Structured sparsity-inducing norms through submodular functions

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Thanks to R. Jenatton, J. Mairal, G. Obozinski

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Outline

- **Introduction: Sparse methods for machine learning**
  - Need for structured sparsity: Going beyond the ℓ_1-norm
- **Submodular functions**
  - Lovász extension
- **Structured sparsity through submodular functions**
  - Relaxation of the penalization of supports
  - Examples
  - Unified algorithms and analysis
- **Extensions to symmetric submodular functions**
  - Shaping level sets

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 $+ \ell_1$-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 $y = (y^1, \dots, y^k) \in \mathbb{R}^{n \times k}$

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

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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 $\forall j,\ \|x^j\|_2 \leqslant 1$

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

  - Olshausen and Field (1997); Elad and Aharon (2006)

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

Sparsity in signal processing

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

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

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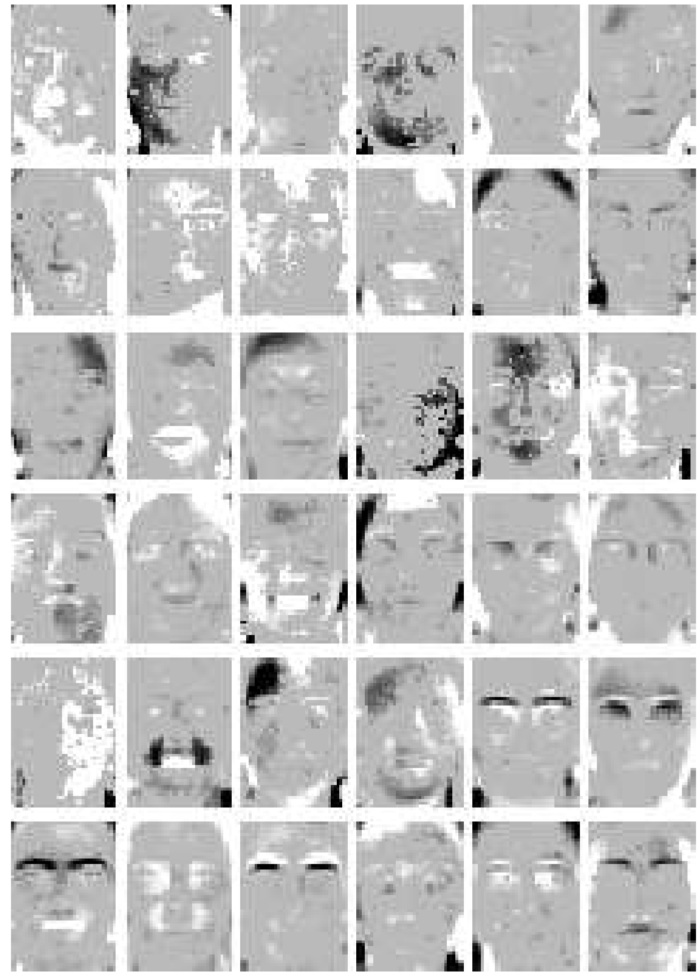
Why structured sparsity?

- **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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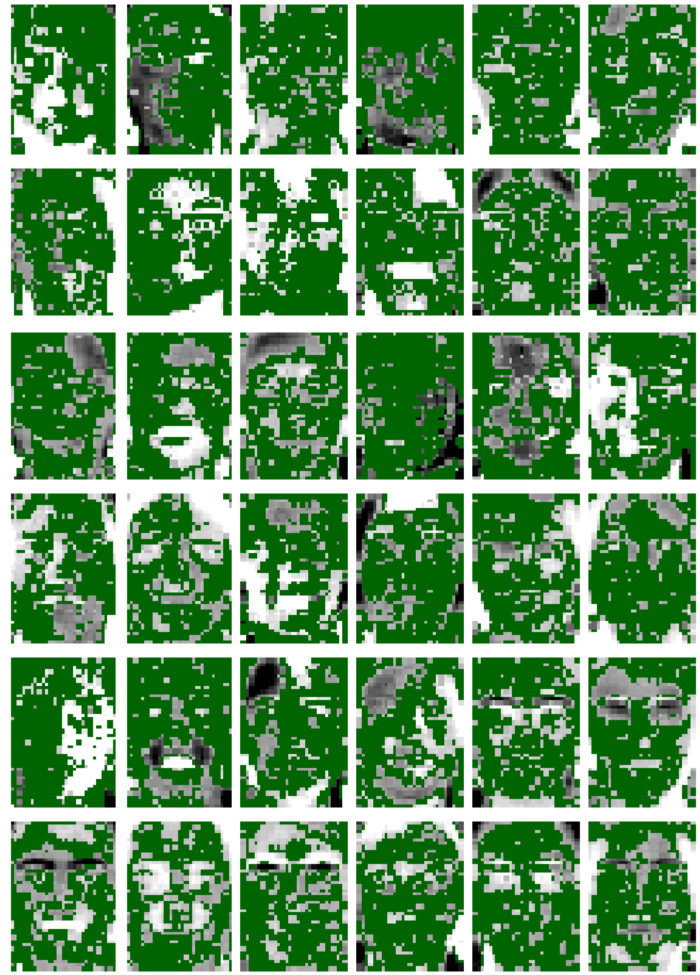

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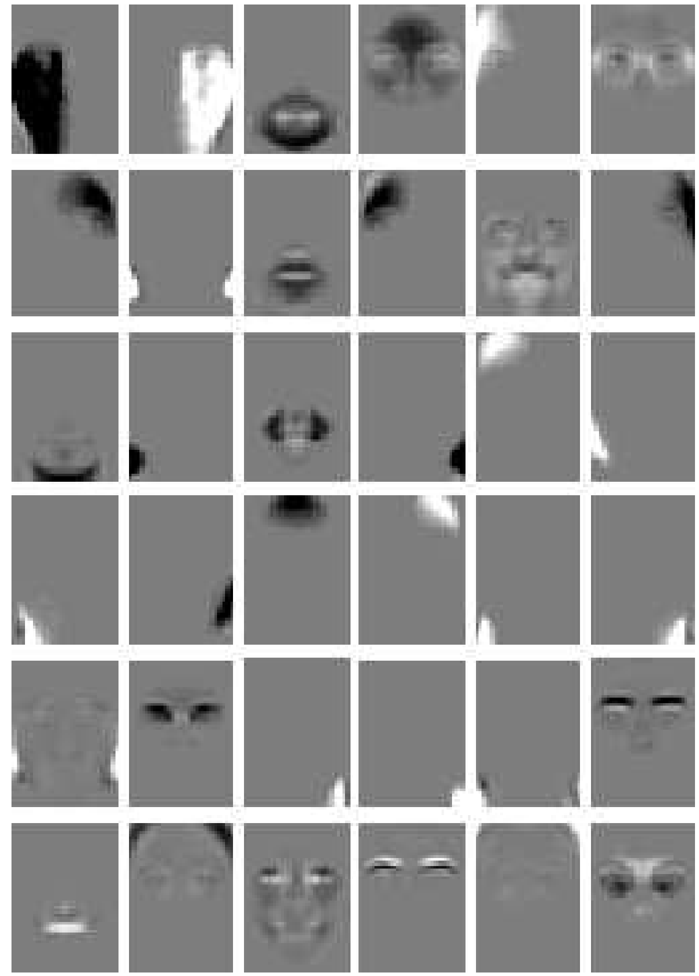

Structured sparse PCA

- Enforce selection of convex nonzero patterns ⇒ robustness to occlusion in face identification

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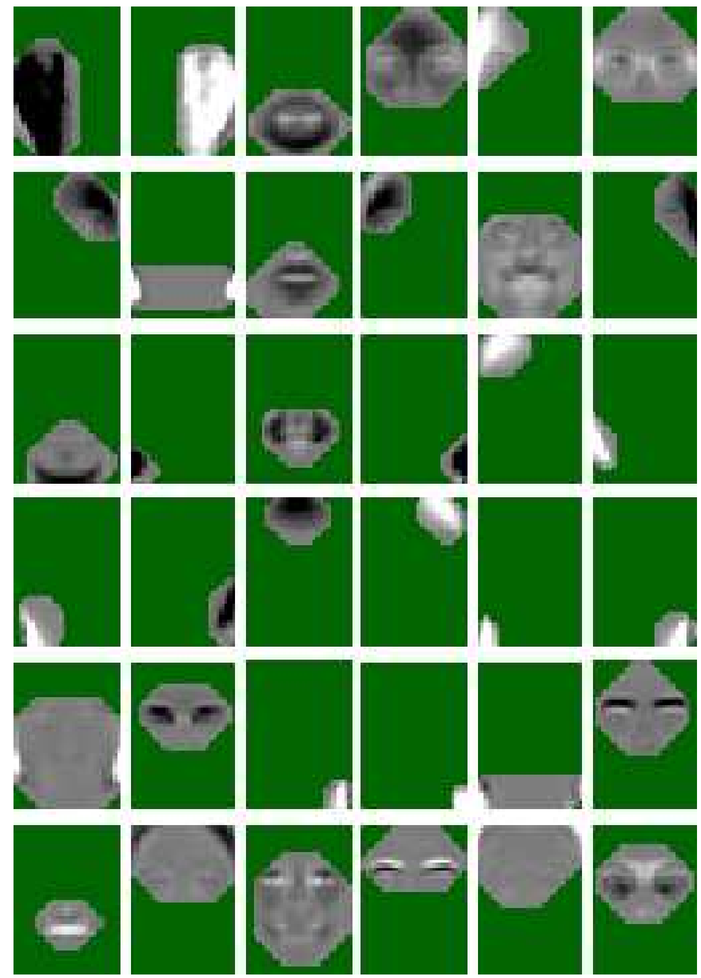

