1, \ldots, A_n \in \mathbb{R}^k$ are coefficient vectors

Learning signal representations

Equivalent formulation

$$X \approx \begin{bmatrix} \Phi_1 & \Phi_2 & \cdots & \Phi_k \end{bmatrix} \begin{bmatrix} A_1 & A_2 & \cdots & A_n \end{bmatrix} = \Phi A$$

 $\Phi \in \mathbb{R}^{d \times k}$, $A \in \mathbb{R}^{k \times n}$

Learning signal representations

▶ k means

- Principal-component analysis
- Nonnegative matrix factorization
- Sparse principal-component analysis
- Dictionary learning

k means

Aim: Divide $x_1, \ldots x_n$ into k classes

Learn Φ_1, \ldots, Φ_k that minimize

$$\sum_{i=1}^{n} ||x_i - \Phi_{c(i)}||_2^2$$

$$c(i) := \arg\min_{1 \le j \le k} ||x_i - \Phi_j||_2$$

k means



Principal-component analysis

Best rank-k approximation

$$\Phi A = U_{1:k} \Sigma_{1:k} V_{1:k}^{T} = \arg \min_{\substack{\{\tilde{M} \mid \operatorname{rank}(\tilde{M}) = k\}}} \left| \left| X - \tilde{M} \right| \right|_{\mathsf{F}}^{2}$$

The atoms Φ_1, \ldots, Φ_k are orthogonal

Principal-component analysis

$$\frac{\sigma_1}{\sqrt{n}} = 1.3490$$
 $\frac{\sigma_2}{\sqrt{n}} = 0.1438$





Nonnegative matrix factorization

Nonnegative atoms/coefficients

$$X \approx \Phi A$$
, $\Phi_{i,j} \ge 0$, $A_{i,j} \ge 0$, for all i, j

Faces dataset





Sparse atoms

 $X \approx \Phi A$, Φ sparse

Faces dataset



Dictionary learning

Sparse coefficients

 $X \approx \Phi A$, A sparse

Dictionary learning



Data-analysis problems

Signal structure

Methods

General techniques Denoising Signal recovery Signal separation Regression Compression / dimensionality reduction Clustering

When is the problem well posed?

Theoretical analysis

Data-analysis problems

Signal structure

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General techniques

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When is the problem well posed?

Theoretical analysis

Promoting sparsity

Find sparse x such that $x \approx y$

Hard thresholding

$$\mathcal{H}_{\eta}\left(y
ight)_{i}:=egin{cases} y_{i} & ext{if } |y_{i}|>\eta \ 0 & ext{otherwise} \end{cases}$$

Promoting group sparsity

Find group sparse x such that $x \approx y$

Block thresholding

$$\mathcal{B}_{\eta}(x)_{i} := \begin{cases} x_{i} & \text{if } i \in \mathcal{G}_{j} \text{ such that } \left| \left| x_{\mathcal{G}_{j}} \right| \right|_{2} > \eta \\ 0 & \text{otherwise} \end{cases}$$

Promoting low-rank structure

Find low rank M such that $M \approx Y \in \mathbb{R}^{m \times n}$

• Truncate singular-value decomposition $Y = U \Sigma V^T$

$$M = U_{1:k} \Sigma_{1:k} V_{1:k}^{T}$$

Solves PCA problem

► Fit M = AB, $A \in \mathbb{R}^{m \times k}$, $B \in \mathbb{R}^{k \times n}$, by solving minimize $\left\| Y - \tilde{A}\tilde{B} \right\|_{F}$

Promoting additional structure in low-rank models

Nonnegative factors

minimize
$$\left| \left| Y - \tilde{A} \tilde{B} \right| \right|_{\mathsf{F}}$$
 subject to $\tilde{A}_{i,j} \ge 0$
 $\tilde{B}_{i,j} \ge 0$ for all i, j

Sparse factors

$$\begin{array}{ll} \text{minimize} & \left\| Y - \tilde{A} \, \tilde{B} \right\|_{\mathsf{F}} + \lambda \sum_{i=1}^{k} \left\| \tilde{A}_{i} \right\|_{1} \\ \text{subject to} & \left\| \tilde{A}_{i} \right\|_{2} = 1, \qquad 1 \leq i \leq k \\ \\ \text{minimize} & \left\| Y - \tilde{A} \, \tilde{B} \right\|_{\mathsf{F}} + \lambda \sum_{i=1}^{k} \left\| \tilde{B}_{i} \right\|_{1} \\ \\ \text{subject to} & \left\| \tilde{A}_{i} \right\|_{2} = 1, \qquad 1 \leq i \leq k \end{array}$$

