Structured Sparsity in Machine Learning:
Models, Algorithms, and Applications

André F. T. Martins

Joint work with:

Mário A. T. Figueiredo, Instituto de Telecomunicações, Lisboa, Portugal
Noah A. Smith, Language Technologies Institute, Carnegie Mellon University, USA

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Outline

Our Setup

- Input set $\mathcal{X}$, output set $\mathcal{Y}$
- Linear model:

$$\widehat{y} := \arg\max_{y \in \mathcal{Y}} \mathbf{w}^\top \mathbf{f}(x, y)$$

  where $\mathbf{f} : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}^D$ is a feature map
- Learning the model parameters from data $\{(x_n, y_n)\}_{n=1}^N \subseteq \mathcal{X} \times \mathcal{Y}$:

$$\widehat{\mathbf{w}} = \arg\min_{\mathbf{w}} \underbrace{\frac{1}{N} \sum_{n=1}^{N} L(\mathbf{w}; x_n, y_n)}_{\text{empirical risk}} + \underbrace{\Omega(\mathbf{w})}_{\text{regularizer}}$$

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This talk: we focus on the **regularizer** Ω

The Bet On Sparsity (Friedman et al., 2004)

Sparsity hypothesis: not all dimensions of $\mathbf{f}$ are needed (many features are *irrelevant*)

Setting the corresponding weights to zero leads to a **sparse** $\mathbf{w}$

Models with just a few features:

- are easier to explain/interpret
- have a smaller memory footprint
- are faster to run (less features need to be evaluated)
- generalize better

(Automatic) Feature Selection

Domain experts are often good at engineering features.

Can we automate the process of selecting which ones to keep?

Three main classes of methods (Guyon and Elisseeff, 2003):

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Embedded Methods for Feature Selection

Formulate the learning problem as a trade-off between

- minimizing loss (fitting the training data, achieving good accuracy on the training data, etc.)
- choosing a desirable model (e.g., with no more features than needed)

$$\min_{\mathbf{w}} \frac{1}{N} \sum_{n=1}^{N} L(\mathbf{w}; x_n, y_n) + \Omega(\mathbf{w})$$

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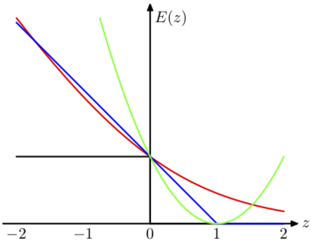
Key advantage: declarative statements of model “desirability” often lead to well-understood, convex optimization problems.

Convex Loss Functions

Squared (linear regression)	$\frac{1}{2}\left(y - \mathbf{w}^\top \mathbf{f}(x)\right)^2$
Log-linear (MaxEnt, CRF, logistic)	$-\mathbf{w}^\top \mathbf{f}(x,y) + \log \sum_{y' \in \mathcal{Y}} \exp(\mathbf{w}^\top \mathbf{f}(x,y'))$
Hinge (SVMs)	$-\mathbf{w}^\top \mathbf{f}(x,y) + \max_{y' \in \mathcal{Y}} \left(\mathbf{w}^\top \mathbf{f}(x,y') + c(y,y')\right)$
Perceptron	$-\mathbf{w}^\top \mathbf{f}(x,y) + \max_{y' \in \mathcal{Y}} \mathbf{w}^\top \mathbf{f}(x,y')$



Regularization Formulations

- Tikhonov regularization: $\widehat{\mathbf{w}} = \arg\min_{\mathbf{w}} \lambda\Omega(\mathbf{w}) + \sum_{n=1}^{N} L(\mathbf{w}; x_n, y_n)$
- Ivanov regularization

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Equivalent, under mild conditions (namely convexity).