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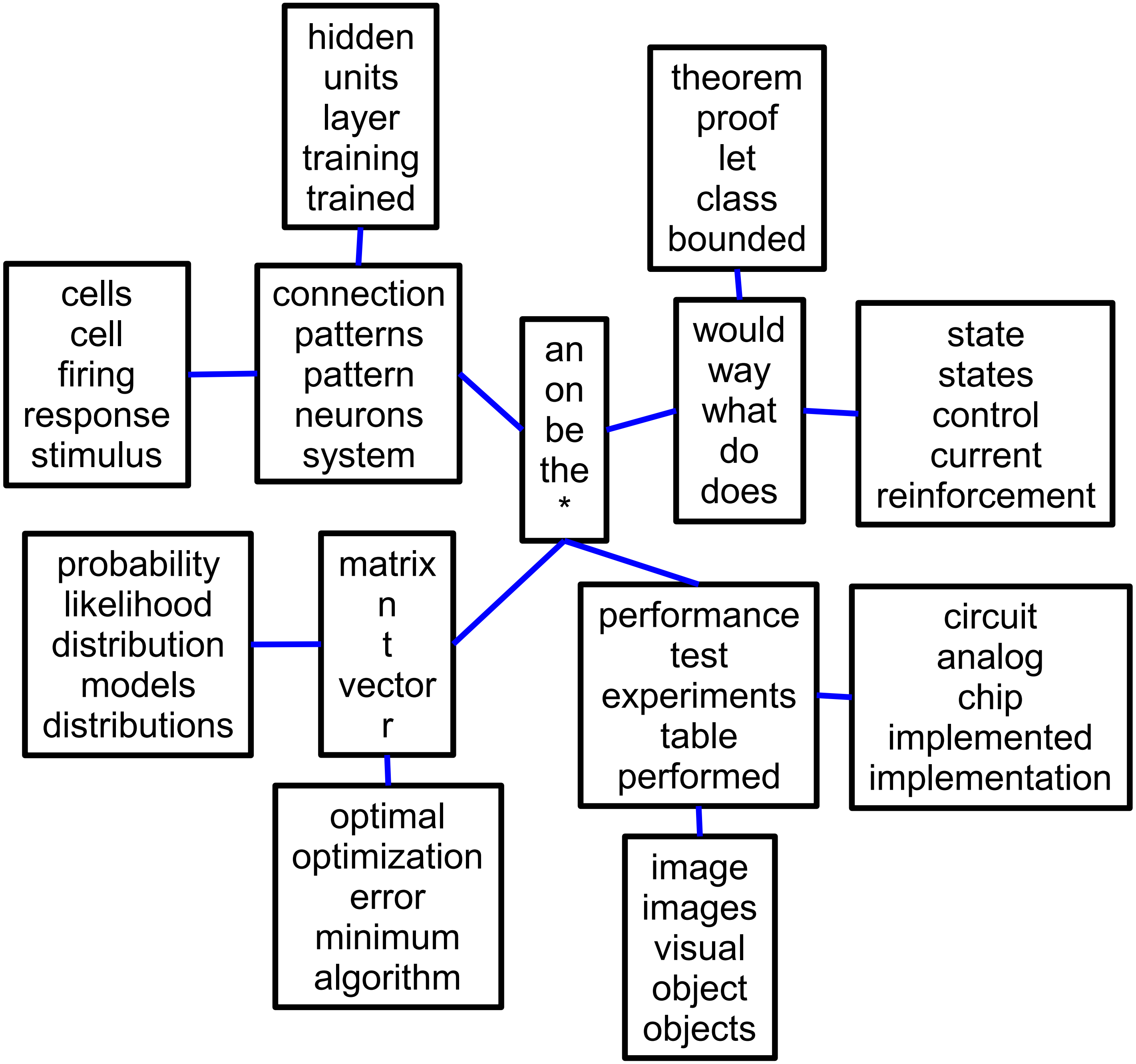
Modelling of text corpora (Jenatton et al., 2010)



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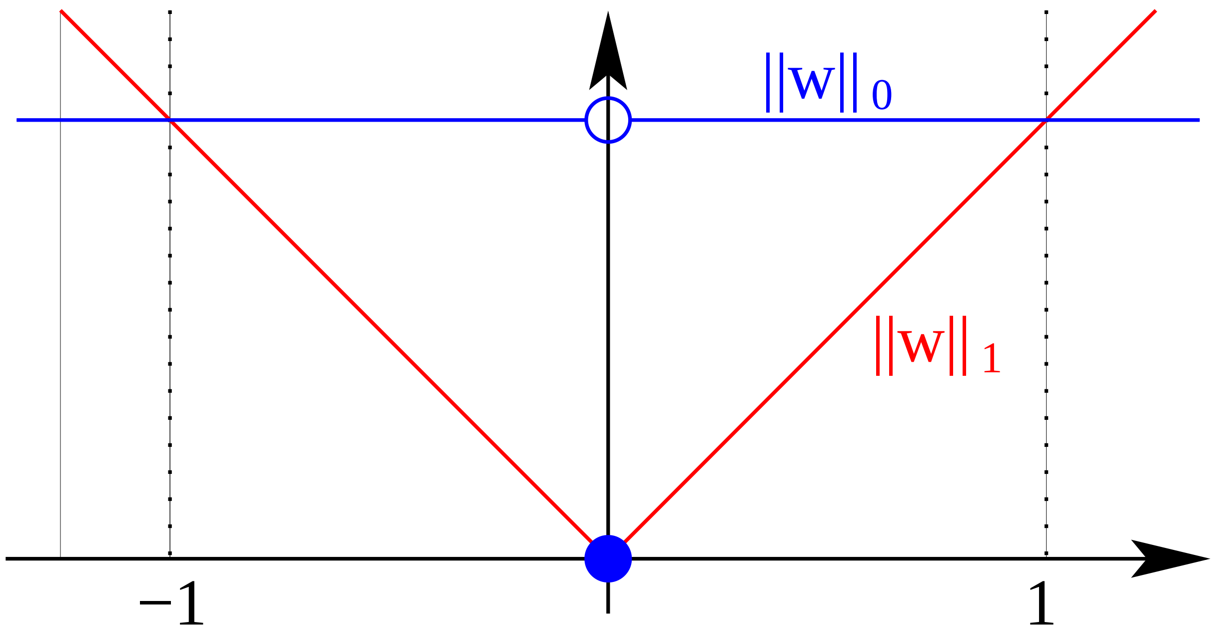
- **Stability and identifiability**
  - Optimization problem $\min_{w \in \mathbb{R}^p} L(y, Xw) + \lambda \|w\|_1$ is unstable
  - "Codes" w^j often used in later processing (Mairal et al., 2009)
- **Prediction or estimation performance**
  - When prior knowledge matches data (Haupt and Nowak, 2006; Baraniuk et al., 2008; Jenatton et al., 2009a; Huang et al., 2009)
- **Numerical efficiency**
  - Non-linear variable selection with 2^p subsets (Bach, 2008)

ℓ_1-norm = convex envelope of cardinality of support

- Let $w \in \mathbb{R}^p$. Let $V = \{1, \dots, p\}$ and $\mathrm{Supp}(w) = \{j \in V,\ w_j \neq 0\}$
- **Cardinality of support**: $\|w\|_0 = \mathrm{Card}(\mathrm{Supp}(w))$
- 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 $F : 2^V \to \mathbb{R}$ be a **set-function**
  - Assume F is **non-decreasing** (i.e., $A \subset B \Rightarrow F(A) \leqslant F(B)$)
  - 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, 2010b)

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

$$\begin{aligned} & \forall A, B \subset V, \quad F(A) + F(B) \geqslant F(A \cap B) + F(A \cup B) \\ \Leftrightarrow \quad & \forall k \in V, \quad A \mapsto F(A \cup \{k\}) - F(A) \text{ is non-increasing} \end{aligned}$$

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- **Intuition 1**: defined like concave functions ("diminishing returns")
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- **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 - Lovász extension

- Subsets may be identified with elements of $\{0,1\}^p$
- Given any set-function F and w such that $w_{j_1} \geqslant \cdots \geqslant w_{j_p}$, 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
  - Minimizing $f(w)$ on $w \in [0,1]^p$ equivalent to minimizing F on 2^V

