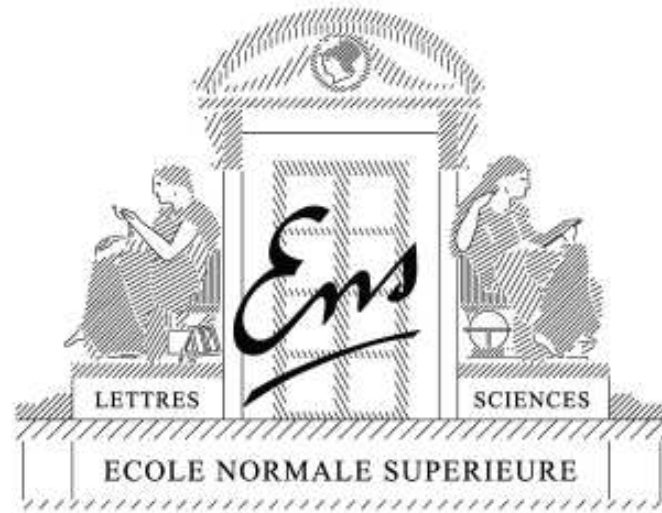


Structured sparsity through convex optimization

Francis Bach

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Joint work with R. Jenatton, J. Mairal, G. Obozinski
November 2011

Outline

- **Introduction: Sparse methods for machine learning**
 - Need for structured sparsity: **Going beyond the ℓ_1 -norm**
- **Classical approaches to structured sparsity**
 - Linear combinations of ℓ_q -norms
- **Structured sparsity through submodular functions**
 - Relaxation of the penalization of supports
 - **Unified algorithms and analysis**
- **Extensions**

Sparsity in supervised machine learning

- Observed data $(x_i, y_i) \in \mathbb{R}^p \times \mathbb{R}$, $i = 1, \dots, n$
 - Response vector $y = (y_1, \dots, y_n)^\top \in \mathbb{R}^n$
 - Design matrix $X = (x_1, \dots, x_n)^\top \in \mathbb{R}^{n \times p}$
- Regularized empirical risk minimization:

$$\min_{w \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^n \ell(y_i, w^\top x_i) + \lambda \Omega(w) = \boxed{\min_{w \in \mathbb{R}^p} L(y, Xw) + \lambda \Omega(w)}$$

- Norm Ω to promote sparsity
 - square loss + ℓ_1 -norm \Rightarrow **basis pursuit** in signal processing (Chen et al., 2001), **Lasso** in statistics/machine learning (Tibshirani, 1996)
 - Proxy for **interpretability**
 - Allow **high-dimensional inference**: $\boxed{\log p = O(n)}$

Sparsity in **unsupervised** machine learning

- **Multiple** responses/signals $y = (y^1, \dots, y^k) \in \mathbb{R}^{n \times k}$

$$\min_{w^1, \dots, w^k \in \mathbb{R}^p} \sum_{j=1}^k \left\{ L(y^j, X w^j) + \lambda \Omega(w^j) \right\}$$

Sparsity in **unsupervised** machine learning

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- **Only responses are observed** \Rightarrow **Dictionary learning**

– Learn $X = (x^1, \dots, x^p) \in \mathbb{R}^{n \times p}$ such that $\forall j, \|x^j\|_2 \leq 1$

$$\min_{X=(x^1, \dots, x^p)} \min_{w^1, \dots, w^k \in \mathbb{R}^p} \sum_{j=1}^k \left\{ L(y^j, X w^j) + \lambda \Omega(w^j) \right\}$$

– Olshausen and Field (1997); Elad and Aharon (2006); Mairal et al. (2009a)

- **sparse PCA**: replace $\|x^j\|_2 \leq 1$ by $\Theta(x^j) \leq 1$

Sparsity in signal processing

- **Multiple** responses/signals $x = (x^1, \dots, x^k) \in \mathbb{R}^{n \times k}$

$$\min_{\alpha^1, \dots, \alpha^k \in \mathbb{R}^p} \sum_{j=1}^k \left\{ L(x^j, D\alpha^j) + \lambda \Omega(\alpha^j) \right\}$$

- **Only responses are observed** \Rightarrow **Dictionary learning**

– Learn $D = (d^1, \dots, d^p) \in \mathbb{R}^{n \times p}$ such that $\forall j, \|d^j\|_2 \leq 1$

$$\min_{D=(d^1, \dots, d^p)} \min_{\alpha^1, \dots, \alpha^k \in \mathbb{R}^p} \sum_{j=1}^k \left\{ L(x^j, D\alpha^j) + \lambda \Omega(\alpha^j) \right\}$$

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Why structured sparsity?

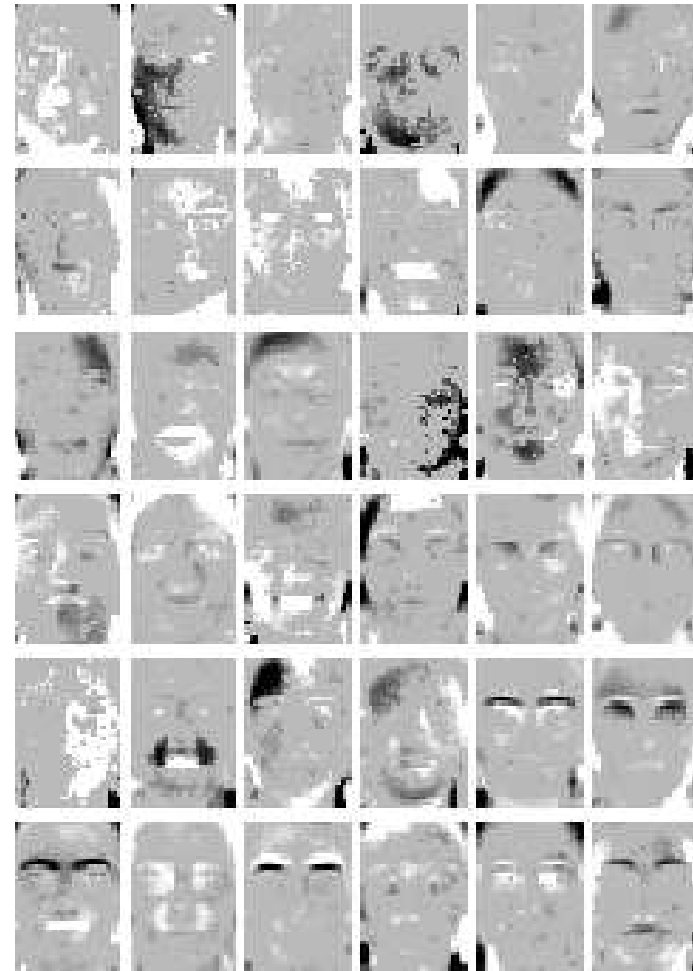
- **Interpretability**

- Structured dictionary elements (Jenatton et al., 2009b)
- Dictionary elements “organized” in a **tree** or a **grid** (Kavukcuoglu et al., 2009; Jenatton et al., 2010; Mairal et al., 2010)

Structured sparse PCA (Jenatton et al., 2009b)



raw data



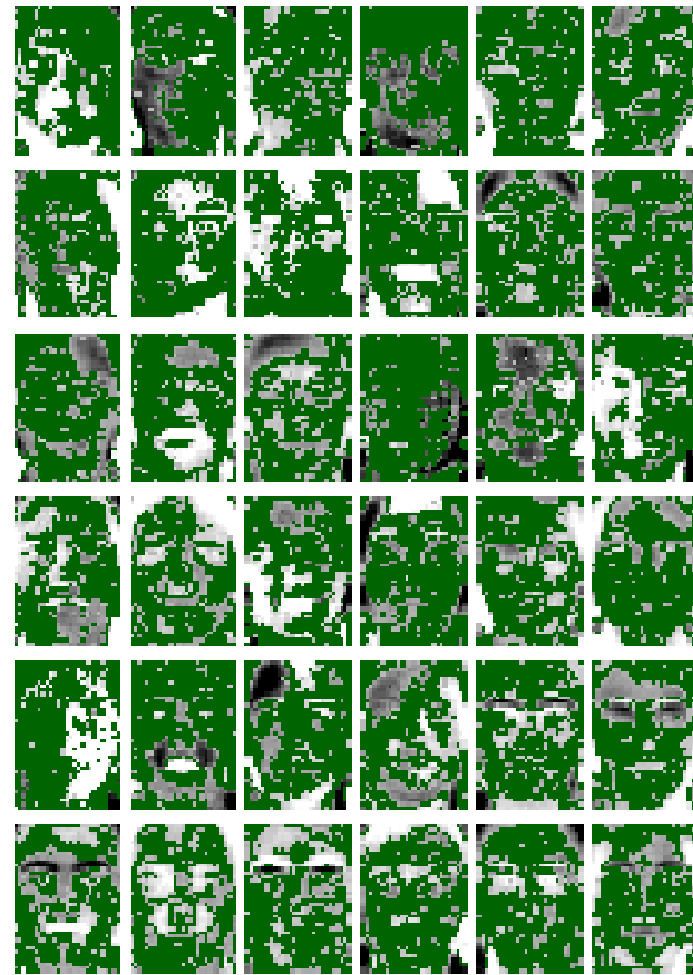
sparse PCA

- Unstructured sparse PCA \Rightarrow many zeros do not lead to better interpretability

