# Convex Optimization in Machine Learning and Inverse Problems Part 1: Applications of Sparse Optimization 

Mário A. T. Figueiredo ${ }^{1}$ and Stephen J. Wright ${ }^{2}$

${ }^{1}$ Instituto de Telecomunicações, Instituto Superior Técnico, Lisboa, Portugal
${ }^{2}$ Computer Sciences Department, University of Wisconsin, Madison, WI, USA

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"There is nothing as practical as a good theory", Lewin, 1952
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## Inference via Optimization

Many inference problems are formulated as optimization problems:

- image reconstruction
- image restoration/denoising
- supervised learning
- unsupervised learning
- statistical inference


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Standard formulation:

- observed data: y
- unknown mathematical object (signal, image, vector, matrix,...):
- inference criterion:

$$
\widehat{x} \in \arg \min _{x} g(x, y)
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Question 1: how to build $g$ ? Where does it come from?
Answer: from the application domain (machine learning, signal processing, inverse problems, system identification, statistics, computer vision, bioinformatics,...);
... examples ahead.

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Question 2: how to solve the optimization problem?
Answer: the focus of this tutorial.

## Regularized Optimization

Inference criterion:

Typical structure of $g$ :

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- $\tau \geq 0$ : the regularization parameter (or constant).
- Since $y$ is fixed, we often write simply $f(x)=h(x, y)$,

$$
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## Probabilistic/Bayesian Interpretations

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- Log-posterior: $\log p(x \mid y)=K(y)-h(x, y)-\tau \psi(x)$


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- Log-posterior: $\log p(x \mid y)=K(y)-h(x, y)-\tau \psi(x)=K(y)-g(x, y)$
- $\hat{x}$ is a maximum a posteriori (MAP) estimate.


## Regularizers

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Common regularizers impose/encourage one (or a combination of) the following characteristics:

- small norm (vector or matrix)
- sparsity (few nonzeros)
- specific nonzero patterns (e.g., group/tree structure)
- low-rank (matrix)
- smoothness or piece-wise smoothness
- ...


## Unconstrained vs Constrained Formulations

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## Unconstrained vs Constrained Formulations

- Tikhonov regularization:
- Morozov regularization:
- Ivanov regularization:
$\min _{x} f(x)+\tau \psi(x)$
$\begin{array}{ll}\min _{x} & \psi(x) \\ \text { subject to } & f(x) \leq \varepsilon\end{array}$
$\min _{x} \quad f(x)$
subject to $\quad \psi(x) \leq \delta$


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Under mild conditions, these are all "equivalent".
Morozov and Ivanov can be written as Tikhonov using indicator functions (more later).

Which one is more convenient is problem-dependent.

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A simple linear inverse problem: from $y=A x$, find $x \quad\left(A \in \mathbb{R}^{m \times n}\right)$

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$\widehat{x}=\arg \min _{x} \sum_{i=1}^{n}\left(y_{i}-(A x)_{i}\right)^{2}=\arg \min _{x}\|y-A x\|_{2}^{2}=\left(A^{T} A\right)^{-1} A^{T} y$


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- Non-trivial cases: resort to optimization and regularization.
- Quadratic (Euclidean) losses and regularizers have a long and rich history: Gauss, Legendre, Wiener, Moore-Penrose, Tikhonov, ...


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Also important (but not a norm): $\|x\|_{0}=\lim _{p \rightarrow 0}\|x\|_{p}^{p}=\left|\left\{i: x_{i} \neq 0\right\}\right|$

## Norm balls

Radius $r$ ball in $\ell_{p}$ norm: $\quad B_{p}(r)=\left\{x \in \mathbb{R}^{n}:\|x\|_{p} \leq r\right\}$


$$
p=1
$$


$p=2$

$p=\infty$

$p=1$

$p=2$

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- Can we hope to recover $x$ ? Yes! ...if $x$ is sparse enough $\left(\|x\|_{0}<k\right)$ and $A$ satisfies some conditions, using

$$
\begin{aligned}
\widehat{x}= & \arg \min _{x}\|x\|_{0} \\
& \text { s.t. } A x=y
\end{aligned}
$$

Several proofs, under different conditions (more later).
But, this is a hard problem! $\ell_{0}$ "norm" is not convex.