Submodular functions and structured sparsity

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

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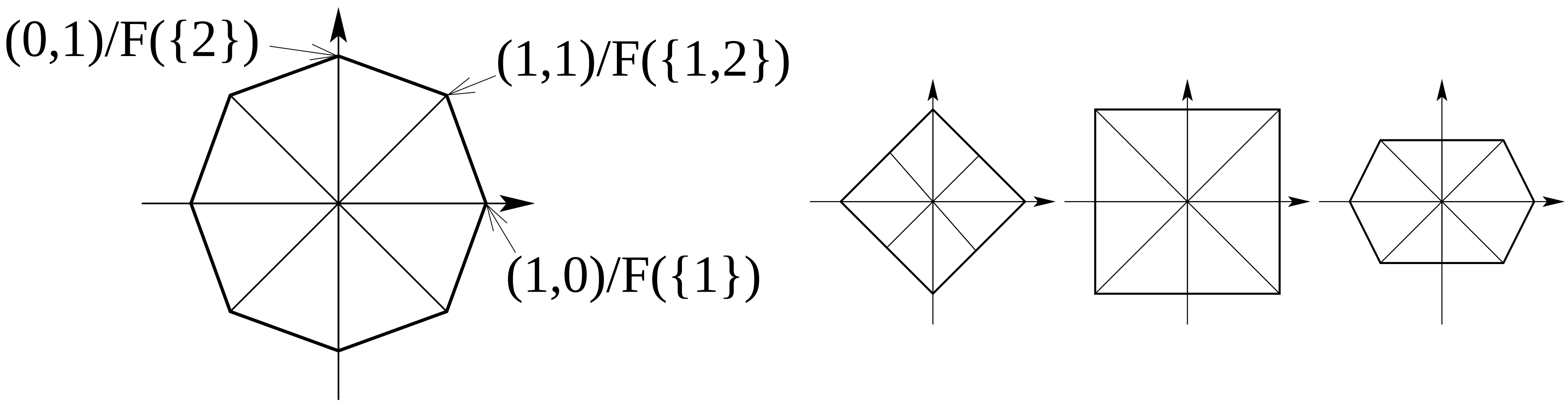
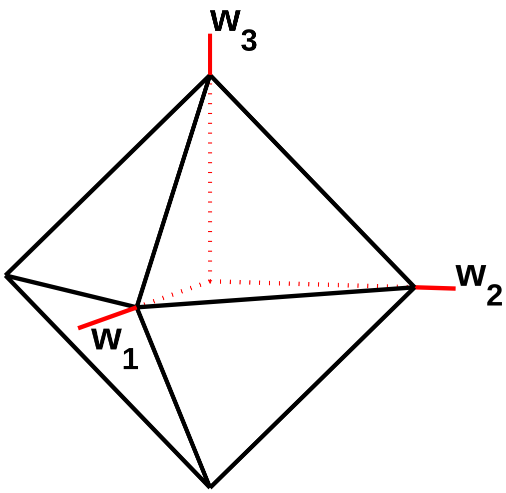
- **Sparsity-inducing properties**: Ω is a polyhedral norm

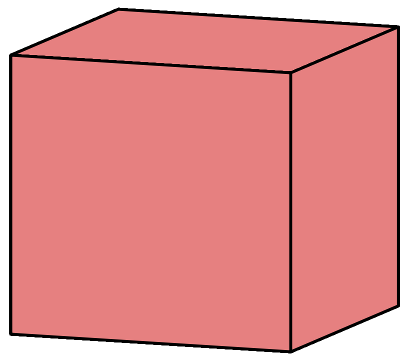


  - A if stable if for all $B \supset A$, $B \neq A \Rightarrow F(B) > F(A)$
  - With probability one, stable sets are the only allowed active sets

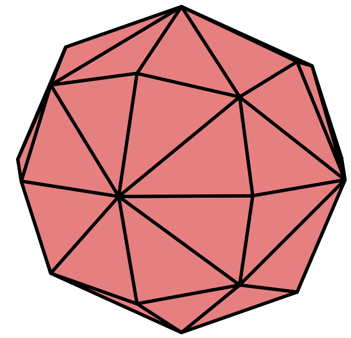
Polyhedral unit balls



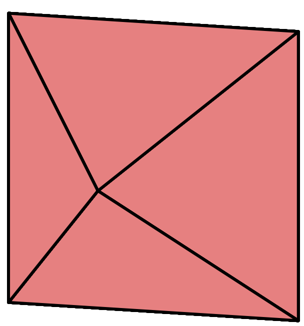
$$F(A) = |A|$$
$$\Omega(w) = \|w\|_1$$



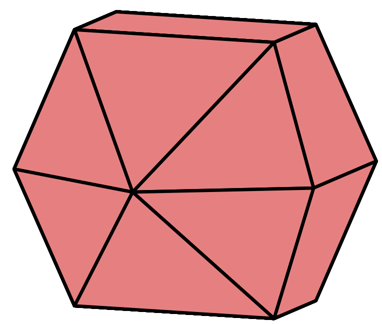
$$F(A) = \min\{|A|, 1\}$$
$$\Omega(w) = \|w\|_\infty$$



$$F(A) = |A|^{1/2}$$
all possible extreme points



$$F(A) = 1_{\{A\cap\{1\}\neq\varnothing\}} + 1_{\{A\cap\{2,3\}\neq\varnothing\}}$$
$$\Omega(w) = |w_1| + \|w_{\{2,3\}}\|_\infty$$



$$F(A) = 1_{\{A\cap\{1,2,3\}\neq\varnothing\}} + 1_{\{A\cap\{2,3\}\neq\varnothing\}} + 1_{\{A\cap\{3\}\neq\varnothing\}}$$
$$\Omega(w) = \|w\|_\infty + \|w_{\{2,3\}}\|_\infty + |w_3|$$

Submodular functions and structured sparsity
Examples

- **From $\Omega(w)$ to $F(A)$:** provides new insights into existing norms
  - Grouped norms with **overlapping** groups (Jenatton et al., 2009a)

$$\Omega(w) = \sum_{G \in \mathcal{G}} \|w_G\|_\infty$$

  - ℓ_1-ℓ_∞ norm $\Rightarrow$ sparsity at the group level
  - Some w_G's are set to zero for some groups G

$$\big(\mathrm{Supp}(w)\big)^c = \bigcup_{G \in \mathcal{H}} G \quad \text{for some } \mathcal{H} \subseteq \mathcal{G}$$

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  - Justification not only limited to allowed sparsity patterns

Selection of contiguous patterns in a sequence

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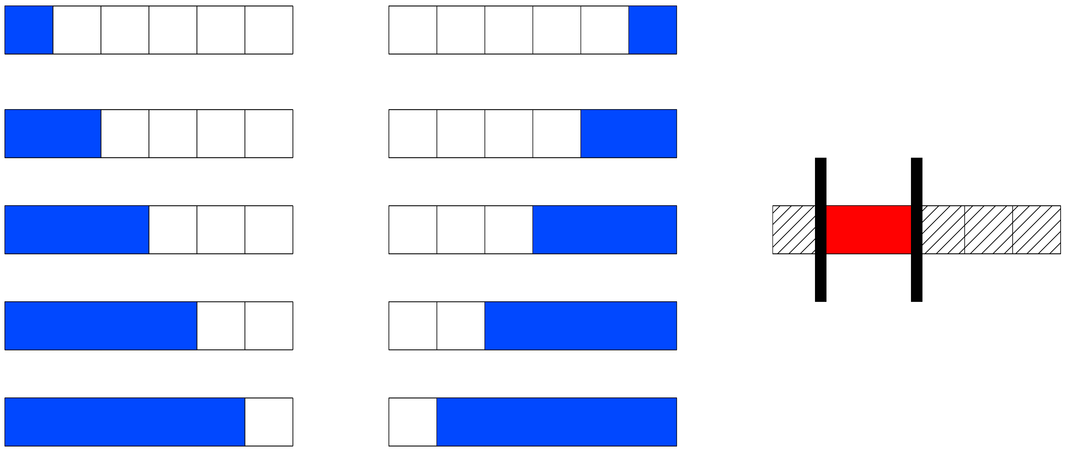

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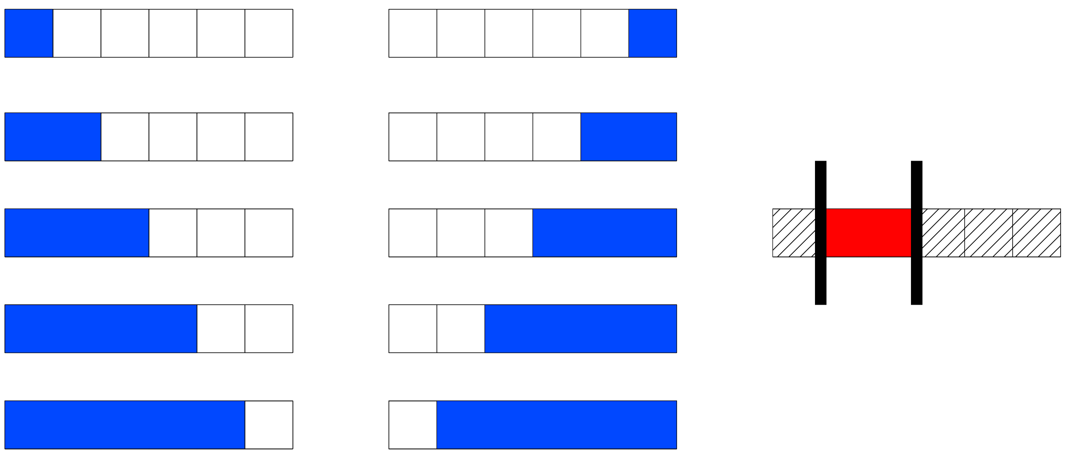