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raw data



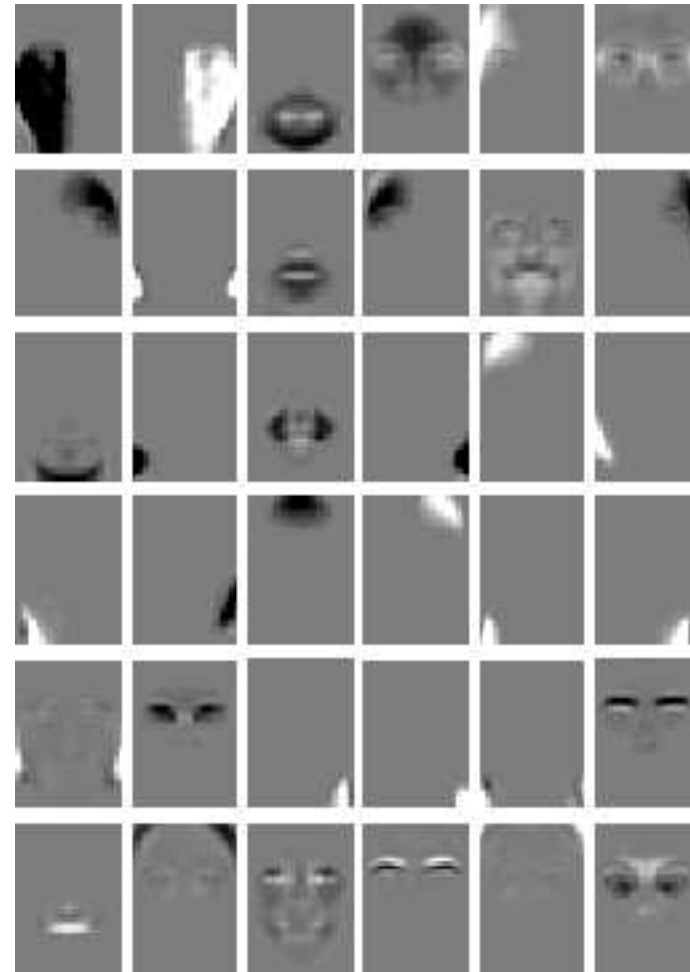
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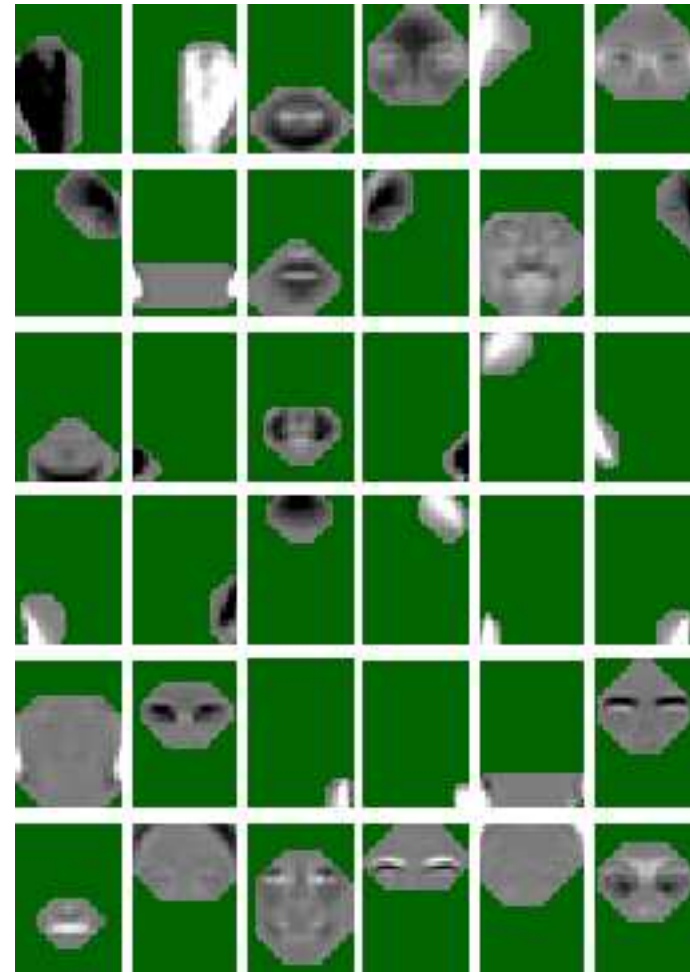
Structured sparse PCA

- Enforce selection of **convex** nonzero patterns \Rightarrow robustness to occlusion in face identification

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raw data



Structured sparse PCA

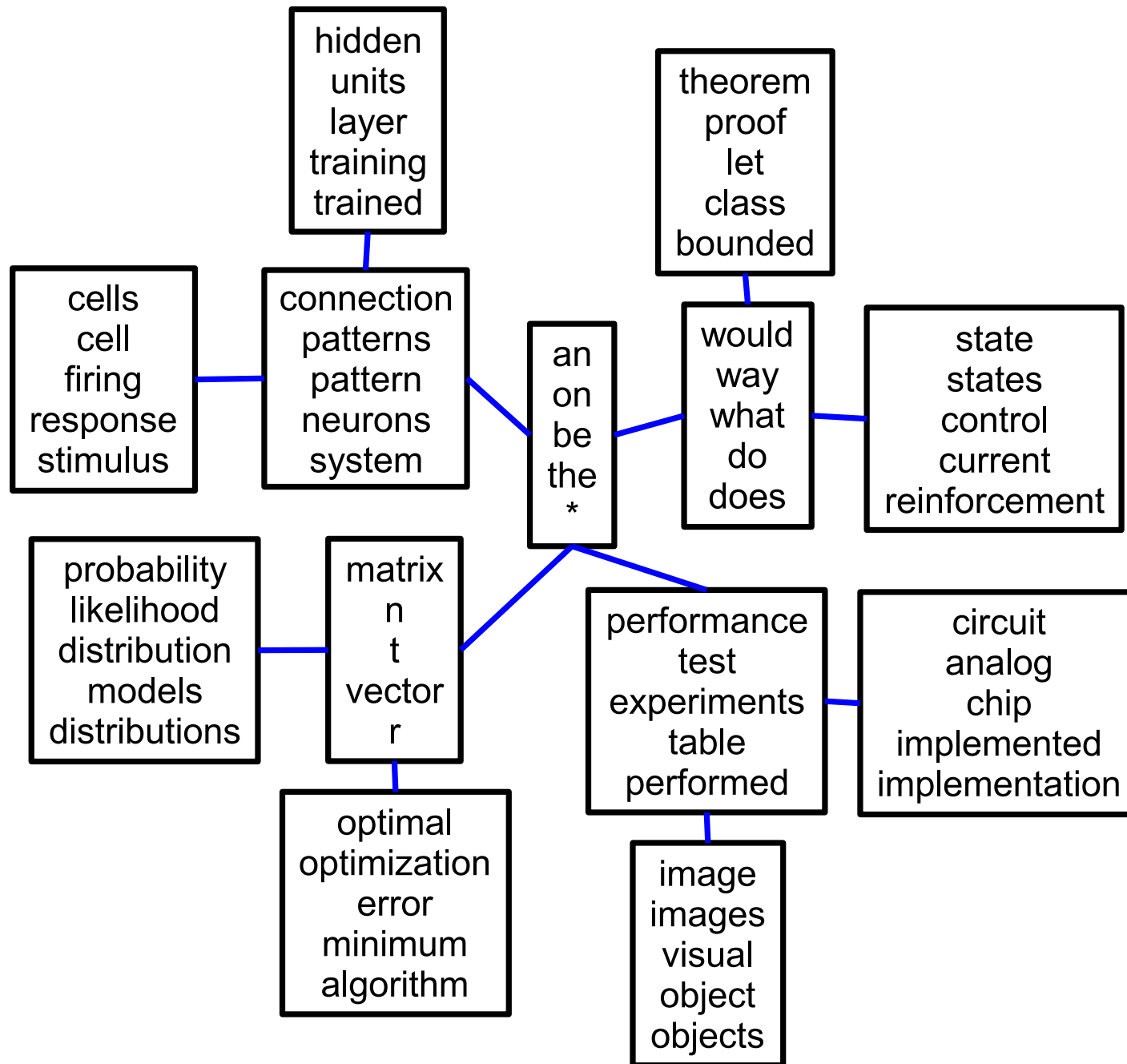
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Modelling of text corpora (Jenatton et al., 2010)



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- **Stability and identifiability**

- Optimization problem $\min_{w \in \mathbb{R}^p} L(y, Xw) + \lambda \|w\|_1$ is unstable
- “Codes” w^j often used in later processing (Mairal et al., 2009c)

- **Prediction or estimation performance**

- When prior knowledge matches data (Haupt and Nowak, 2006; Baraniuk et al., 2008; Jenatton et al., 2009a; Huang et al., 2009)

- **Numerical efficiency**

- Non-linear variable selection with 2^p subsets (Bach, 2008)

Classical approaches to structured sparsity

- **Many application domains**

- Computer vision (Cevher et al., 2008; Mairal et al., 2009b)
- Neuro-imaging (Gramfort and Kowalski, 2009; Jenatton et al., 2011)
- Bio-informatics (Rapaport et al., 2008; Kim and Xing, 2010)

- **Non-convex approaches**

- Haupt and Nowak (2006); Baraniuk et al. (2008); Huang et al. (2009)

- **Convex approaches**

- Design of sparsity-inducing norms

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Sparsity-inducing norms

- Popular choice for Ω

- The ℓ_1 - ℓ_2 norm,

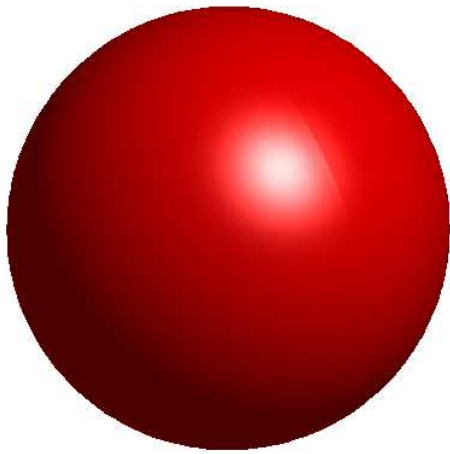
$$\sum_{G \in \mathbf{H}} \|w_G\|_2 = \sum_{G \in \mathbf{H}} \left(\sum_{j \in G} w_j^2 \right)^{1/2}$$

- with \mathbf{H} a **partition** of $\{1, \dots, p\}$
- The ℓ_1 - ℓ_2 norm sets to zero **groups of non-overlapping variables** (as opposed to single variables for the ℓ_1 -norm)
- For the square loss, group Lasso (Yuan and Lin, 2006)