## Review of Basics: Convex Sets

## Convex and strictly convex sets

$$
\mathcal{S} \text { is convex if } x, x^{\prime} \in \mathcal{S} \Rightarrow \forall \lambda \in[0,1], \quad \lambda x+(1-\lambda) x^{\prime} \in \mathcal{S}
$$


$\mathcal{S}$ is strictly convex if $x, x^{\prime} \in \mathcal{S} \Rightarrow \forall \lambda \in(0,1), \quad \lambda x+(1-\lambda) x^{\prime} \in \operatorname{int}(\mathcal{S})$


## Review of Basics: Convex Functions

Extended real valued function: $f: \mathbb{R}^{N} \rightarrow \overline{\mathbb{R}}=\mathbb{R} \cup\{+\infty\}$
Domain: $\operatorname{dom}(f)=\{x: f(x) \neq+\infty\}$
$f$ is proper if $\operatorname{dom}(f) \neq \emptyset$
$f$ is convex if
$\forall \lambda \in[0,1], x, x^{\prime} \in \operatorname{dom}(f) f\left(\lambda x+(1-\lambda) x^{\prime}\right) \leq \lambda f(x)+(1-\lambda) f\left(x^{\prime}\right)$
$f$ is strictly convex if

$$
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$$


non-convex

strictly convex

convex, not strictly

## Lower Semi-Continuity: Why Is It Important?

A function $f: \mathbb{R}^{n} \rightarrow \overline{\mathbb{R}}$ is lower semi-continuous (l.s.c.) if

$$
\liminf _{x \rightarrow x_{0}} \geq f\left(x_{0}\right), \text { for any } x_{0} \in \operatorname{dom}(f)
$$

or, equivalently, $\{x: f(x) \leq \alpha\}$ is a closed set, for any $\alpha \in \mathbb{R}$

$$
f(x)= \begin{cases}e^{-x}, & \text { if } x<0 \\ +\infty, & \text { if } x \geq 0\end{cases}
$$


$\operatorname{dom}(f)=]-\infty, 0\left[, \quad \arg \min _{x} f(x)=\emptyset\right.$

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Unless stated otherwise, we only consider I.s.c. functions.

## Coercivity, Convexity, and Minima

$$
f: \mathbb{R}^{N} \rightarrow \overline{\mathbb{R}}=\mathbb{R} \cup\{+\infty\}
$$

$f$ is coercive if $\lim _{\|x\| \rightarrow+\infty} f(x)=+\infty$
if $f$ is coercive, then $G \equiv \arg \min _{x} f(x)$ is a non-empty set
if $f$ is strictly convex, then $G$ has at most one element


## Another Important Concept: Strong Convexity

Recall the definition of convex function: $\forall \lambda \in[0,1]$,

$$
f\left(\lambda x+(1-\lambda) x^{\prime}\right) \leq \lambda f(x)+(1-\lambda) f\left(x^{\prime}\right)
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A $\beta$-strongly convex function satisfies a stronger condition: $\forall \lambda \in[0,1]$

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f\left(\lambda x+(1-\lambda) x^{\prime}\right) \leq \lambda f(x)+(1-\lambda) f\left(x^{\prime}\right)-\frac{\beta}{2} \lambda(1-\lambda)\left\|x-x^{\prime}\right\|_{2}^{2}
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convexity

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Strong convexity $\underset{ }{\nRightarrow}$ strict convexity.

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- $f: \mathbb{R}^{n} \rightarrow \overline{\mathbb{R}}$, defined as $f(x)=\max \left\{f_{1}(x), \ldots, f_{N}(x)\right\}$, is convex.


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- $f: \mathbb{R}^{n} \rightarrow \overline{\mathbb{R}}$, defined as $f(x)=\max \left\{f_{1}(x), \ldots, f_{N}(x)\right\}$, is convex.
- $g: \mathbb{R}^{n} \rightarrow \overline{\mathbb{R}}$, defined as $g(x)=f_{1}(L(x))$, where $L$ is affine, is convex. Note: $L$ is affine $\Leftrightarrow L(x)-L(0)$ is linear; e.g. $L(x)=A x+b$.


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An important function: the indicator of a set $C \subset \mathbb{R}^{n}$,

$$
\iota_{C}: \mathbb{R}^{n} \rightarrow \overline{\mathbb{R}}, \iota_{C}(x)= \begin{cases}0 & \Leftarrow x \in C \\ +\infty & \Leftarrow x \notin C\end{cases}
$$

If $C$ is a closed convex set, $\iota_{C}$ is a l.s.c. convex function.