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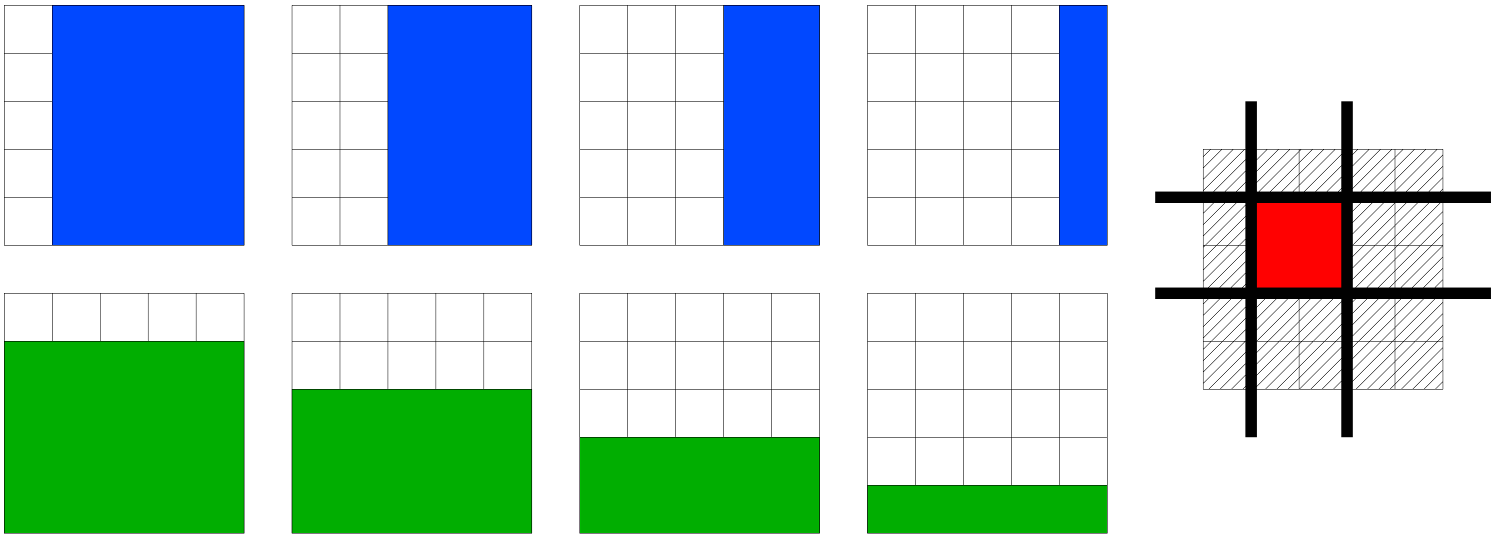
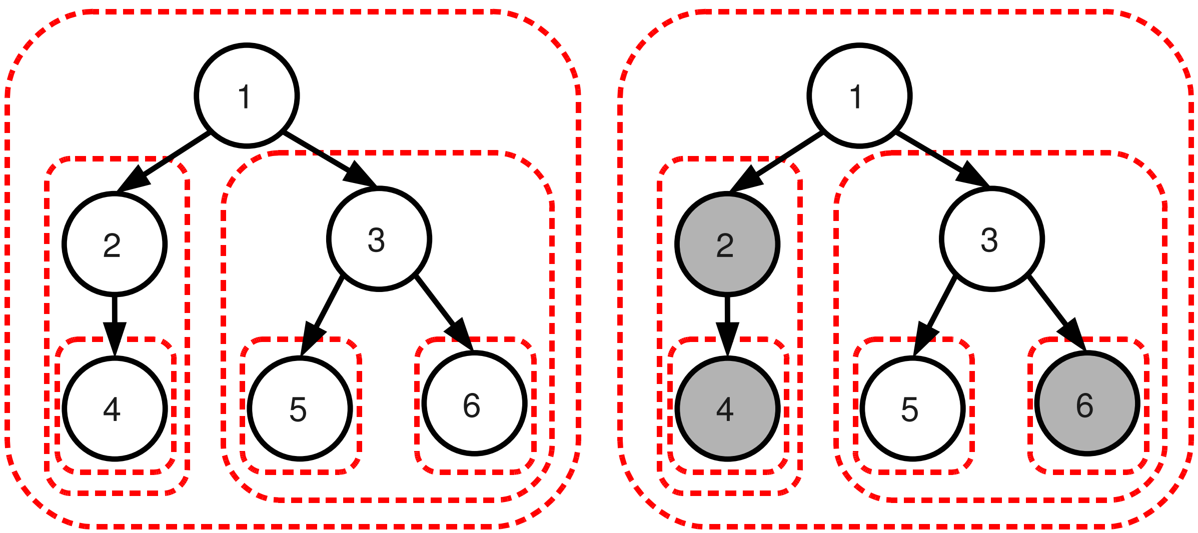
- $\sum_{G\in\mathcal{G}} \|w_G\|_\infty \;\Rightarrow\; F(A) = p - 2 + \mathrm{Range}(A)$ if $A \neq \varnothing$
  - Jump from 0 to $p-1$: tends to include all variables simultaneously
  - Add $\nu|A|$ to smooth the kink: all sparsity patterns are possible
  - **Contiguous patterns are favored (and not forced)**