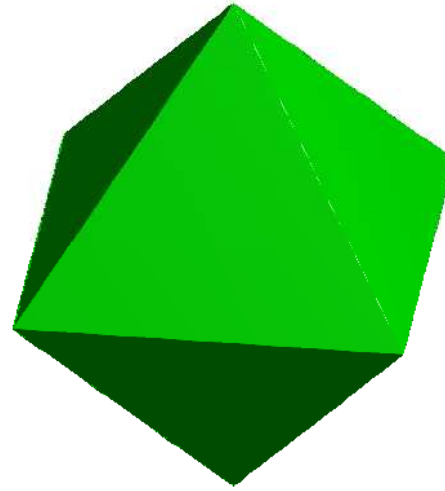


Unit norm balls

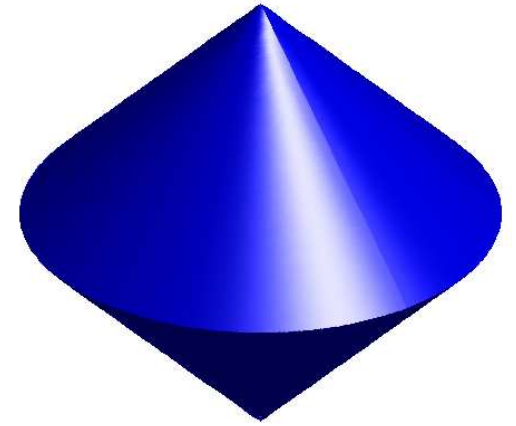
Geometric interpretation



$$\|w\|_2$$



$$\|w\|_1$$



$$\sqrt{w_1^2 + w_2^2} + |w_3|$$

Sparsity-inducing norms

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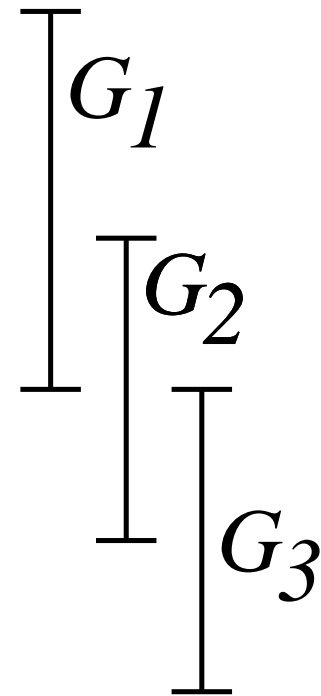
- However, the ℓ_1 - ℓ_2 norm encodes **fixed/static prior information**, requires to know in advance how to group the variables
- What happens if the set of groups \mathbf{H} is not a partition anymore?

Structured sparsity with **overlapping** groups (Jenatton, Audibert, and Bach, 2009a)

- When penalizing by the ℓ_1 - ℓ_2 norm,

$$\sum_{G \in \mathcal{H}} \|w_G\|_2 = \sum_{G \in \mathcal{H}} \left(\sum_{j \in G} w_j^2 \right)^{1/2}$$

- The ℓ_1 norm induces sparsity at the group level:
 - * Some w_G 's are set to zero
- Inside the groups, the ℓ_2 norm does not promote sparsity

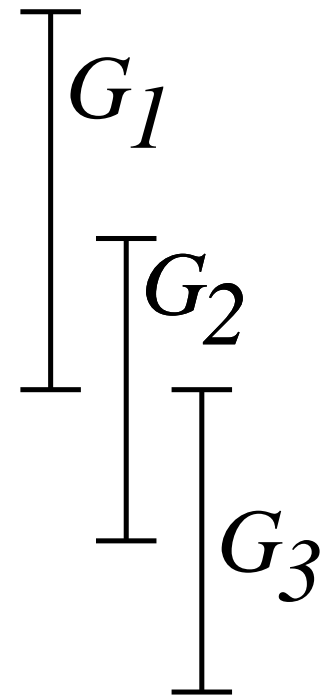


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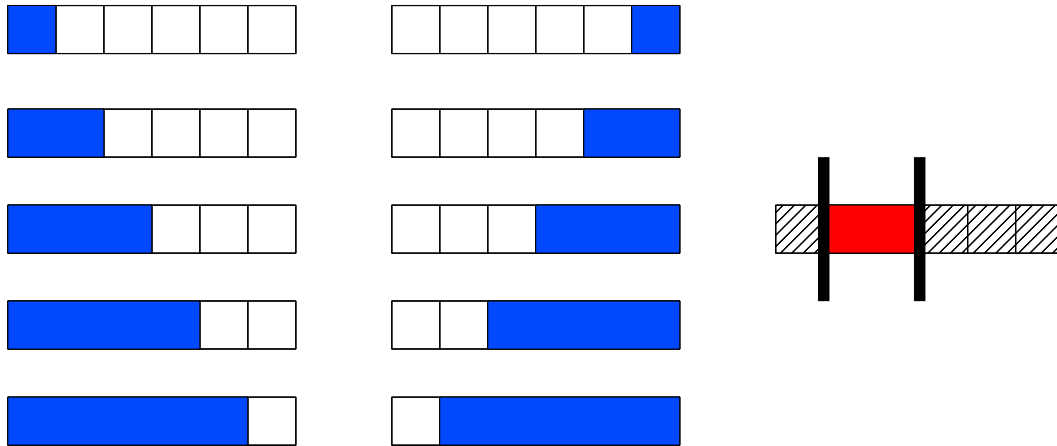
- The zero pattern of w is given by

$$\{j, w_j = 0\} = \bigcup_{G \in \mathbf{H}'} G \text{ for some } \mathbf{H}' \subseteq \mathbf{H}$$

- **Zero patterns are unions of groups**

Examples of set of groups \mathbf{H}

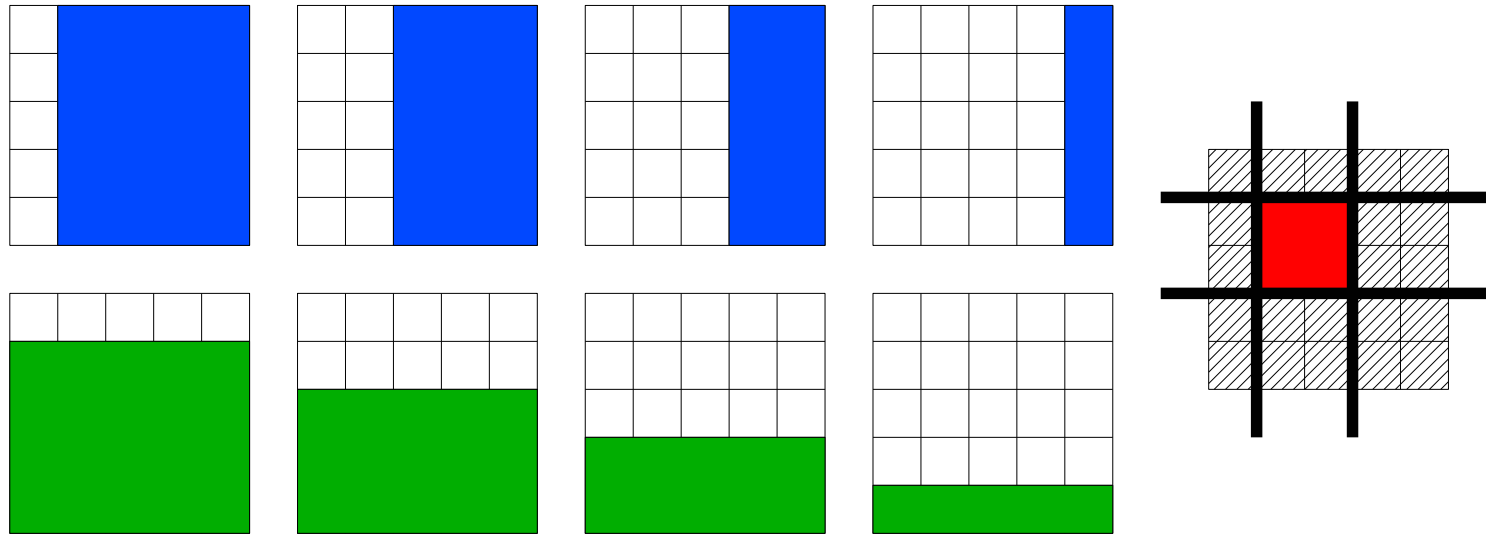
- Selection of contiguous patterns on a sequence, $p = 6$



- \mathbf{H} is the set of blue groups
- Any union of blue groups set to zero leads to the selection of a contiguous pattern

Examples of set of groups \mathbf{H}

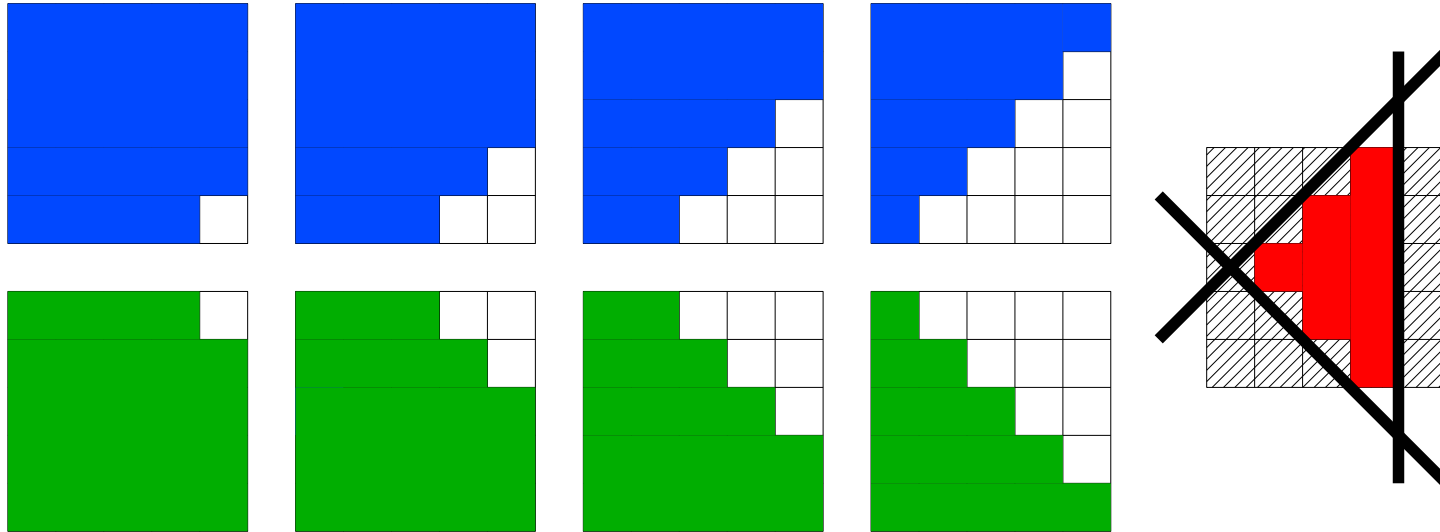
- Selection of rectangles on a 2-D grids, $p = 25$