## The Case of Differentiable Functions

Let $f: \mathbb{R}^{n} \rightarrow \mathbb{R}$ be twice differentiable and consider its Hessian matrix at $x$, denoted $\nabla^{2} f(x)$ (or $\left.H f(x)\right)$ :

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\left(\nabla^{2} f(x)\right)_{i j}=\frac{\partial f}{\partial x_{i} \partial x_{j}}, \text { for } i, j=1, \ldots, n
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- $f$ is $\beta$-strongly convex $\Leftrightarrow$ its Hessian $\nabla^{2} f(x) \succeq \beta I$, with $\beta>0, \forall_{x}$.


## More on the Relationship Between $\ell_{1}$ and $\ell_{0}$

Finding the sparsest solution is NP-hard (Muthukrishnan, 2005).

$$
\begin{aligned}
\widehat{w}= & \arg \min _{w}\|w\|_{0} \\
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Under conditions, replacing $\ell_{0}$ with $\ell_{1}$ yields "similar" results: see compressive sensing (CS) (Candès et al., 2006; Donoho, 2006)

## The Ubiquitous $\ell_{1}$ Norm

- Lasso (least absolute shrinkage and selection operator) (Tibshirani, 1996) a.k.a. basis pursuit denoising (Chen et al., 1995):

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\min _{x} \frac{1}{2}\|A x-y\|_{2}^{2}+\tau\|x\|_{1} \text { or } \min _{x}\|A x-y\|_{2}^{2} \text { s.t. }\|x\|_{1} \leq \delta
$$

or, more generally,

$$
\min _{x} f(x)+\lambda\|x\|_{1} \text { or } \min _{x} f(x) \text { s.t. }\|x\|_{1} \leq \delta
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or, more gene
- Geology/geophysics
- Claerbout and Muir (1973)
- Taylor et al. (1979)
- Levy and Fullager (1981)
- Oldenburg et al. (1983)
- Santosa and Symes (1988)
- Radio astronomy
- Högbom (1974)
- Schwarz (1978)
- Fourier transform spectroscopy
s.t. $\|x\|_{1} \leq \delta$
- Kawata et al. (1983)
- Mammone (1983)
- Minami et al. (1985)
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- Widely used o (statistics, sig
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- Newman (1988)
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- Many extensions: namely to express structured sparsity (more later).
- Why does $\ell_{1}$ yield sparse solutions? (next slides)
- How to solve these problems? (this tutorial)


## Why $\ell_{1}$ Yields Sparse Solution

$$
\begin{array}{clcc}
w^{*}=\begin{array}{ll}
\arg \min _{w} & \|A w-y\|_{2}^{2}
\end{array} \quad \text { vs } \quad w^{*}= & \arg \min _{w} & \|A w-y\|_{2}^{2} \\
\text { s.t. } & \|w\|_{2} \leq \delta & & \text { s.t. }
\end{array}\|w\|_{1} \leq \delta
$$




## Why $\ell_{1}$ Yields Sparse Solution

The simplest problem with $\ell_{1}$ regularization

$$
\widehat{w}=\arg \min _{w} \frac{1}{2}(w-y)^{2}+\lambda|w|=\operatorname{soft}(y, \lambda)= \begin{cases}y-\lambda \Leftarrow y>\lambda \\ 0 & \Leftarrow|y| \leq \lambda \\ y+\lambda & \Leftarrow y<-\lambda\end{cases}
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...by the way, how is this solved? (more later).

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...by the way, how is this solved? (more later).
Contrast with the squared $\ell_{2}$ (ridge) regularizer (linear scaling):

$$
\widehat{w}=\arg \min _{w} \frac{1}{2}(w-y)^{2}+\frac{\lambda}{2} w^{2}=\frac{1}{1+\lambda} y
$$

## More on the Relationship Between $\ell_{1}$ and $\ell_{0}$

The $\ell_{0}$ "norm" (number of non-zeros): $\|w\|_{0}=\left|\left\{i: w_{i} \neq 0\right\}\right|$. Not a norm, not convex, but in the simple case...
$\widehat{w}=\arg \min _{w} \frac{1}{2}(w-y)^{2}+\lambda|w|_{0}=\operatorname{hard}(y, \sqrt{2 \lambda})= \begin{cases}y & \Leftarrow|y|>\sqrt{2 \lambda} \\ 0 & \Leftarrow|y| \leq \sqrt{2 \lambda}\end{cases}$

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Natural images are well represented by a few coefficients in some bases.

- Images ( $N \times M \equiv n$ pixels) are represented by vectors $x \in \mathbb{R}^{n}$


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Original $1000 \times 1000$ image $x \in \mathbb{R}^{10^{6}} \quad$...only its 25000 largest coefficients.