Extensions of norms with overlapping groups

- Selection of **rectangles** (at any position) in a 2-D grids

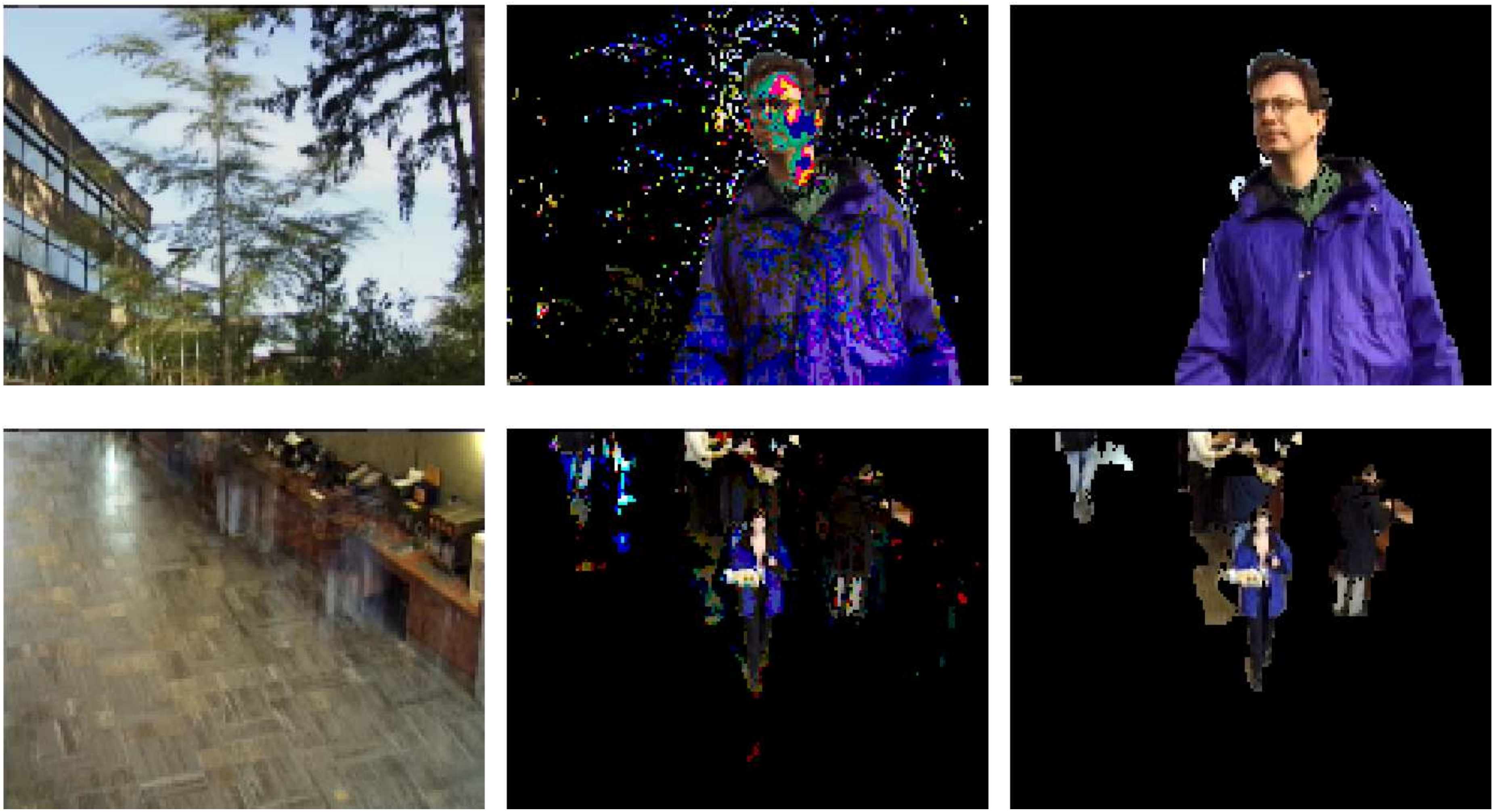


- **Hierarchies**

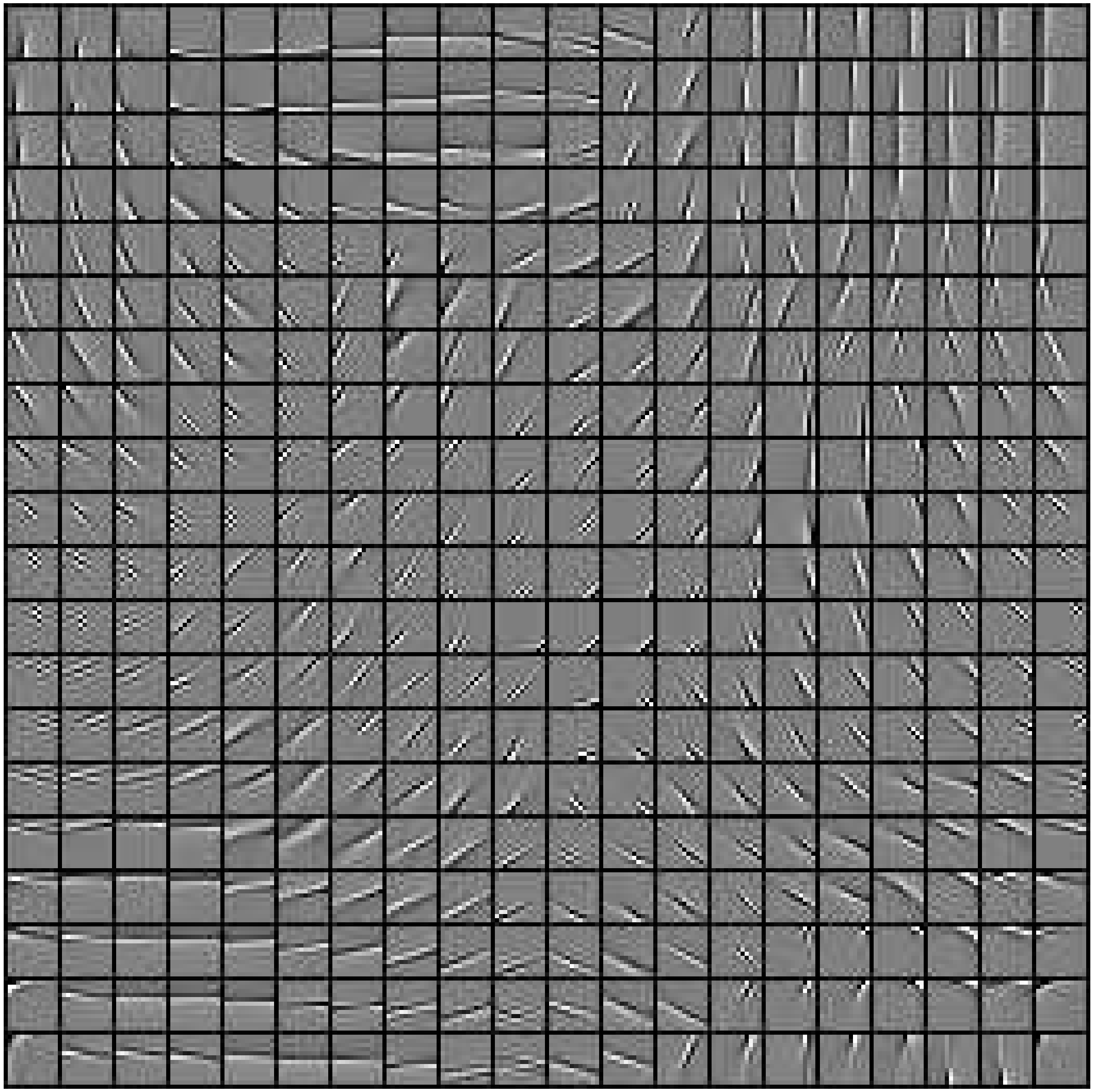


Application to background subtraction (Mairal, Jenatton, Obozinski, and Bach, 2010)

Background ℓ_1-norm Structured norm



Topographic dictionaries
(Mairal, Jenatton, Obozinski, and Bach, 2010)



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- **From $F(A)$ to $\Omega(w)$:** provides new sparsity-inducing norms
  - $F(A) = g(\mathrm{Card}(A)) \ \Rightarrow\ \Omega$ is a combination of **order statistics**
  - **Non-factorial priors** for supervised learning: Ω depends on the eigenvalues of $X_A^\top X_A$ and not simply on the cardinality of A

Non-factorial priors for supervised learning

- Selection of subset A from design $X \in \mathbb{R}^{n \times p}$ with ℓ_2-penalization
- **Frequentist analysis** (Mallow's C_L): $\operatorname{tr} X_A^\top X_A (X_A^\top X_A + \lambda I)^{-1}$
  - Not submodular
- **Bayesian analysis** (marginal likelihood): $\log\det(X_A^\top X_A + \lambda I)$
  - Submodular (also true for $\operatorname{tr}(X_A^\top X_A)^{1/2}$)

p	n	k	submod.	ℓ_2 vs. submod.	ℓ_1 vs. submod.	greedy vs. submod.
120	120	80	40.8 $\pm$ 0.8	-2.6 $\pm$ 0.5	**0.6** $\pm$ **0.0**	**21.8** $\pm$ **0.9**
120	120	40	35.9 $\pm$ 0.8	**2.4** $\pm$ **0.4**	**0.3** $\pm$ **0.0**	**15.8** $\pm$ **1.0**
120	120	20	29.0 $\pm$ 1.0	**9.4** $\pm$ **0.5**	-0.1 $\pm$ 0.0	**6.7** $\pm$ **0.9**
120	120	10	20.4 $\pm$ 1.0	**17.5** $\pm$ **0.5**	-0.2 $\pm$ 0.0	-2.8 $\pm$ 0.8
120	20	20	49.4 $\pm$ 2.0	0.4 $\pm$ 0.5	**2.2** $\pm$ **0.8**	**23.5** $\pm$ **2.1**
120	20	10	49.2 $\pm$ 2.0	0.0 $\pm$ 0.6	1.0 $\pm$ 0.8	**20.3** $\pm$ **2.6**
120	20	6	43.5 $\pm$ 2.0	**3.5** $\pm$ **0.8**	**0.9** $\pm$ **0.6**	**24.4** $\pm$ **3.0**
120	20	4	41.0 $\pm$ 2.1	**4.8** $\pm$ **0.7**	-1.3 $\pm$ 0.5	**25.1** $\pm$ **3.5**

Unified optimization algorithms

- **Polyhedral norm** with $O(3^p)$ faces and extreme points
  - Not suitable to linear programming toolboxes
- **Subgradient** ($w \mapsto \Omega(w)$ non-differentiable)
  - subgradient may be obtained in polynomial time $\Rightarrow$ too slow

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- **Proximal methods** (e.g., Beck and Teboulle, 2009)
  - $\min_{w \in \mathbb{R}^p} L(y, Xw) + \lambda\Omega(w)$: differentiable + non-differentiable
  - Efficient when (P) : $\min_{w \in \mathbb{R}^p} \frac{1}{2}\|w - v\|_2^2 + \lambda\Omega(w)$ is "easy"

- **Proposition**: (P) is equivalent to $\min\limits_{A \subset V} \lambda F(A) - \sum_{j \in A} |v_j|$ with minimum-norm-point algorithm
  - Possible complexity bound $O(p^6)$, but empirically $O(p^2)$ (or more)
  - Faster algorithm for special case (Mairal et al., 2010)

Proximal methods for Lovász extensions

- **Proposition** (Chambolle and Darbon, 2009): let w^* be the solution of $\min_{w\in\mathbb{R}^p} \frac{1}{2}\|w-v\|_2^2 + \lambda f(w)$. Then the solutions of