- \mathbf{H} is the set of blue/green groups (with their not displayed complements)
- Any union of blue/green groups set to zero leads to the selection of a rectangle

Examples of set of groups H

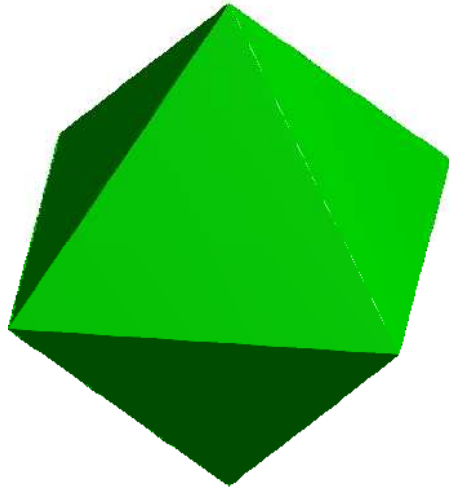
- Selection of diamond-shaped patterns on a 2-D grids, $p = 25$.



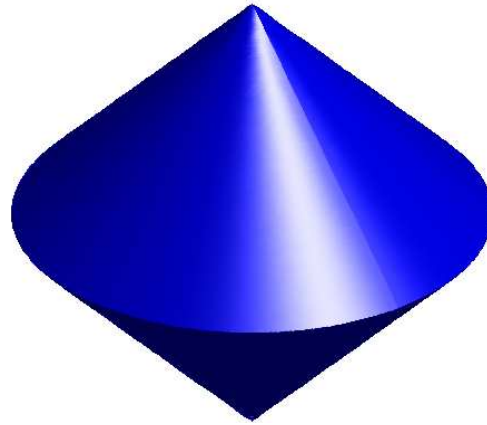
- It is possible to extend such settings to 3-D space, or more complex topologies

Unit norm balls

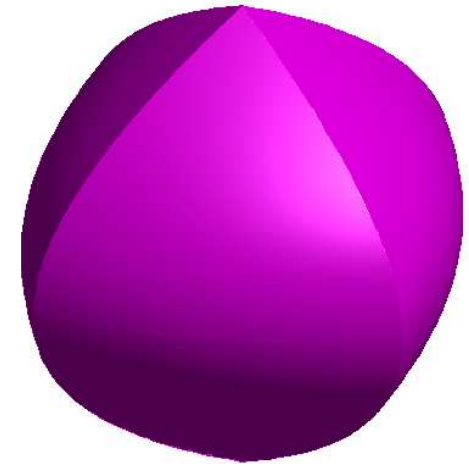
Geometric interpretation



$$\|w\|_1$$



$$\sqrt{w_1^2 + w_2^2} + |w_3|$$



$$\|w\|_2 + |w_1| + |w_2|$$

Optimization for sparsity-inducing norms

(see Bach, Jenatton, Mairal, and Obozinski, 2011)

- Gradient descent as a **proximal method** (differentiable functions)

$$- w_{t+1} = \arg \min_{w \in \mathbb{R}^p} J(w_t) + (w - w_t)^\top \nabla J(w_t) + \frac{L}{2} \|w - w_t\|_2^2$$

$$- w_{t+1} = w_t - \frac{1}{L} \nabla J(w_t)$$

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- Problems of the form:
$$\min_{w \in \mathbb{R}^p} L(w) + \lambda \Omega(w)$$

$$- w_{t+1} = \arg \min_{w \in \mathbb{R}^p} L(w_t) + (w - w_t)^\top \nabla L(w_t) + \lambda \Omega(w) + \frac{L}{2} \|w - w_t\|_2^2$$

$$- \Omega(w) = \|w\|_1 \Rightarrow \text{Thresholded gradient descent}$$

- Similar convergence rates than smooth optimization

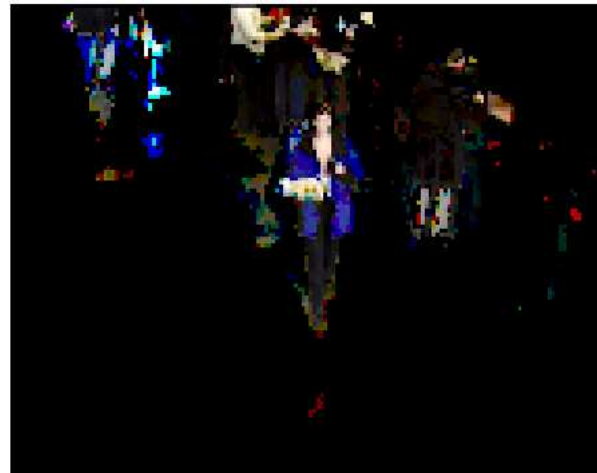
– Acceleration methods (Nesterov, 2007; Beck and Teboulle, 2009)

Application to background subtraction (Mairal, Jenatton, Obozinski, and Bach, 2010)

Input

ℓ_1 -norm

Structured norm



Application to background subtraction (Mairal, Jenatton, Obozinski, and Bach, 2010)

Background

ℓ_1 -norm

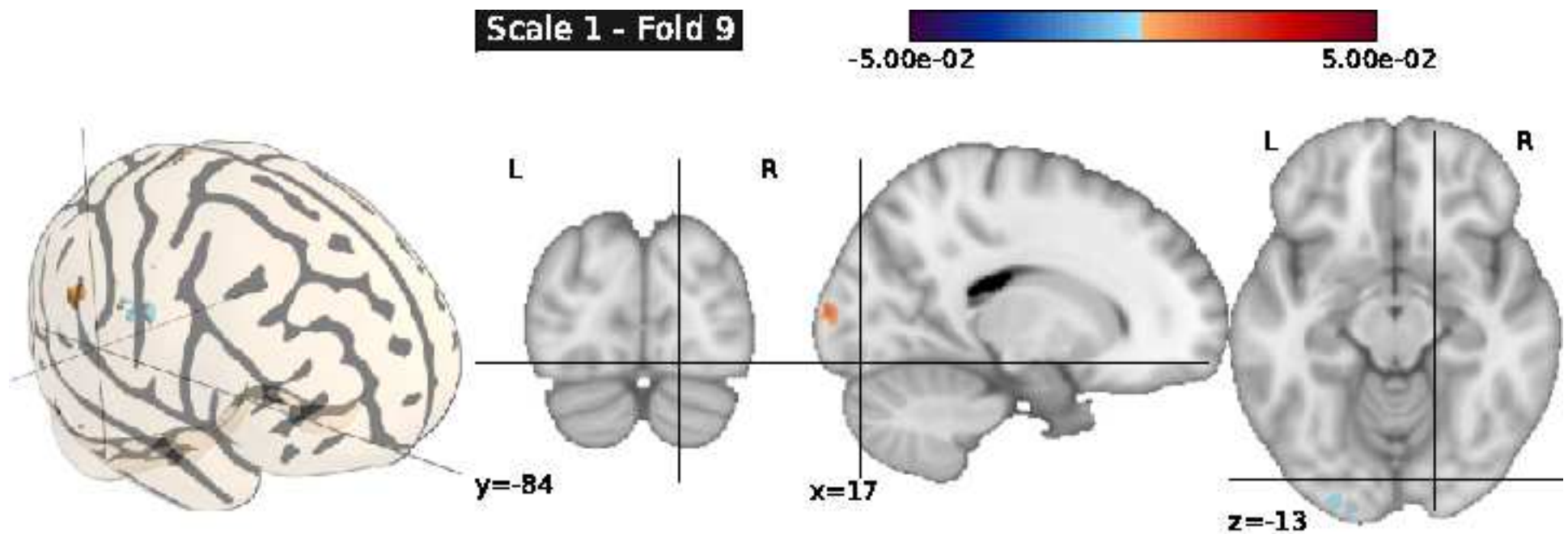
Structured norm



Application to neuro-imaging

Structured sparsity for fMRI (Jenatton et al., 2011)

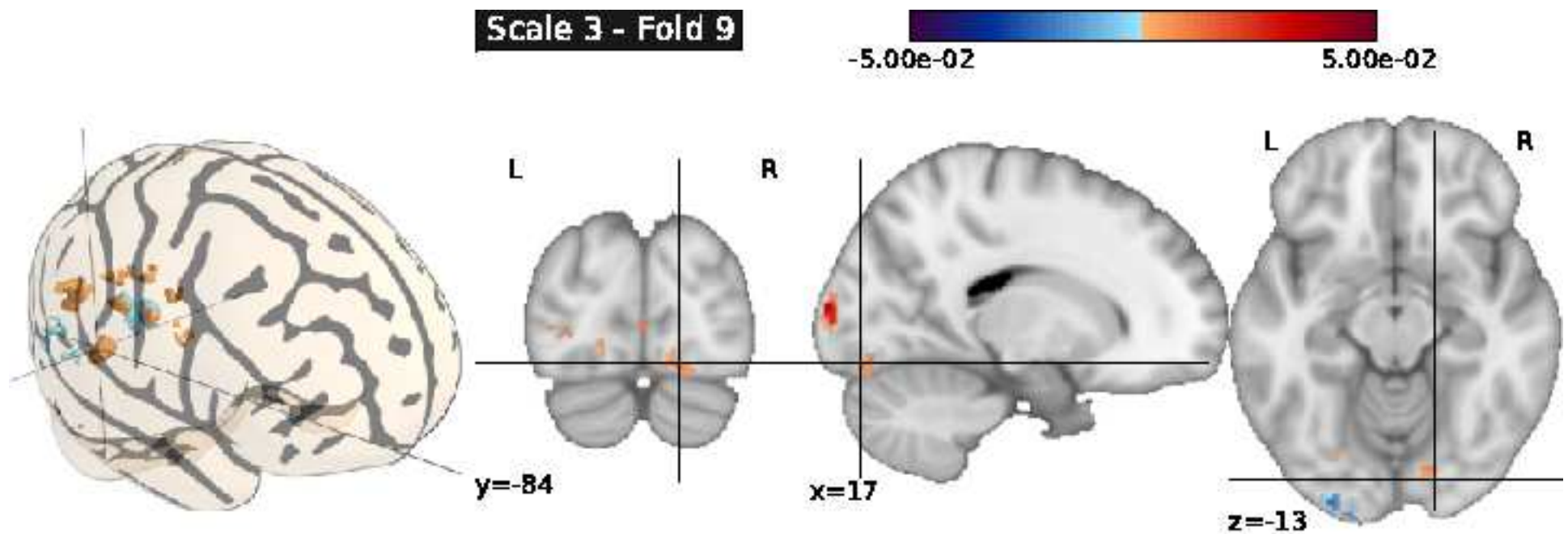
- “Brain reading”: prediction of (seen) object size
- Multi-scale activity levels through hierarchical penalization