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Original $1000 \times 1000$ image $x \in \mathbb{R}^{10^{6}} \quad$...only its 25000 largest coefficients.

- Also (even more) true with an over-complete tight frame; $W$ is "fat" (more columns than rows) and $W W^{T}=I$, but $W^{\top} W \neq I$.


## Application to Image Deblurring/Deconvolution

blurred

restored

$\widehat{\mathbf{x}} \in \arg \min _{\mathbf{x}} \frac{1}{2}\|\mathbf{A} \mathbf{x}-\mathbf{y}\|_{2}^{2}+\tau\|\mathbf{x}\|_{1}$


## Application to Magnetic Resonance Imaging

$$
\widehat{\mathbf{x}} \in \arg \min _{\mathbf{x}} \frac{1}{2}\|\mathbf{A} \mathbf{x}-\mathbf{y}\|_{2}^{2}+\tau\|\mathbf{x}\|_{1}
$$

## A = MUW


discrete Fourier transform
 acquired slices in DFT domain
reconstruction $\mathbf{W} \widehat{\mathbf{x}}$


## Machine/Statistical Learning: Linear Regression

Data $N$ pairs $\left(x_{1}, y_{1}\right), \ldots,\left(x_{N}, y_{N}\right)$, where $x_{i} \in \mathbb{R}^{d}$ (feature/variable vectors) and $y_{i} \in \mathbb{R}$ (outputs).

Goal: find "good" linear function: $\hat{y}=\sum_{j=1}^{d} w_{j} x_{j}+w_{d+1}=\left[x^{T} 1\right] w$

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Mean squared error: $\min _{w} \mathbb{E}\left(Y-\left[X^{T} 1\right] w\right)^{2} \quad$ impossible! $P_{X, Y}$ unknown

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Regularization: $\min _{w}\|y-A w\|_{2}^{2}+\tau \psi(w)$

## Machine/Statistical Learning: Linear Classification

Data $N$ pairs $\left(x_{1}, y_{1}\right), \ldots,\left(x_{N}, y_{N}\right)$, where $x_{i} \in \mathbb{R}^{d}$ (feature vectors) and $y_{i} \in\{-1,+1\}$ (labels).
Goal: find "good" linear classifier (i.e., find the optimal weights):

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\widehat{y}=\operatorname{sign}\left(\left[x^{T} 1\right] w\right)=\operatorname{sign}\left(w_{d+1}+\sum_{j=1}^{d} w_{j} x_{j}\right)
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Convexification: EE neither convex nor differentiable (NP-hard problem). Solution: replace $h: \mathbb{R} \rightarrow\{0,1\}$ with convex loss $L: \mathbb{R} \rightarrow \mathbb{R}_{+}$.

## Machine/Statistical Learning: Linear Classification

Criterion: $\min _{w} \underbrace{\sum_{i=1}^{N} L(\underbrace{y_{i}\left(w^{T} x_{i}+b\right)}_{\text {margin }})}_{f(w)}+\tau \psi(w)$
Regularizer: $\psi=\ell_{1} \Rightarrow$ encourage sparseness $\Rightarrow$ feature selection Convex losses: $L: \mathbb{R} \rightarrow \mathbb{R}_{+}$is a (preferably convex) loss function.

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- Misclassification loss: $L(z)=1_{z<0}$
- Hinge loss: $L(z)=\max \{1-z, 0\}$
- Logistic loss: $L(z)=\frac{\log (1+\exp (-z))}{\log 2}$
- Squared loss: $L(z)=(z-1)^{2}$



## Machine/Statistical Learning: General Formulation

This formulation covers a wide range of linear ML methods:

$$
\min _{w} \underbrace{\sum_{i=1}^{N} L\left(y_{i}\left(\left[x^{T} 1\right] w\right)\right)}_{f(w)}+\tau \psi(w)
$$

- Least squares regression: $L(z)=(z-1)^{2}, \psi(w)=0$.
- Ridge regression: $L(z)=(z-1)^{2}, \psi(w)=\|w\|_{2}^{2}$.
- Lasso regression: $L(z)=(z-1)^{2}, \psi(w)=\|w\|_{1}$
- Logistic regression: $L(z)=\log (1+\exp (-z))$ (ridge, if $\psi(w)=\|w\|_{2}^{2}$
- Sparse logistic regression: $L(z)=\log (1+\exp (-z)), \psi(w)=\|w\|_{1}$
- Support vector machines: $L(z)=\max \{1-z, 0\}, \psi(w)=\|w\|_{2}^{2}$
- Boosting: $L(z)=\exp (-z)$,
- ...