Signal representation

x = D c

Columns of D are designed/learned atoms

Inverse problems

y = A x

Linear models

Linear regression

 $y = X \beta$

► X contains the predictors

Find x such that $Ax \approx y$

minimize
$$||y - A\tilde{x}||_2$$

Alternatives: Logistic loss for classification

Promoting sparsity

Find sparse x such that $Ax \approx y$

- Greedy methods: Choose entries of x sequentially to minimize residual (matching pursuit, orthogonal m. p., forward stepwise regression)
- Penalize ℓ_1 norm of x

minimize
$$||y - A\tilde{x}||_2^2 + \lambda ||\tilde{x}||_1$$

Implementation:

gradient descent + soft-thresholding / coordinate descent
Promoting group sparsity

Find group sparse x such that $Ax \approx y$

• Penalize ℓ_1/ℓ_2 norm of x

minimize
$$||y - A\tilde{x}||_2^2 + \lambda ||\tilde{x}||_{1,2}$$

Implementation:

gradient descent + block soft-thresholding / coordinate descent

Promoting low-rank structure

Find low rank M such that $M_\Omega \approx Y_\Omega \in \mathbb{R}^{m \times n}$ for a set of entries Ω

Penalize nuclear norm of x

minimize
$$\left\| Y_{\Omega} - \tilde{M}_{\Omega} \right\|_{2}^{2} + \lambda \left\| \tilde{M} \right\|_{*}$$

Implementation: gradient descent + soft-thresholding of singular values

▶ Fit M = AB, $A \in \mathbb{R}^{m \times k}$, $B \in \mathbb{R}^{k \times n}$, by solving

minimize
$$\left\| Y_{\Omega} - \left(\tilde{A} \, \tilde{B} \right)_{\Omega} \right\|_{F}$$

Data-analysis problems

Signal structure

Methods General techniques Denoising Signal recovery Signal separation Regression Compression / dimensionality reduction Clustering

When is the problem well posed?

Theoretical analysis

Denoising



Denoising via thresholding



Denoising

DCT coefficients





Denoising via thresholding in DCT basis







Denoising



Denoising



2D wavelet coefficients



Original coefficients



Thresholded coefficients



Denoising via thresholding in a wavelet basis



Denoising via thresholding in a wavelet basis



Denoising via thresholding in a wavelet basis

Original



Noisy



Estimate



Speech denoising



Time thresholding



Spectrum



Frequency thresholding



Frequency thresholding



Spectrogram (STFT)



Frequency

STFT thresholding



Frequency

Time

STFT thresholding



STFT block thresholding



Time

STFT block thresholding



Sines and spikes



Denoising



Denoising via $\ell_1\text{-norm}$ regularized least squares



Denoising via $\ell_1\text{-norm}$ regularized least squares



Denoising

Signal ñ H ü i I

Data













Small λ


Small λ



${\rm Medium}\ \lambda$



${\rm Medium}\ \lambda$



Large λ



Large λ



Denoising via TV regularization

Original



Noisy



Estimate



Data-analysis problems

Signal structure

Methods General techniques Denoising Signal recovery Signal separation Regression Compression / dimensionality reductio Clustering

When is the problem well posed?

Theoretical analysis

Compressed sensing

Signal

Spectrum

Data

$\ell_1\text{-norm}$ minimization



x2 undersampling





$\ell_1\text{-norm}$ minimization

Regular



Random



Super-resolution

The resolving power of lenses, however perfect, is limited (Lord Rayleigh)



Diffraction imposes a fundamental limit on the resolution of optical systems

Super-resolution



Super-resolution: ℓ_1 -norm regularization





Spectral Super-resolution



Spectrum

Spectral super-resolution: Pseudospectrum from low-rank model (MUSIC)



Deconvolution



Deconvolution with the ℓ_1 norm (Taylor, Banks, McCoy '79)



Matrix completion



Matrix completion via nuclear-norm minimization



Data-analysis problems

Signal structure

Methods

General techniques Denoising Signal recovery Signal separation Regression Compression / dimensionality redu

When is the problem well posed?

Theoretical analysis

Electrocardiogram



Spectrum









Temperature data



Temperature data



Model fitted by least squares



Model fitted by least squares



Model fitted by least squares



Trend: Increase of 0.75 $^\circ\text{C}$ / 100 years (1.35 $^\circ\text{F})$



Demixing of sines and spikes



 $\mathcal{F}_{c} x$ s

Demixing of sines and spikes



Spikes



Sines (spectrum)

Background subtraction



Low-rank component


Sparse component



Data-analysis problems

Signal structure

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General techniques Denoising Signal recovery Signal separation Regression Compression / dimensionality r

When is the problem well posed?

Theoretical analysis

Assumption: Response only depends on a subset S of $s \ll p$ predictors

Model-selection problem: Determine what predictors are relevant

Lasso



Arrhythmia prediction

- Predict whether patient has arrhythmia from n = 271 examples and p = 182 predictors
- Age, sex, height, weight
- Features obtained from electrocardiogram recordings

Best sparse model uses around 60 predictors

Lasso (logistic regression)





Correlated predictors: Lasso path



Correlated predictors: Ridge-regression path



Correlated predictors: Elastic net path



Several responses y_1, y_2, \ldots, y_k modeled with the same predictors

Assumption: Responses depend on the same subset of predictors

Aim: Learn a group-sparse model

Multitask learning

Lasso





Data-analysis problems

Signal structure

Methods

General techniques Denoising Signal recovery Signal separation Regression Compression / dimensionality reduction Clustering

When is the problem well posed?