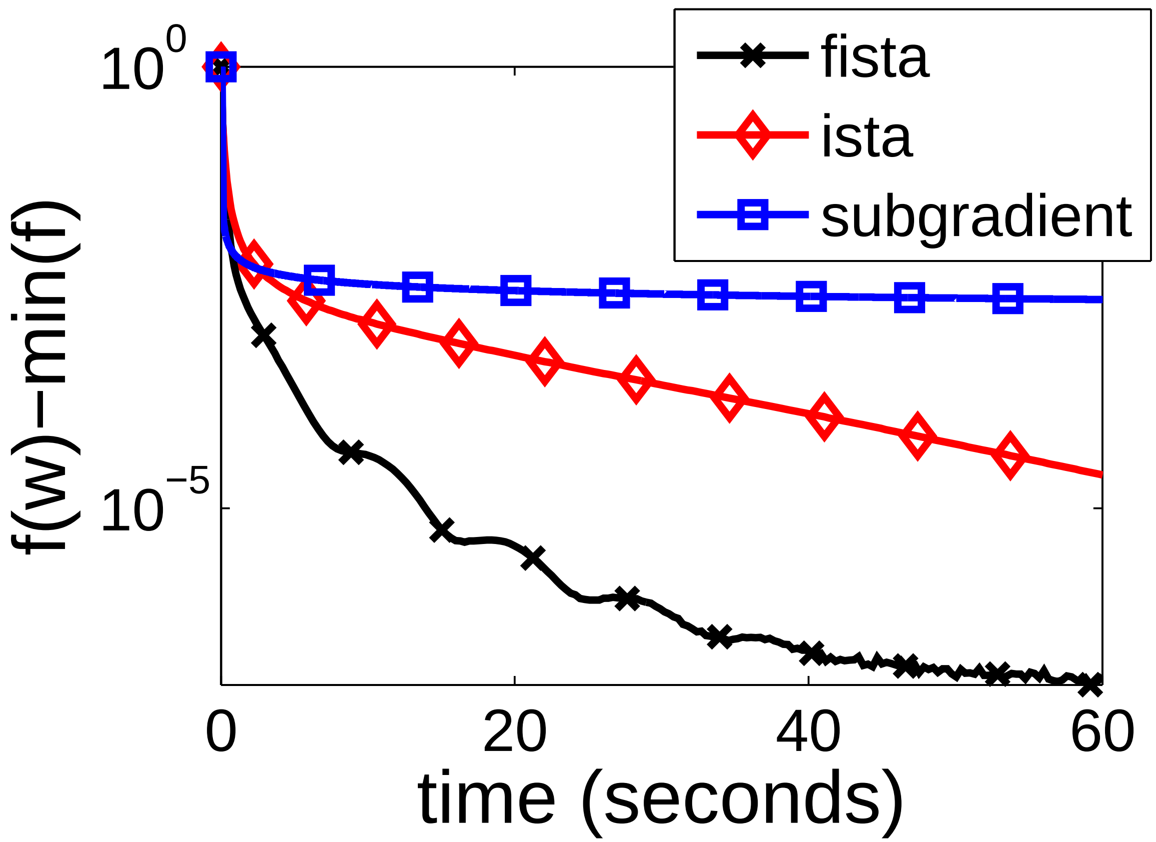
$$\min_{A\subset V} \lambda F(A) + \sum_{j\in A}(\alpha - v_j)$$

are the sets A^α such that $\{w^* > \alpha\} \subset A^\alpha \subset \{w^* \geqslant \alpha\}$

- **Parametric submodular function optimization**
  - General decomposition strategy for $f(|w|)$ and $f(w)$ (Groenevelt, 1991)
  - Efficient only when submodular minimization is efficient
  - Otherwise, minimum-norm-point algorithm (a.k.a. Frank Wolfe) is preferable

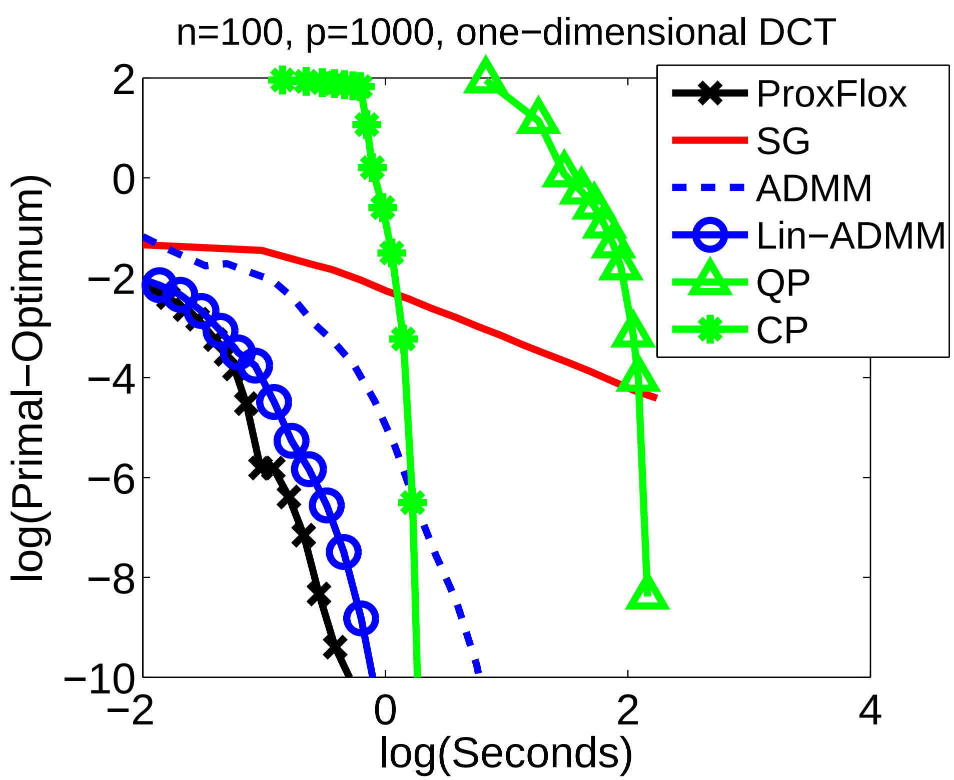
Comparison of optimization algorithms

- Synthetic example with $p = 1000$ and $F(A) = |A|^{1/2}$
- ISTA: proximal method
- FISTA: accelerated variant (Beck and Teboulle, 2009)



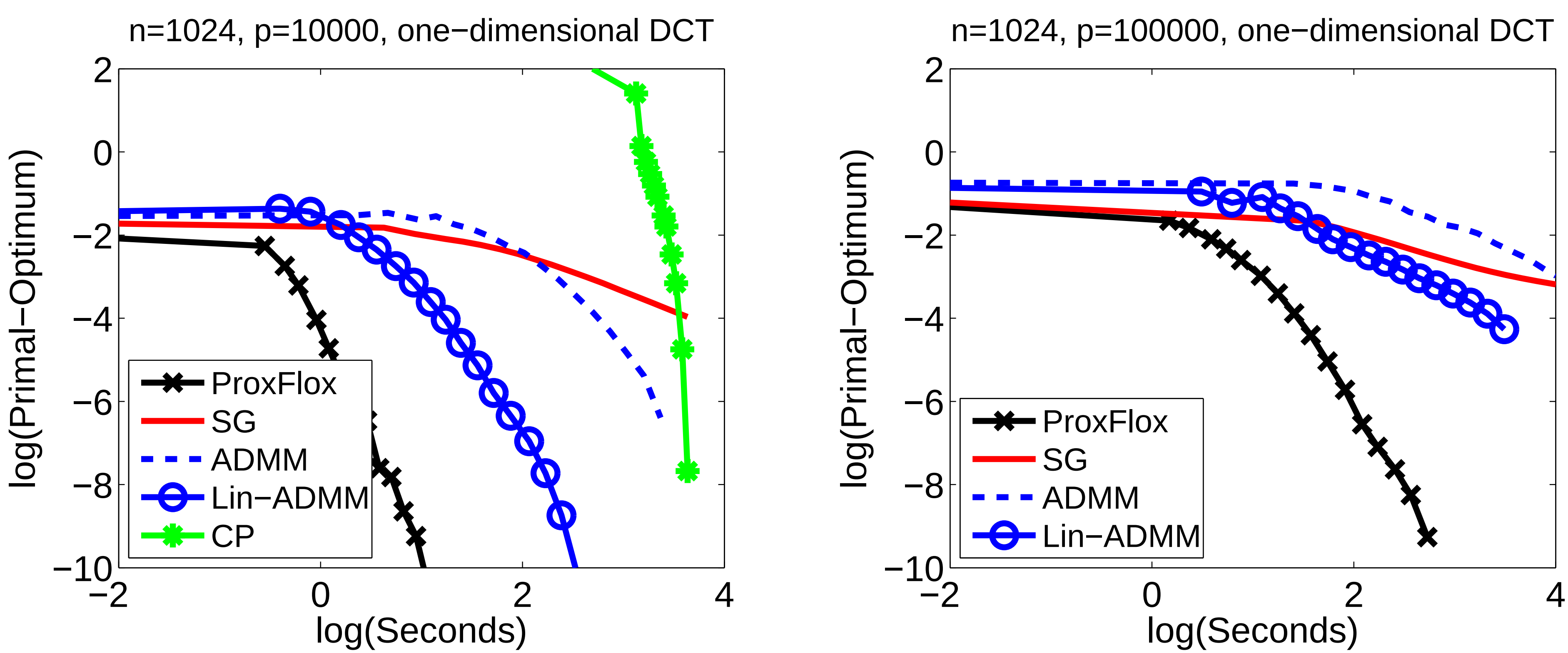
Comparison of optimization algorithms
(Mairal, Jenatton, Obozinski, and Bach, 2010)
Small scale