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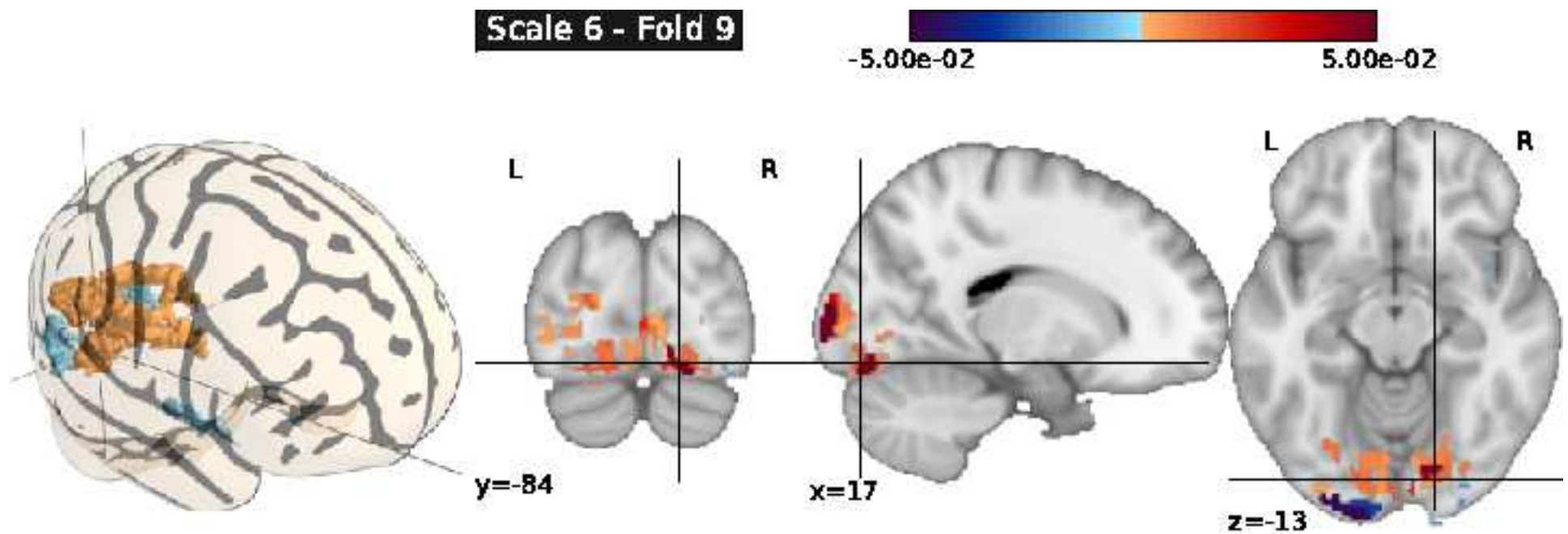
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Sparse Structured PCA

(Jenatton, Obozinski, and Bach, 2009b)

- Learning **sparse and structured dictionary elements**:

$$\min_{W \in \mathbb{R}^{k \times n}, X \in \mathbb{R}^{p \times k}} \frac{1}{n} \sum_{i=1}^n \|y^i - X w^i\|_2^2 + \lambda \sum_{j=1}^p \Omega(x^j) \text{ s.t. } \forall i, \|w^i\|_2 \leq 1$$

Application to face databases (1/3)



raw data



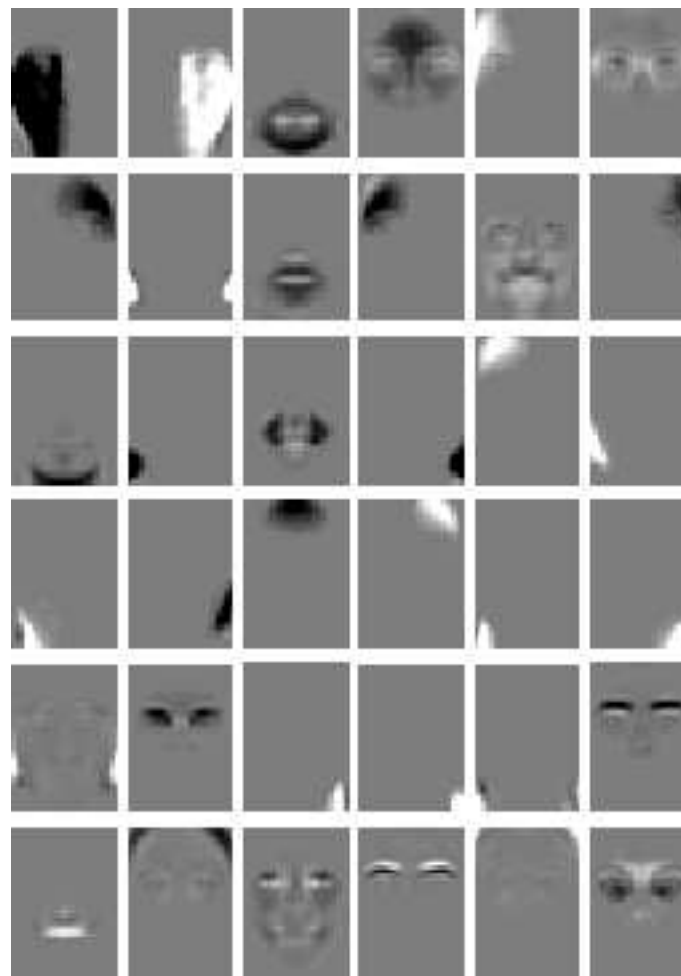
(unstructured) NMF

- NMF obtains partially local features

Application to face databases (2/3)



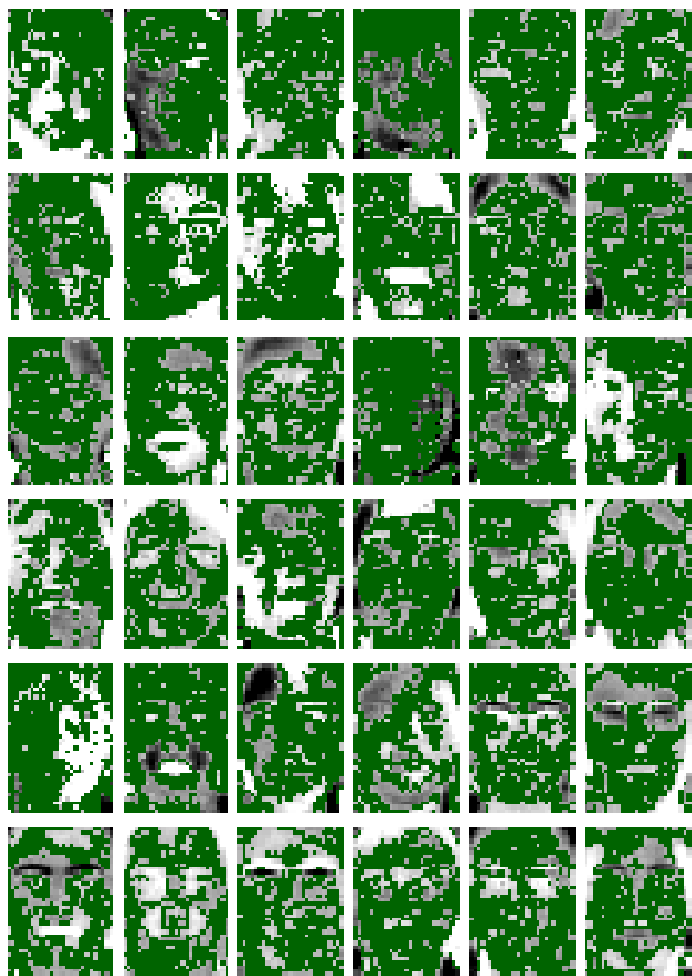
(unstructured) sparse PCA



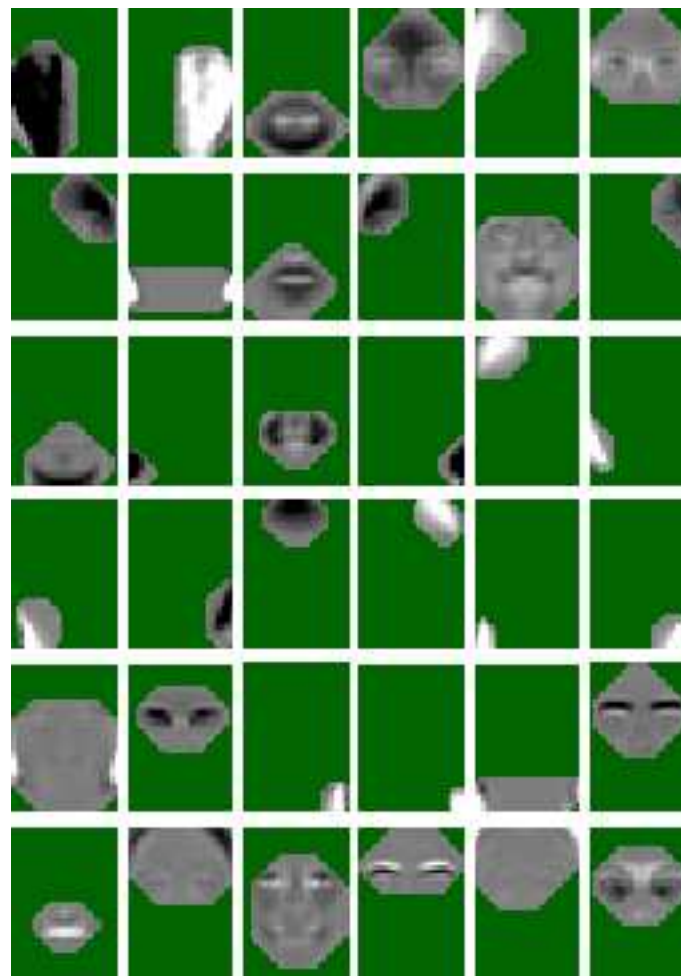
Structured sparse PCA

- Enforce selection of **convex** nonzero patterns \Rightarrow robustness to occlusion