Theoretical analysis

Compression



Original

Compression via frequency representation



10 % largest DCT coeffs

Compression via frequency representation



2% largest DCT coeffs

Dimensionality reduction

Seeds from three different varieties of wheat: Kama, Rosa and Canadian

Dimensions:

- Area
- Perimeter
- Compactness
- Length of kernel
- Width of kernel
- Asymmetry coefficient
- Length of kernel groove

PCA: Projection onto two first PCs



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PCA: Projection onto two last PCs



Random projections



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Data-analysis problems

Signal structure

Methods

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When is the problem well posed?

Theoretical analysis

Clustering



k means using Lloyd's algorithm



Collaborative filtering



First left singular vector clusters movies

D. Knight Sp. 3 Love Act. B.J.'s Diary P. Woman Sup. 2 $U_1 = \begin{pmatrix} -0.45 & -0.39 & 0.39 & 0.39 & 0.39 & -0.45 \end{pmatrix}$

First right singular vector clusters users

Bob Molly Mary Larry
$$V_1=egin{pmatrix} 0.48 & 0.52 & -0.48 & -0.52 \end{pmatrix}$$

Topic modeling

singer	GDP	senate	election	vote	stock	bass	market	band	Articles
/ 6	1	1	0	0	1	9	0	8 \	а
1	0	9	5	8	1	0	1	0	b
8	1	0	1	0	0	9	1	7	с
0	7	1	0	0	9	1	7	0	d
0	5	6	7	5	6	0	7	2	е
$\setminus 1$	0	8	5	9	2	0	0	1 /	f

Right nonnegative factors cluster words

singer GDP senate election vote stock bass market band $H_1 = (0.34 \quad 0 \quad 3.73 \quad 2.54$ 0.35)3.67 0.52 0 0.35 $H_2 = (0 \quad 2.21 \quad 0.21 \quad 0.45)$ 0.22)0 2.64 0.21 2.43 $H_3 = (3.22)$ 0.37 0.19 0.2 0 0.12 4.13 0.13 3.43) Left nonnegative factors cluster documents

Data-analysis problems

Signal structure

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When is the problem well posed?

Theoretical analysis

Denoising based on sparsity

Signal is sparse in the chosen representation

Noise is not sparse in the chosen representation

Signal recovery

MeasurementsClass of signalsCompressed
sensingGaussian, random
Fourier coeffs.SparseSuper-resolutionLow passSignals with min.
separation

Matrix completion

Random sampling

Incoherent low-rank matrices





Measurement operator = random frequency samples





Aim: Study effect of measurement operator on sparse vectors



Operator is well conditioned when acting upon any sparse signal (restricted isometry property)
Compressed sensing



Operator is well conditioned when acting upon any sparse signal (restricted isometry property)



No discretization



Data: Low-pass Fourier coefficients



Data: Low-pass Fourier coefficients



Problem: If the support is clustered, the problem may be ill posed In super-resolution sparsity is not enough!



If the support is spread out, there is still hope We need conditions beyond sparsity

Matrix completion



The signals are identifiable

Example: For low rank + sparse model, low rank component cannot be sparse and vice versa

Enough examples to prevent overfitting

For sparse models, enough examples with respect to the number of relevant predictors

Least-squares regression



Lasso (logistic regression)

n = 271 examples



Data-analysis problems

Signal structure

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When is the problem well posed?

Theoretical analysis

Optimization problem

minimize $f(\tilde{x})$ subject to Ax = y

f is a nondifferentiable convex function

Examples: ℓ_1 norm, nuclear norm

Aim: Show that the original signal x is the solution

Dual certificate

Subgradient of f at x of the form

$$q := A^T v$$

For any h such that Ah = 0

$$\langle q,h\rangle = \left\langle A^T v,h\right\rangle = \langle v,Ah\rangle = 0$$

$$f(x+h) \geq f(x) + \langle q, h \rangle = f(x)$$

Certificates

	Subgradient	Row space of A
Compressed sensing	$egin{array}{l} { m sign}\left(x ight)+z,\ {\left \left z ight ight _{\infty}}<1 \end{array}$	Random sinusoids
Super-resolution	$egin{array}{l} { m sign}\left(x ight)+z,\ {\left \left z ight ight _{\infty}}<1 \end{array}$	Low-pass sinusoids
Matrix completion	$UV^{T} + Z$, $ Z < 1$	Observed entries

Certificate for compressed sensing



Certificate for super-resolution