## Machine/Statistical Learning: Nonlinear Problems

What about non-linear functions?
Simply use $\widehat{y}=\phi(x, w)=\sum_{j=1}^{D} w_{j} \phi_{j}(x)$, where $\phi_{j}: \mathbb{R}^{d} \rightarrow \mathbb{R}$
Essentially, nothing changes; computationally, a lot may change!

$$
\min _{w} \underbrace{\sum_{i=1}^{N} L\left(y_{i} \phi(x, w)\right)}_{f(w)}+\tau \psi(w)
$$

Key feature: $\phi(x, w)$ is still linear with respect to $w$, thus $f$ inherits the convexity of $L$.

Examples: polynomials, radial basis functions, wavelets, splines, kernels,... Recover the linear case, letting $D=d+1, f_{j}(x)=x_{j}, \quad$ and $f_{d+1}=1$.

## Structured Sparsity

$\ell_{1}$ regularization promotes sparsity
A very simple sparsity pattern: prefer models with small cardinality

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Group/structured regularization.

## Structured Sparsity and Groups

Main goal: to promote structural patterns, not just penalize cardinality

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Main goal: to promote structural patterns, not just penalize cardinality
Group sparsity: discard/keep entire groups of features (Bach et al., 2012)

- density inside each group
- sparsity with respect to the groups which are selected
- choice of groups: prior knowledge about the intended sparsity patterns


## Structured Sparsity and Groups

Main goal: to promote structural patterns, not just penalize cardinality
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Yields statistical gains if the assumption is correct (Stojnic et al., 2009)
Many applications:

- feature template selection (Martins et al., 2011)
- multi-task learning (Caruana, 1997; Obozinski et al., 2010)
- learning the structure of graphical models (Schmidt and Murphy, 2010)


## "Grid" Sparsity

For feature spaces that can be arranged as a grid (examples next)


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Goal: push entire columns to have zero weights
The groups are the columns of the grid

## Example: Sparsity with Multiple Classes

In multi-class (more than just 2 classes) classification, a common formulation is

$$
\hat{y}=\arg \max _{y \in\{1, \ldots, K\}} x^{T} w_{y}
$$

Weight vector $w=\left(w_{1}, \ldots, w_{K}\right) \in \mathbb{R}^{K d}$ has a natural group/grid organization:

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Weight vector $w=\left(w_{1}, \ldots, w_{K}\right) \in \mathbb{R}^{K d}$ has a natural group/grid organization:


sparse


Simple sparsity is wasteful: may still need to keep all the features Structured sparsity: discard some input features (feature selection)

## Example: Multi-Task Learning

Same thing, except now rows are tasks and columns are features Example: simultaneous regression (seek function into $\mathbb{R}^{d} \rightarrow \mathbb{R}^{b}$ )



## Example: Multi-Task Learning

Same thing, except now rows are tasks and columns are features Example: simultaneous regression (seek function into $\mathbb{R}^{d} \rightarrow \mathbb{R}^{b}$ )


Goal: discard features that are irrelevant for all tasks
Approach: one group per feature (Caruana, 1997; Obozinski et al., 2010)

## Example: Magnetoencephalograpy (MEG)

Group: localized cortex area at localized time period (Bolstad et al., 2009)


## Group Sparsity

## $\square_{\square}^{\square} \square_{\square}^{\square}$ ■ ロ

## Group Sparsity

- $D$ features
- $M$ groups $G_{1}, \ldots, G_{M}$, each $G_{m} \subseteq\{1, \ldots, D\}$
- parameter subvectors $x_{G_{1}}, \ldots, x_{G_{M}}$


## Group Sparsity



$$
\psi(x)=\sum_{m=1}^{M}\left\|x_{G_{m}}\right\|_{2}
$$

## Group Sparsity



- Intuitively: the $\ell_{1}$ norm of the $\ell_{2}$ norms
- Technically, still a norm (called a mixed norm, denoted $\ell_{2,1}$ )


## Lasso versus group-Lasso



$$
\Omega(\boldsymbol{w})=\left|w_{1}\right|+\left|w_{2}\right|+\left|w_{3}\right|
$$