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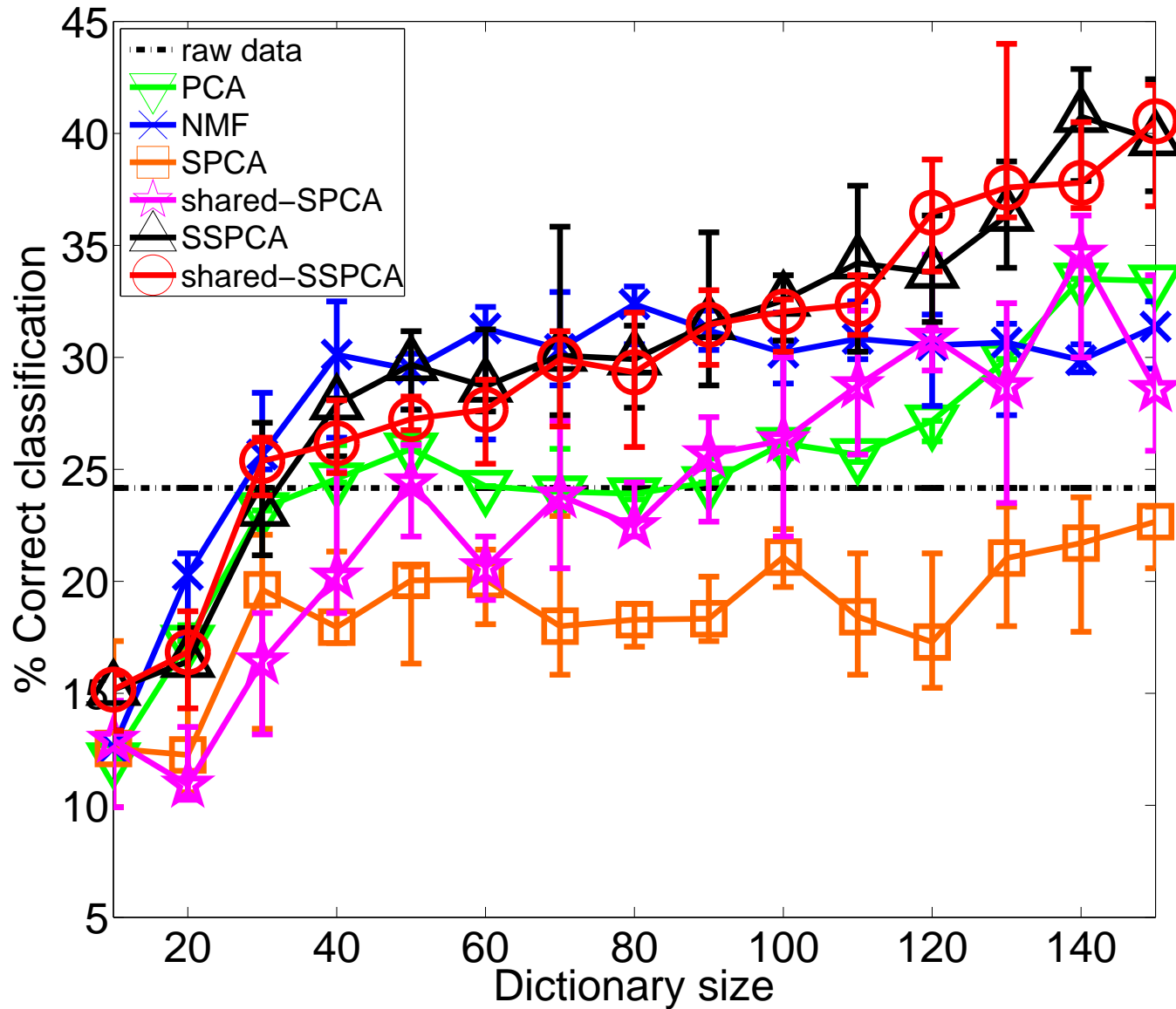


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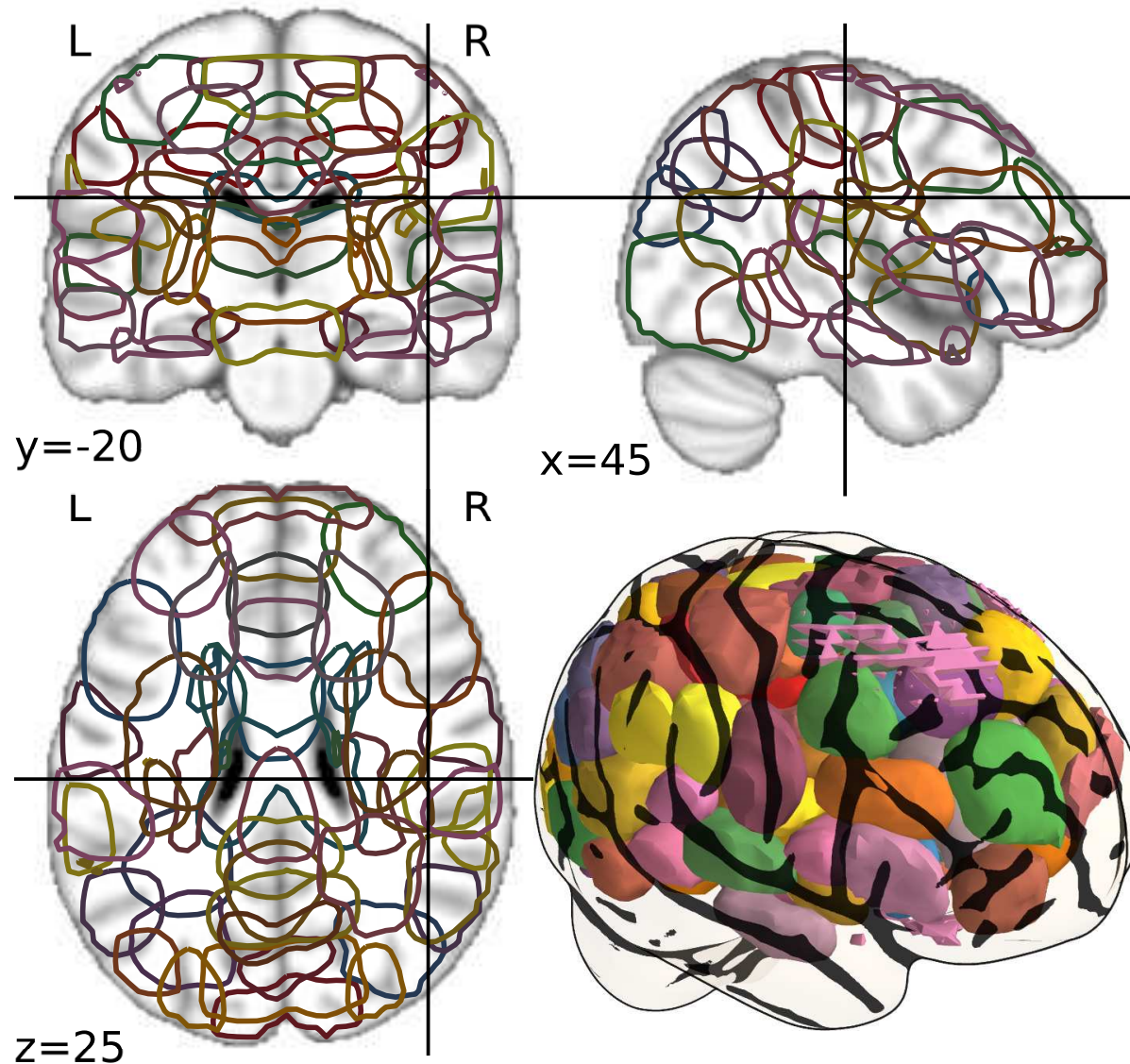
Application to face databases (3/3)

- Quantitative performance evaluation on classification task



Structured sparse PCA on resting state activity

(Varoquaux, Jenatton, Gramfort, Obozinski, Thirion, and Bach, 2010)



Dictionary learning vs. sparse structured PCA

Exchange roles of X and w

- Sparse structured PCA (**structured dictionary elements**):

$$\min_{W \in \mathbb{R}^{k \times n}, X \in \mathbb{R}^{p \times k}} \frac{1}{n} \sum_{i=1}^n \|y^i - Xw^i\|_2^2 + \lambda \sum_{j=1}^k \Omega(x^j) \text{ s.t. } \forall i, \|w^i\|_2 \leq 1.$$

- Dictionary learning with **structured sparsity for codes** w :