- Specific norms which can be implemented through network flows



Comparison of optimization algorithms (Mairal, Jenatton, Obozinski, and Bach, 2010) Large scale

- Specific norms which can be implemented through network flows



Unified theoretical analysis

- **Decomposability**
  - Key to theoretical analysis (Negahban et al., 2009)
  - **Property**: $\forall w \in \mathbb{R}^p$, and $\forall J \subset V$, if $\min_{j \in J} |w_j| \geqslant \max_{j \in J^c} |w_j|$, then $\Omega(w) = \Omega_J(w_J) + \Omega^J(w_{J^c})$
- **Support recovery**
  - Extension of known sufficient condition (Zhao and Yu, 2006; Negahban and Wainwright, 2008)
- **High-dimensional inference**
  - Extension of known sufficient condition (Bickel et al., 2009)
  - Matches with analysis of Negahban et al. (2009) for common cases

Support recovery - $\min_{w\in\mathbb{R}^p} \frac{1}{2n}\|y - Xw\|_2^2 + \lambda\Omega(w)$

- **Notation**
  - $\rho(J) = \min_{B\subset J^c} \frac{F(B\cup J)-F(J)}{F(B)} \in (0,1]$ (for J stable)
  - $c(J) = \sup_{w\in\mathbb{R}^p} \Omega_J(w_J)/\|w_J\|_2 \leqslant |J|^{1/2} \max_{k\in V} F(\{k\})$

- **Proposition**
  - Assume $y = Xw^* + \sigma\varepsilon$, with $\varepsilon \sim \mathcal{N}(0, I)$
  - J = smallest stable set containing the support of w^*
  - Assume $\nu = \min_{j, w_j^*\neq 0} |w_j^*| > 0$
  - Let $Q = \frac{1}{n}X^\top X \in \mathbb{R}^{p\times p}$. Assume $\kappa = \lambda_{\min}(Q_{JJ}) > 0$
  - Assume that for $\eta > 0$, $\boxed{(\Omega^J)^*[(\Omega_J(Q_{JJ}^{-1}Q_{Jj}))_{j\in J^c}] \leqslant 1 - \eta}$
  - If $\lambda \leqslant \frac{\kappa\nu}{2c(J)}$, $\hat{w}$ has support equal to J, with probability larger than

$$1 - 3P\Big(\Omega^*(z) > \frac{\lambda\eta\rho(J)\sqrt{n}}{2\sigma}\Big)$$

  - z is a multivariate normal with covariance matrix Q

Consistency - $\min_{w\in\mathbb{R}^p} \frac{1}{2n}\|y - Xw\|_2^2 + \lambda\Omega(w)$

- **Proposition**
  - Assume $y = Xw^* + \sigma\varepsilon$, with $\varepsilon \sim \mathcal{N}(0, I)$
  - J = smallest stable set containing the support of w^*
  - Let $Q = \frac{1}{n}X^\top X \in \mathbb{R}^{p\times p}$.
  - Assume that $\forall\Delta$ s.t. $\Omega^J(\Delta_{J^c}) \leqslant 3\Omega_J(\Delta_J)$, $\Delta^\top Q\Delta \geqslant \kappa\|\Delta_J\|_2^2$
  - Then $\boxed{\Omega(\hat{w} - w^*) \leqslant \dfrac{24c(J)^2\lambda}{\kappa\rho(J)^2}}$ and $\boxed{\dfrac{1}{n}\|X\hat{w} - Xw^*\|_2^2 \leqslant \dfrac{36c(J)^2\lambda^2}{\kappa\rho(J)^2}}$

    with probability larger than $1 - P\big(\Omega^*(z) > \frac{\lambda\rho(J)\sqrt{n}}{2\sigma}\big)$
  - z is a multivariate normal with covariance matrix Q

- **Concentration inequality** (z normal with covariance matrix Q):
  - $\mathcal{T}$ set of stable inseparable sets
  - Then $P(\Omega^*(z) > t) \leqslant \sum_{A\in\mathcal{T}} 2^{|A|} \exp\big(-\frac{t^2F(A)^2/2}{1^\top Q_{AA}1}\big)$

Outline

- **Introduction: Sparse methods for machine learning**
  - Need for structured sparsity: Going beyond the ℓ_1-norm
- **Submodular functions**
  - Lovász extension
- **Structured sparsity through submodular functions**
  - Relaxation of the penalization of supports
  - Examples
  - Unified algorithms and analysis
- **Extensions to symmetric submodular functions**
  - Shaping level sets

Symmetric submodular functions (Bach, 2010a)

- Let $F : 2^V \to \mathbb{R}$ be a **symmetric submodular set-function**

- **Proposition**: The Lovász extension $f(w)$ is the convex envelope of the function $w \mapsto \max_{\alpha \in \mathbb{R}} F(\{w \geqslant \alpha\})$ on the set $[0,1]^p + \mathbb{R}1_V = \{w \in \mathbb{R}^p, \ \max_{k \in V} w_k - \min_{k \in V} w_k \leqslant 1\}$.

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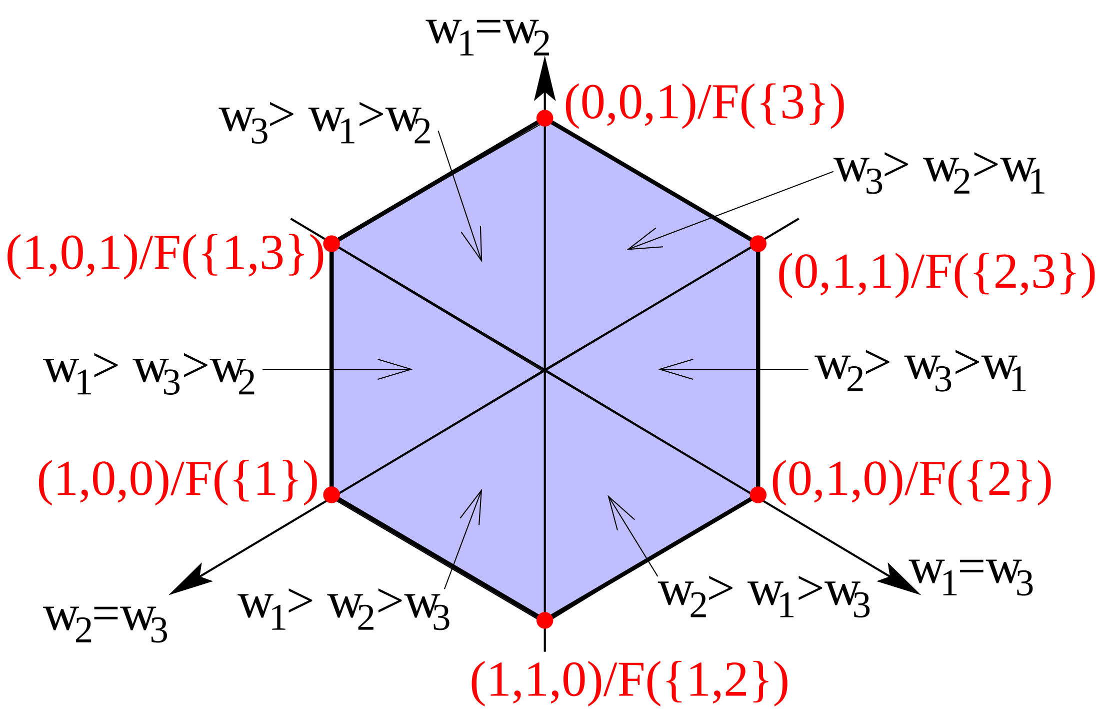
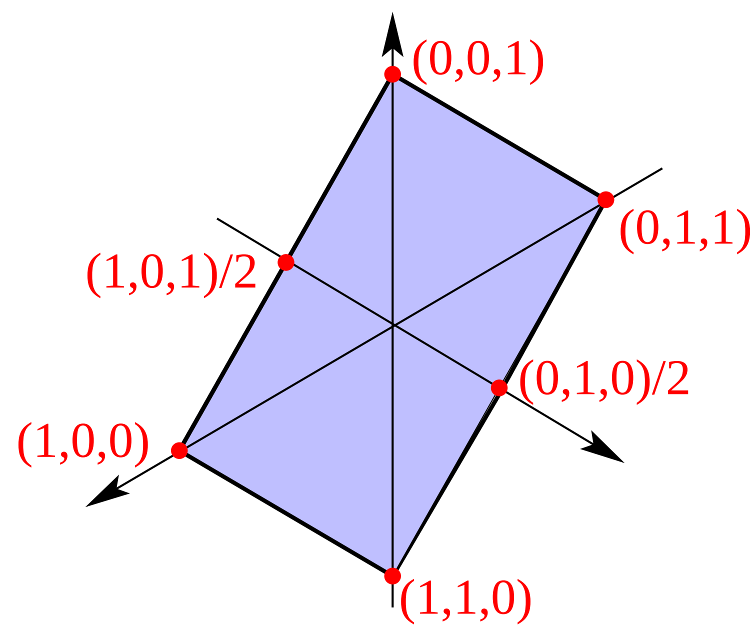
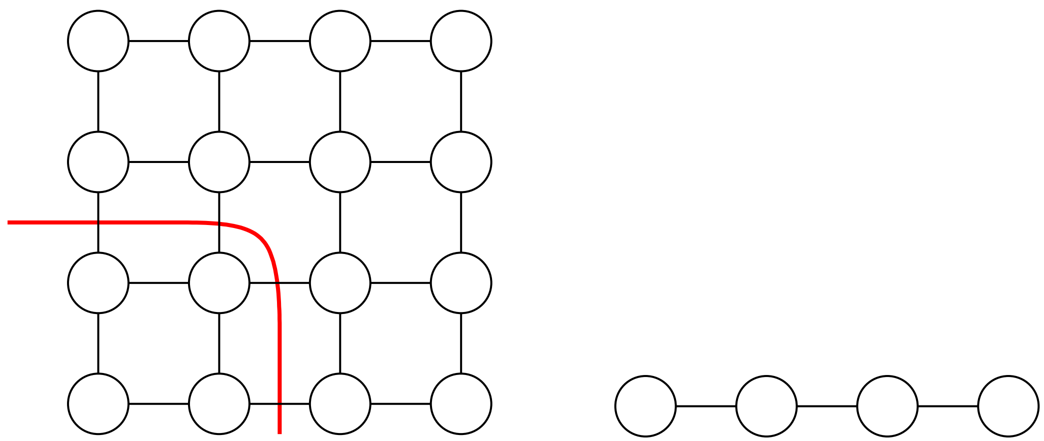