## Lasso versus group-Lasso



## Composite Absolute Penalties

A mixed-norm regularization:

$$
\psi(x)=\left(\sum_{m=1}^{M}\left\|x_{m}\right\|_{q}^{r}\right)^{1 / r}
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The $r$-norm of the $q$-norms $(r \geq 1, q \geq 1)$
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- The most common choice: $\ell_{2,1}$ norm
- Another frequent choice: $\ell_{\infty, 1}$ norm (Quattoni et al., 2009; Graça et al., 2009; Eisenstein et al., 2011; Wright et al., 2009)


## Three Scenarios

- Non-overlapping Groups
- Tree-structured Groups
- Graph-structured Groups


## Non-overlapping Groups

Assume that $G_{1}, \ldots, G_{M}$ (where $G_{m} \subset\{1, \ldots, d\}$ ) constitute a partition:

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\bigcup_{i=1}^{M} G_{m}=\{1, \ldots, d\} \quad \text { and } \quad i \neq j \Rightarrow G_{i} \cap G_{j}=\emptyset
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Examples of non-trivial groups:

- label-based groups
- task-based groups


## Tree-Structured Groups

Assumption: if two groups overlap, one is contained in the other $\Rightarrow$ hierarchical structure (Kim and Xing, 2010; Mairal et al., 2010)

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- If a group is discarded, all its descendants are also discarded


## Matrix Inference Problems

Sparsest solution:

- From $B x=b \in \mathbb{R}^{p}$, find
$x \in \mathbb{R}^{n}(p<n)$.
- $\min _{x}\|x\|_{0}$ s.t. $B x=b$
- Yields exact solution, under some conditions.


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Lowest rank solution:

- From $\mathcal{B}(X)=b \in \mathbb{R}^{p}$, find $X \in \mathbb{R}^{m \times n}(p<m n)$.
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Both NP-hard (in general); the same is true of noisy versions:

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Under some conditions, the same solution is obtained by replacing $\operatorname{rank}(X)$ by the nuclear norm $\|X\|_{*}$ (as any norm, it is convex) (Recht et al., 2010)

## Matrix Nuclear Norm (and Other Norms)

- Also known as trace norm; the $\ell_{1}$-type norm for matrices $X \in \mathbb{R}^{m \times n}$
- Definition: $\|X\|_{*}=\operatorname{trace}\left(\sqrt{X^{\top} X}\right)=\sum_{i=1}^{\min \{m, n\}} \sigma_{i}$, the $\sigma_{i}$ are the singular values of $X$.


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- Particular case of Schatten $q$-norm: $\|X\|_{q}=\left(\sum_{i=1}^{\min \{m, n\}}\left(\sigma_{i}\right)^{q}\right)^{1 / q}$.
- Two other notable Schatten norms:
- Frobenius norm: $\|X\|_{2}=\|X\|_{F}=\sqrt{\sum_{i=1}^{\min \{m, n\}}\left(\sigma_{i}\right)^{2}}=\sqrt{\sum_{i, i} X_{i, j}^{2}}$
- Spectral norm: $\|X\|_{\infty}=\max \left\{\sigma_{1}, \ldots, \sigma_{\min \{m, n\}}\right\}$


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Tikhonov formulation: $\min _{X} \underbrace{\|\mathcal{B}(X)-b\|_{2}^{2}}_{f(X)}+\underbrace{\tau\|X\|_{*}}_{\tau \psi(X)}$

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Why does the nuclear norm favor low rank solutions? Let $Y=U \wedge V^{T}$ be the singular value decomposition, where $\Lambda=\operatorname{diag}\left(\sigma_{1}, \ldots, \sigma_{\min \{m, n\}}\right)$; then

$$
\arg \min _{X} \frac{1}{2}\|Y-X\|_{F}^{2}+\tau\|X\|_{*}=U \underbrace{\operatorname{soft}(X, \tau)}_{\text {may yield zeros }} V^{T}
$$

...singular value thresholding (Ma et al., 2011; Cai et al., 2010)

## Another Matrix Inference Problem: Inverse Covariance

Consider $n$ samples $y_{1}, \ldots, y_{n} \in \mathbb{R}^{d}$ of a Gaussian r.v. $Y \sim \mathcal{N}(\mu, C)$; the log-likelihood is

$$
L(P)=\log p\left(y_{1}, \ldots, y_{n} \mid P\right)=\log \operatorname{det}(P)-\operatorname{trace}(S P)+\text { constant }
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where $S=\frac{1}{n} \sum_{i=1}^{n}\left(y_{i}-\mu\right)\left(y_{i}-\mu\right)^{T}$ and $P=C^{-1}$ (inverse covariance).