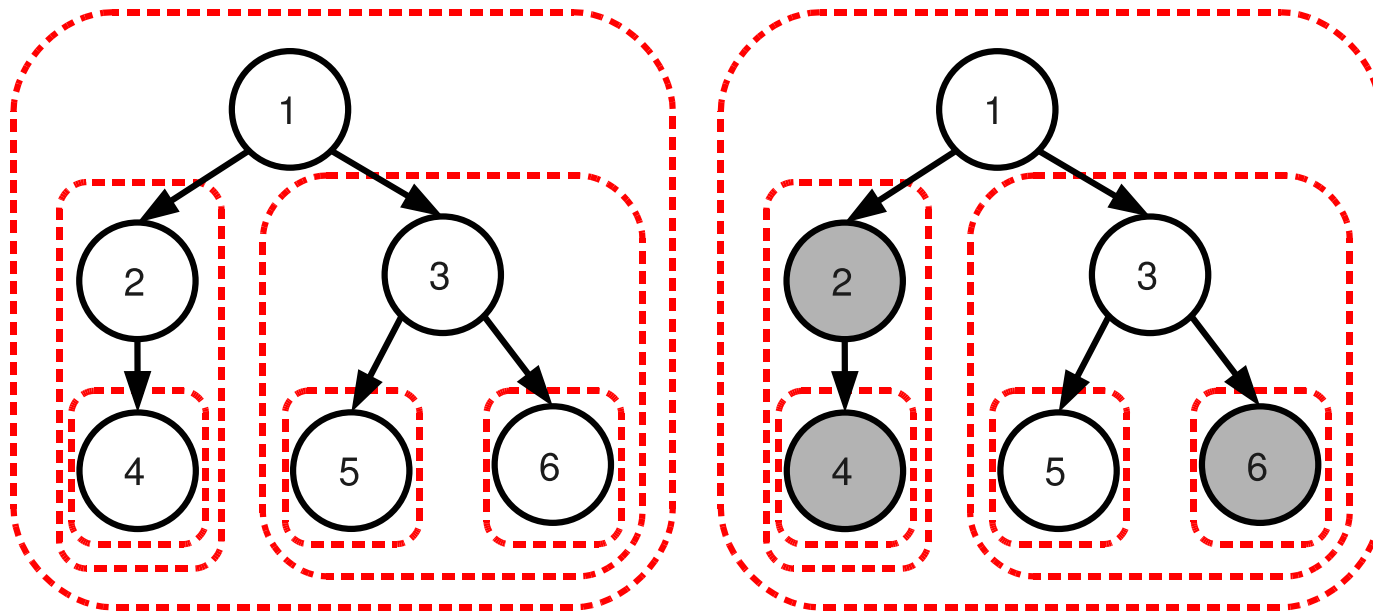
$$\min_{W \in \mathbb{R}^{k \times n}, X \in \mathbb{R}^{p \times k}} \frac{1}{n} \sum_{i=1}^n \|y^i - Xw^i\|_2^2 + \lambda \Omega(w^i) \text{ s.t. } \forall j, \|x^j\|_2 \leq 1.$$

- **Optimization:**

- Alternating optimization
- **Modularity of implementation** if proximal step is efficient (Jenatton et al., 2010; Mairal et al., 2010)

Hierarchical dictionary learning (Jenatton, Mairal, Obozinski, and Bach, 2010)

- Structure on codes w (not on dictionary X)
- Hierarchical penalization: $\Omega(w) = \sum_{G \in \mathbf{H}} \|w_G\|_2$ where groups G in \mathbf{H} are equal to **set of descendants** of some nodes in a tree



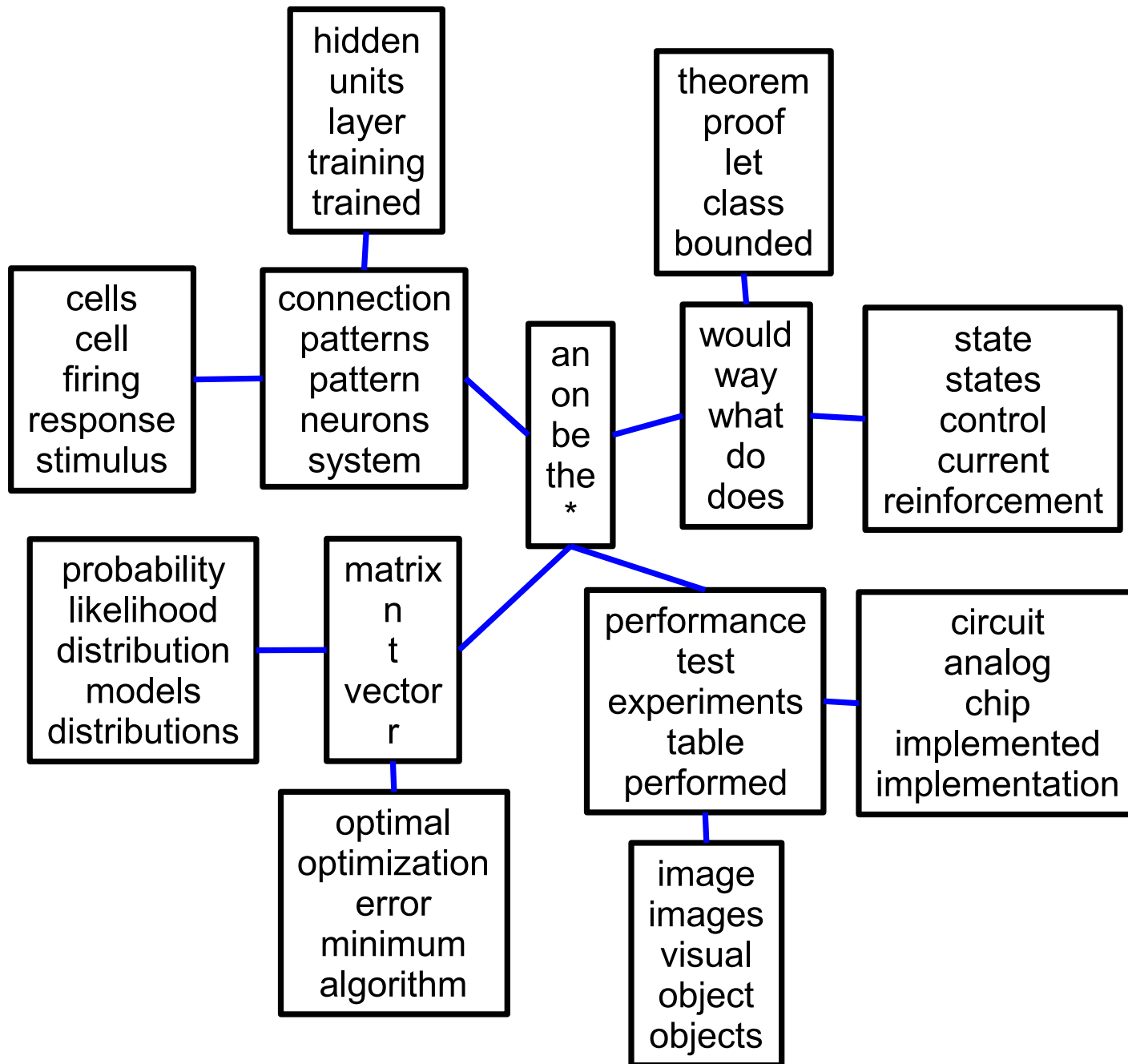
- Variable selected after its ancestors (Zhao et al., 2009; Bach, 2008)

Hierarchical dictionary learning

Modelling of text corpora

- Each document is modelled through word counts
- Low-rank matrix factorization of word-document matrix
- Probabilistic topic models (Blei et al., 2003)
 - Similar structures based on non parametric Bayesian methods (Blei et al., 2004)
 - **Can we achieve similar performance with simple matrix factorization formulation?**

Modelling of text corpora - Dictionary tree

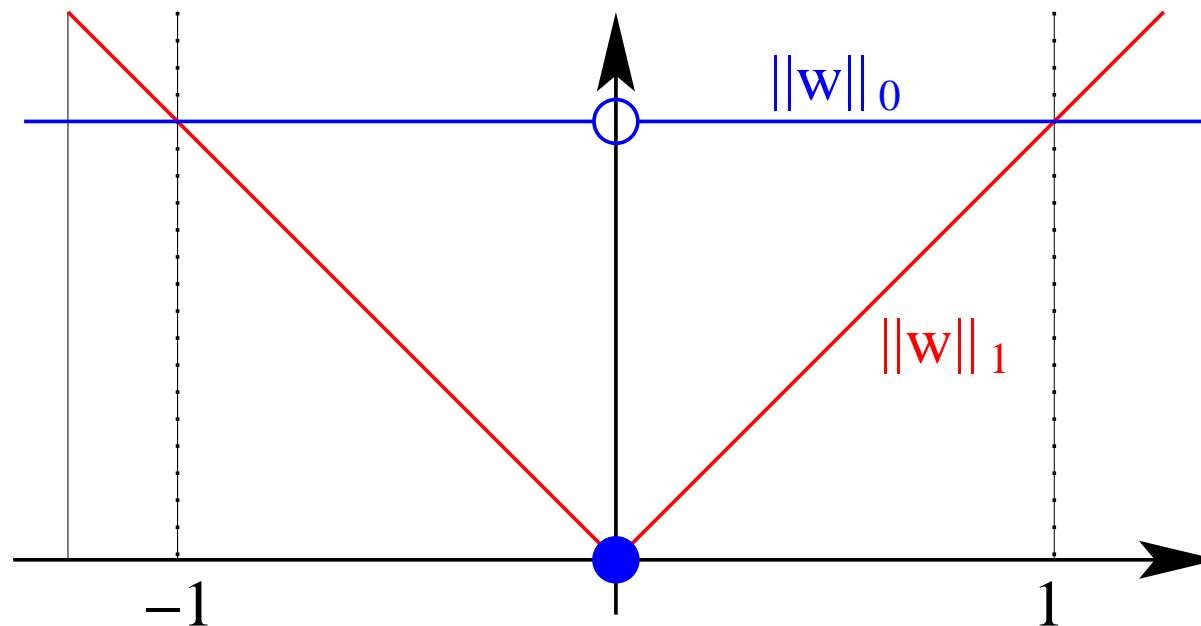


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ℓ_1 -norm = convex envelope of cardinality of support

- Let $w \in \mathbb{R}^p$. Let $V = \{1, \dots, p\}$ and $\text{Supp}(w) = \{j \in V, w_j \neq 0\}$
- **Cardinality of support:** $\|w\|_0 = \text{Card}(\text{Supp}(w))$
- Convex envelope = largest convex lower bound (see, e.g., Boyd and Vandenberghe, 2004)