Symmetric submodular functions - Examples

- **From $\Omega(w)$ to $F(A)$:** provides new insights into existing norms
  - **Cuts - total variation**

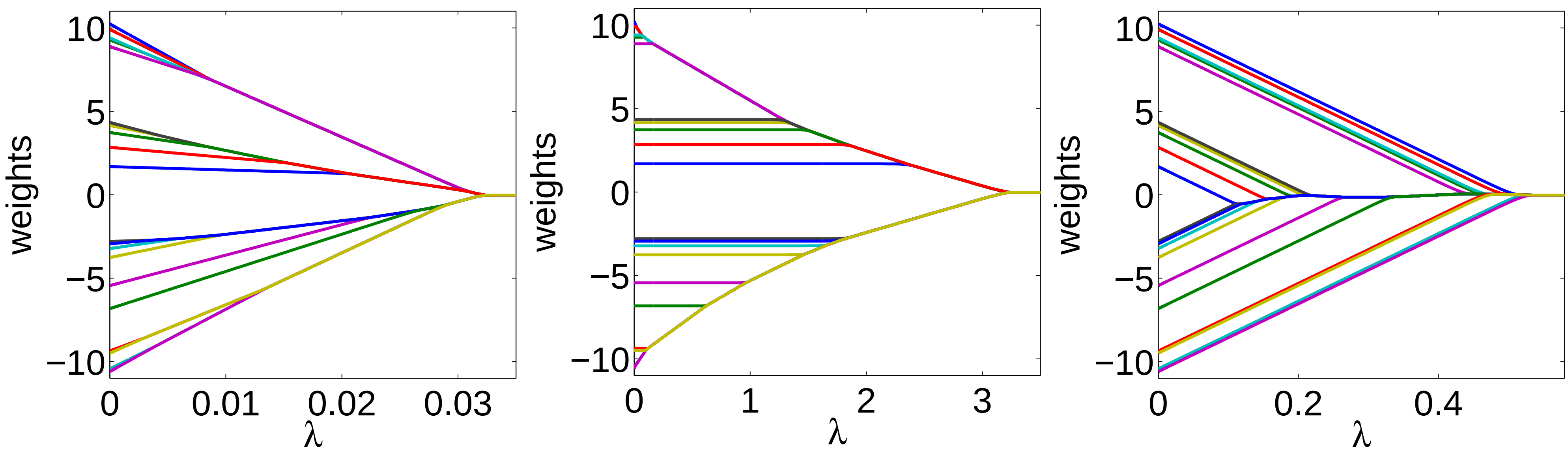
$$F(A) = \sum_{k \in A, j \in V \backslash A} d(k,j) \quad \Rightarrow \quad f(w) = \sum_{k,j \in V} d(k,j)(w_k - w_j)_+$$



  - NB: graph may be directed

Symmetric submodular functions - Examples

- **From $F(A)$ to $\Omega(w)$:** provides new sparsity-inducing norms
  - $F(A) = g(\mathrm{Card}(A)) \Rightarrow$ priors on the size and numbers of clusters



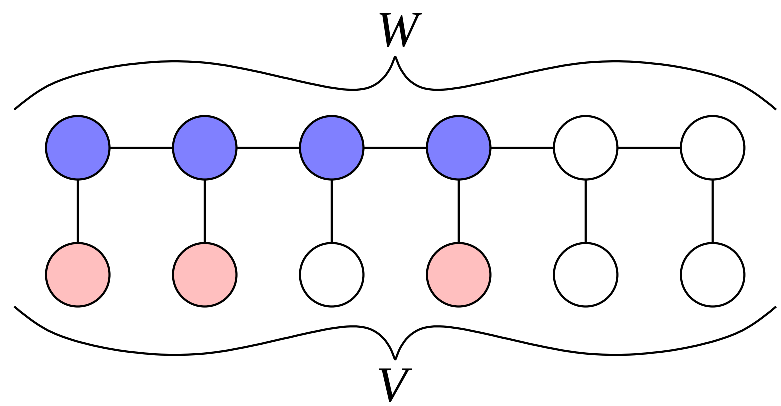
$|A|(p - |A|)$ $\quad\quad$ $1_{|A| \in (0,p)}$ $\quad\quad$ $\max\{|A|, p - |A|\}$

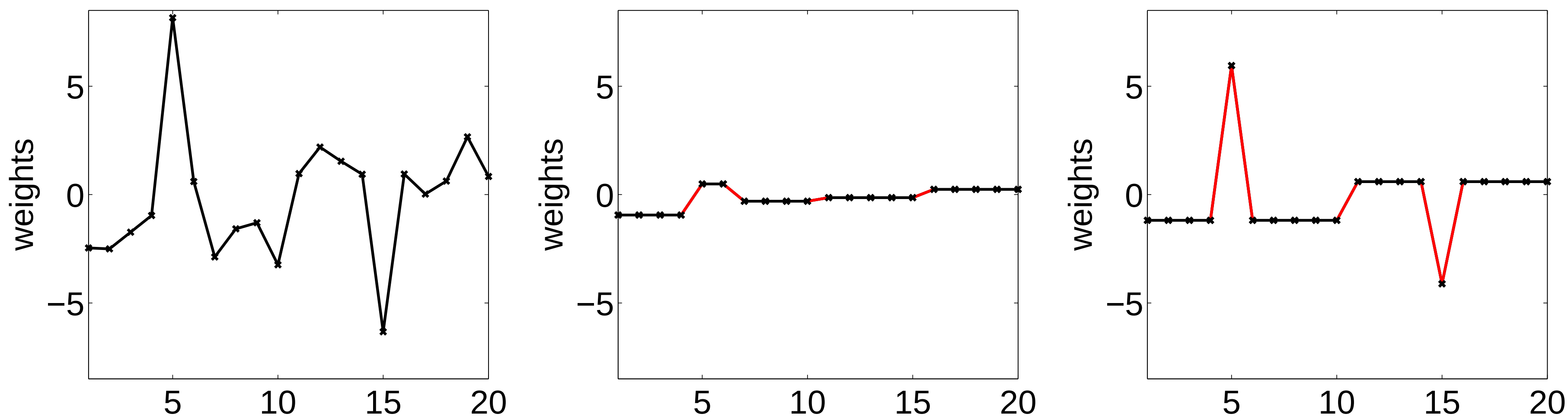
  - Convex formulations for clustering (Hocking, Joulin, Bach, and Vert, 2011)

Symmetric submodular functions - Examples

- **From $F(A)$ to $\Omega(w)$**: provides new sparsity-inducing norms
  - **Regular functions** (Boykov et al., 2001; Chambolle and Darbon, 2009)

$$F(A) = \min_{B \subset W} \sum_{k \in B,\ j \in W \backslash B} d(k,j) + \lambda |A \Delta B|$$





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 work on structured sparsity**
  - Norm design beyond submodular functions
  - Links with greedy methods (Haupt and Nowak, 2006; Baraniuk et al., 2008; Huang et al., 2009)
  - Extensions to matrices

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