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Zeros in $P$ reveal conditional independencies between components of $Y$ :

$$
P_{i j}=0 \Leftrightarrow Y_{i} \Perp Y_{j} \mid\left\{Y_{k}, k \neq i, j\right\}
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...exploited to infer (in)dependencies among Gaussian variables. Widely used in computational biology and neuroscience, social network analysis, ...

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Sparsity (presence of zeros) in $P$ is encouraged by solving

$$
\min _{P \succ 0} \underbrace{-\log \operatorname{det}(P)+\operatorname{trace}(S P)}_{f(P)}+\tau \underbrace{\|\operatorname{vect}(P)\|_{1}}_{\psi(P)}
$$

where $\operatorname{vect}(P)=\left[P_{1,1}, \ldots, P_{d, d}\right]^{T}$.

## Atomic-Norm Regularization

Key concept in sparse modeling: synthesize "object" using a few atoms:

$$
x=\sum_{i=1}^{|\mathcal{A}|} c_{i} a_{i}
$$

- $\mathcal{A}$ is the set of atoms (the atomic set), or building blocks.
- $c_{i} \geq 0$ are weights; $x$ is simple/sparse object $\Rightarrow\|c\|_{0} \ll|\mathcal{A}|$
- Formally, $\mathcal{A}$ is a compact subset of $\mathbb{R}^{n}$


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The (Minkowski) gauge of $\mathcal{A}$ is:

$$
\|x\|_{\mathcal{A}}=\inf \{t>0: x \in t \operatorname{conv}(\mathcal{A})\}
$$

Assuming that $\mathcal{A}$ centrally symmetry about the origin $(a \in \mathcal{A} \Rightarrow-a \in \mathcal{A}),\|\cdot\|_{\mathcal{A}}$ is a norm, called the atomic norm
Chandrasekaran et al. (2012).

## Atomic-Norm Regularization

The atomic norm

$$
\begin{aligned}
\|x\|_{\mathcal{A}} & =\inf \{t>0: x \in t \operatorname{conv}(\mathcal{A})\} \\
& =\inf \left\{\sum_{i=1}^{|\mathcal{A}|} c_{i}: x=\sum_{i=1}^{|\mathcal{A}|} c_{i} a_{i}, c_{i} \geq 0\right\}
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...assuming that the centroid of $\mathcal{A}$ is at the origin.

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...assuming that the centroid of $\mathcal{A}$ is at the origin.
Example: the $\ell_{1}$ norm as an atomic norm

- $\mathcal{A}=\left\{\left[\begin{array}{l}0 \\ 1\end{array}\right],\left[\begin{array}{l}1 \\ 0\end{array}\right],\left[\begin{array}{c}0 \\ -1\end{array}\right],\left[\begin{array}{c}-1 \\ 0\end{array}\right]\right\}$



## Atomic Norms: More Examples

## Examples with easy forms:

- sparse vectors

$$
\begin{aligned}
& \mathcal{A}=\left\{ \pm e_{i}\right\}_{i=1}^{N} \\
& \operatorname{conv}(\mathcal{A})=\text { cross-polytope } \\
& \|x\|_{\mathcal{A}}=\|x\|_{1}
\end{aligned}
$$

- low-rank matrices

$$
\begin{aligned}
& \mathcal{A}=\left\{A: \operatorname{rank}(A)=1,\|A\|_{F}=1\right\} \\
& \operatorname{conv}(\mathcal{A})=\text { nuclear norm ball } \\
& \|x\|_{\mathcal{A}}=\|x\|_{\star}
\end{aligned}
$$

- binary vectors

$$
\begin{aligned}
& \mathcal{A}=\{ \pm 1\}^{N} \\
& \operatorname{conv}(\mathcal{A})=\text { hypercube } \\
& \|x\|_{\mathcal{A}}=\|x\|_{\infty}
\end{aligned}
$$

## Atomic-Norm Regularization

Given an atomic set $\mathcal{A}$, we can adopt an Ivanov formulation

$$
\min f(x) \text { s.t. }\|x\|_{\mathcal{A}} \leq \delta
$$

(for some $\delta>0$ ) tends to recover $x$ with sparse atomic representation.

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Can formulate algorithms for the various special cases - but is a general approach available for this formulation?

Yes! The conditional gradient (more later.)