- ℓ_1 -norm = convex envelope of ℓ_0 -quasi-norm on the ℓ_∞ -ball $[-1, 1]^p$

Convex envelopes of general functions of the support (Bach, 2010)

- Let $F : 2^V \rightarrow \mathbb{R}$ be a **set-function**
 - Assume F is **non-decreasing** (i.e., $A \subset B \Rightarrow F(A) \leq F(B)$)
 - Explicit prior knowledge on supports (Haupt and Nowak, 2006; Baraniuk et al., 2008; Huang et al., 2009)
- Define $\Theta(w) = F(\text{Supp}(w))$: **How to get its convex envelope?**
 1. Possible if F is also **submodular**
 2. Allows **unified** theory and algorithm
 3. Provides **new** regularizers

Submodular functions (Fujishige, 2005; Bach, 2010)

- $F : 2^V \rightarrow \mathbb{R}$ is **submodular** if and only if

$$\forall A, B \subset V, \quad F(A) + F(B) \geq F(A \cap B) + F(A \cup B)$$

$$\Leftrightarrow \forall k \in V, \quad A \mapsto F(A \cup \{k\}) - F(A) \text{ is non-increasing}$$

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- **Intuition 1:** defined like concave functions (“diminishing returns”)
 - Example: $F : A \mapsto g(\text{Card}(A))$ is submodular if g is concave

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- **Intuition 1:** defined like concave functions (“diminishing returns”)
 - Example: $F : A \mapsto g(\text{Card}(A))$ is submodular if g is concave
- **Intuition 2:** behave like convex functions
 - Polynomial-time minimization, conjugacy theory

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$$\forall A, B \subset V, \quad F(A) + F(B) \geq F(A \cap B) + F(A \cup B)$$

$$\Leftrightarrow \forall k \in V, \quad A \mapsto F(A \cup \{k\}) - F(A) \text{ is non-increasing}$$

- **Intuition 1: defined like concave functions** (“diminishing returns”)
 - Example: $F : A \mapsto g(\text{Card}(A))$ is submodular if g is concave
- **Intuition 2: behave like convex functions**
 - Polynomial-time minimization, conjugacy theory
- Used in several areas of signal processing and machine learning
 - Total variation/graph cuts (Chambolle, 2005; Boykov et al., 2001)
 - Optimal design (Krause and Guestrin, 2005)

Submodular functions - Examples

- Concave functions of the cardinality: $g(|A|)$
- Cuts
- Entropies
 - $H((X_k)_{k \in A})$ from p random variables X_1, \dots, X_p
- Network flows
 - Efficient representation for set covers
- Rank functions of matroids

Submodular functions - Lovász extension

- Subsets may be identified with elements of $\{0, 1\}^p$
- Given **any** set-function F and w such that $w_{j_1} \geq \dots \geq w_{j_p}$, define:

$$f(w) = \sum_{k=1}^p w_{j_k} [F(\{j_1, \dots, j_k\}) - F(\{j_1, \dots, j_{k-1}\})]$$

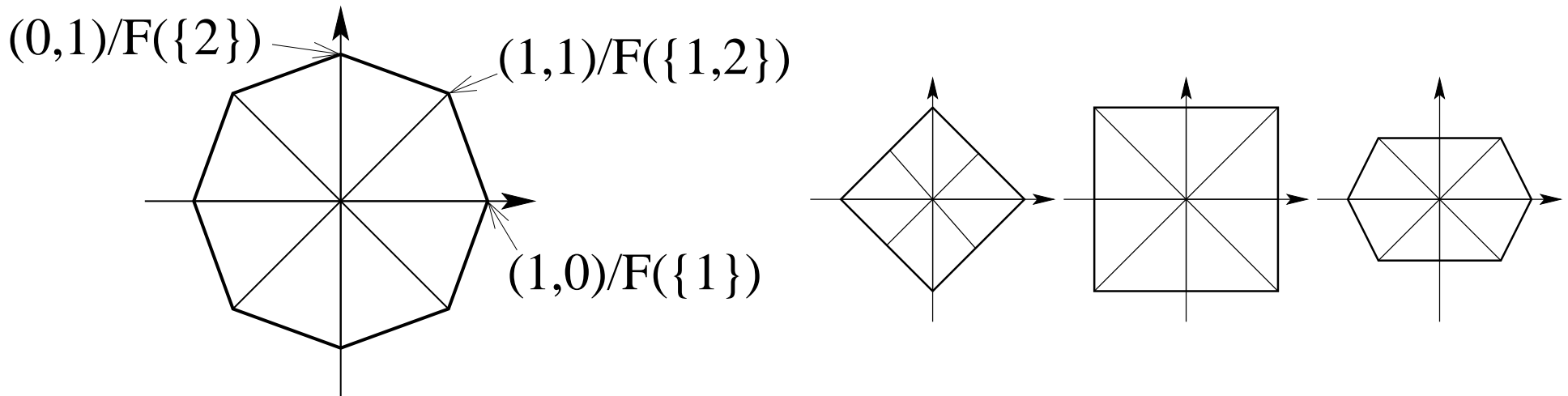
- If $w = 1_A$, $f(w) = F(A) \Rightarrow$ extension from $\{0, 1\}^p$ to \mathbb{R}^p
- f is piecewise affine and positively homogeneous
- **F is submodular if and only if f is convex** (Lovász, 1982)
 - Minimizing $f(w)$ on $w \in [0, 1]^p$ equivalent to minimizing F on 2^V

Submodular functions and structured sparsity

- Let $F : 2^V \rightarrow \mathbb{R}$ be a **non-decreasing submodular set-function**
- **Proposition:** the convex envelope of $\Theta : w \mapsto F(\text{Supp}(w))$ on the ℓ_∞ -ball is $\Omega : w \mapsto f(|w|)$ where f is the Lovász extension of F

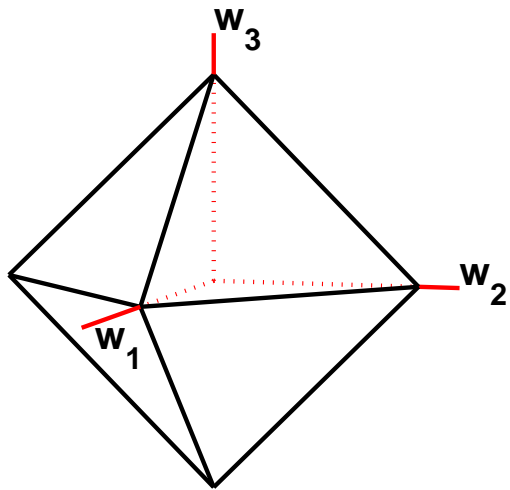
Submodular functions and structured sparsity

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- **Sparsity-inducing properties:** Ω is a **polyhedral** norm



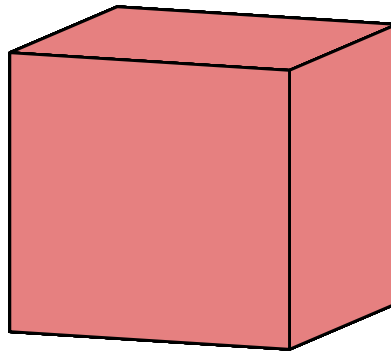
- A is stable if for all $B \supset A$, $B \neq A \Rightarrow F(B) > F(A)$
- With probability one, stable sets are the only allowed active sets

Polyhedral unit balls



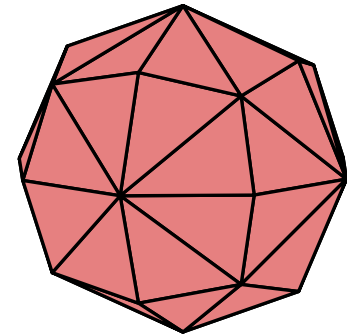
$$F(A) = |A|$$

$$\Omega(w) = \|w\|_1$$



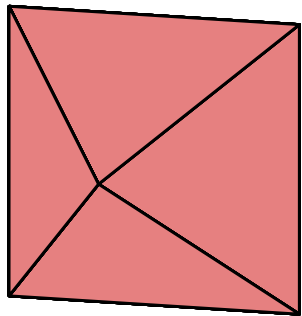
$$F(A) = \min\{|A|, 1\}$$

$$\Omega(w) = \|w\|_\infty$$



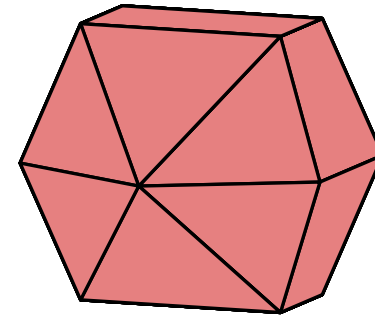
$$F(A) = |A|^{1/2}$$

all possible extreme points



$$F(A) = 1_{\{A \cap \{1\} \neq \emptyset\}} + 1_{\{A \cap \{2,3\} \neq \emptyset\}}$$

$$\Omega(w) = |w_1| + \|w_{\{2,3\}}\|_\infty$$



$$F(A) = 1_{\{A \cap \{1,2,3\} \neq \emptyset\}} + 1_{\{A \cap \{2,3\} \neq \emptyset\}} + 1_{\{A \cap \{3\} \neq \emptyset\}}$$

$$\Omega(w) = \|w\|_\infty + \|w_{\{2,3\}}\|_\infty + |w_3|$$

Conclusion

- **Structured sparsity for machine learning and statistics**
 - Many applications (image, audio, text, etc.)
 - May be achieved through structured sparsity-inducing norms
 - Link with submodular functions: unified analysis and algorithms

Conclusion

- **Structured sparsity for machine learning and statistics**
 - Many applications (image, audio, text, etc.)
 - May be achieved through structured sparsity-inducing norms
 - Link with submodular functions: unified analysis and algorithms
- **On-going/related work on structured sparsity**
 - **Norm design** beyond submodular functions
 - Complementary approach of Jacob, Obozinski, and Vert (2009)
 - Links with greedy methods (Haupt and Nowak, 2006; Baraniuk et al., 2008; Huang et al., 2009)
 - Achieving $\log p = O(n)$ algorithmically (Bach, 2008)

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