## Summary

- Many inference, learning, signal/image processing problems can be formulated as optimization problems.
- Sparsity-inducing regularizers play an important role in these problems
- There are several way to induce sparsity
- It is possible to formulate structured sparsity
- It is possible to extend the sparsity rationale to other objects, namely matrices
- Atomic norms provide a unified framework for sparsity/simplicity regularization


## References I

Amaldi, E. and Kann, V. (1998). On the approximation of minimizing non zero variables or unsatisfied relations in linear systems. Theoretical Computer Science, 209:237-260.
Bach, F., Jenatton, R., Mairal, J., and Obozinski, G. (2012). Structured sparsity through convex optimization. Statistical Science, 27:450-468.
Bakin, S. (1999). Adaptive regression and model selection in data mining problems. PhD thesis, Australian National University.
Bolstad, A., Veen, B. V., and Nowak, R. (2009). Space-time event sparse penalization for magnetoelectroencephalography. Neurolmage, 46:1066-1081.
Cai, J.-F., Candès, E., and Shen, Z. (2010). A singular value thresholding algorithm for matrix completion. SIAM JOurnal on Optimization, 20:1956-1982.
Candès, E., Romberg, J., and Tao, T. (2006). Robust uncertainty principles: Exact signal reconstruction from highly incomplete frequency information. IEEE Transactions on Information Theory, 52:489-509.
Caruana, R. (1997). Multitask learning. Machine Learning, 28(1):41-75.
Chandrasekaran, V., Recht, B., Parrilo, P., and Willsky, A. (2012). The convex geometry of linear inverse problems. Foundations of Computational Mathematics, 12:805-849.
Chen, S., Donoho, D., and Saunders, M. (1995). Atomic decomposition by basis pursuit. Technical report, Department of Statistics, Stanford University.

## References II

Davis, G., Mallat, S., and Avellaneda, M. (1997). Greedy adaptive approximation. Journal of Constructive Approximation, 13:57-98.
Donoho, D. (2006). Compressed sensing. IEEE Transactions on Information Theory, 52:1289-1306.
Eisenstein, J., Smith, N. A., and Xing, E. P. (2011). Discovering sociolinguistic associations with structured sparsity. In Proc. of ACL.
Graça, J., Ganchev, K., Taskar, B., and Pereira, F. (2009). Posterior vs. parameter sparsity in latent variable models. Advances in Neural Information Processing Systems.
Kim, S. and Xing, E. (2010). Tree-guided group lasso for multi-task regression with structured sparsity. In Proc. of ICML.
Ma, S., Goldfarb, D., and Chen, L. (2011). Fixed point and Bregman iterative methods for matrix rank minimization. Mathematical Programming (Series A), 128:321-353.
Mairal, J., Jenatton, R., Obozinski, G., and Bach, F. (2010). Network flow algorithms for structured sparsity. In Advances in Neural Information Processing Systems.
Martins, A. F. T., Smith, N. A., Aguiar, P. M. Q., and Figueiredo, M. A. T. (2011). Structured Sparsity in Structured Prediction. In Proc. of Empirical Methods for Natural Language Processing.
Muthukrishnan, S. (2005). Data Streams: Algorithms and Applications. Now Publishers, Boston, MA.

## References III

Obozinski, G., Taskar, B., and Jordan, M. (2010). Joint covariate selection and joint subspace selection for multiple classification problems. Statistics and Computing, 20(2):231-252.
Quattoni, A., Carreras, X., Collins, M., and Darrell, T. (2009). An efficient projection for $I_{1, \infty}$ regularization. In Proc. of ICML.
Recht, B., Fazel, M., and Parrilo, P. (2010). Guaranteed minimum-rank solutions of linear matrix equations via nuclear norm minimization. SIAM Review, 52:471-501.
Schmidt, M. and Murphy, K. (2010). Convex structure learning in log-linear models: Beyond pairwise potentials. In Proc. of AISTATS.
Stojnic, M., Parvaresh, F., and Hassibi, B. (2009). On the reconstruction of block-sparse signals with an optimal number of measurements. Signal Processing, IEEE Transactions on, 57(8):3075-3085.
Tibshirani, R. (1996). Regression shrinkage and selection via the lasso. Journal of the Royal Statistical Society B., pages 267-288.
Wright, S., Nowak, R., and Figueiredo, M. (2009). Sparse reconstruction by separable approximation. IEEE Transactions on Signal Processing, 57:2479-2493.
Yuan, M. and Lin, Y. (2006). Model selection and estimation in regression with grouped variables. Journal of the Royal Statistical Society (B), 68(1):49.
Zhao, P., Rocha, G., and Yu, B. (2009). Grouped and hierarchical model selection through composite absolute penalties. Annals of Statistics, 37(6A):3468-3497.