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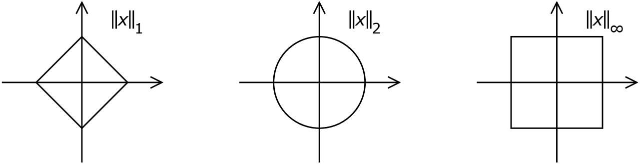

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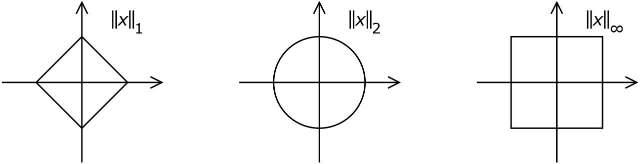

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- **Side note:** the infamous ℓ_0 "norm" (**non-convex, not a norm**):

$$\|\mathbf{w}\|_0 = \lim_{p \to 0} \|\mathbf{w}\|_p^p = |\{i : w_i \neq 0\}|$$

Ridge and Lasso Regularizers

Ridge or ℓ_2 regularization: $\boxed{\Omega(\mathbf{w}) = \frac{\lambda}{2}\|\mathbf{w}\|_2^2}$

- goes back to Tikhonov (1943) and Wiener (1949)
- corresponds to a zero-mean Gaussian prior
- **Pros**: smooth and convex, thus benign for optimization.
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Lasso or ℓ_1 regularization: $\boxed{\Omega(\mathbf{w}) = \lambda\|\mathbf{w}\|_1}$

- goes back to Claerbout and Muir (1973); Taylor et al. (1979); Tibshirani (1996)
- corresponds to zero-mean Laplacian prior
- **Pros**: encourages sparsity: embedded feature selection.
- **Cons**: convex, but non-smooth: more challenging optimization.

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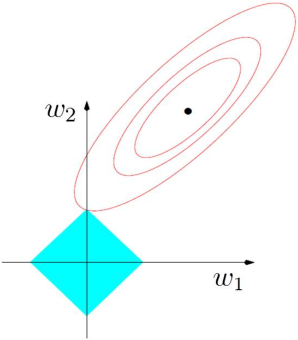

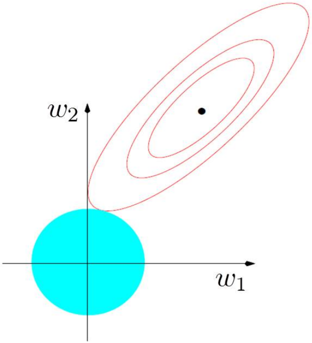

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Take-Home Messages

- Sparsity is desirable for interpretability, computational savings, and generalization
- ℓ_1-regularization gives an embedded method for feature selection
- Another view of ℓ_1: a convex surrogate for direct penalization of cardinality (ℓ_0)
- Under some conditions, ℓ_1 guarantees exact support recovery (Candès et al., 2006; Donoho, 2006)
- However: the currently known sufficient conditions are too strong and not met in typical ML problems

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ℓ_1 regularization promotes **sparse models**

A very simple sparsity pattern: **small cardinality**

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Main question: how to promote less trivial sparsity patterns?

Structured Sparsity and Groups

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Group sparsity: discard entire *groups* of features

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

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- **density** inside each group
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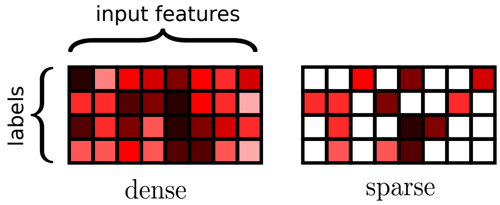
- choice of groups: prior knowledge about the intended *sparsity patterns*

Yields statistical gains if prior assumptions are correct (Stojnic et al., 2009)

Example: Sparsity in a Grid

Assume the feature map decomposes as $\mathbf{f}(x, y) = \mathbf{f}(x) \otimes \mathbf{e}_y$

In words: we're conjoining each input feature with each output class



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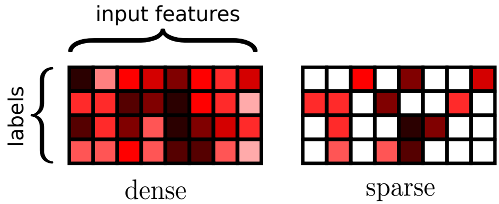

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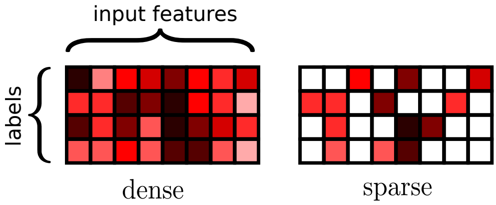

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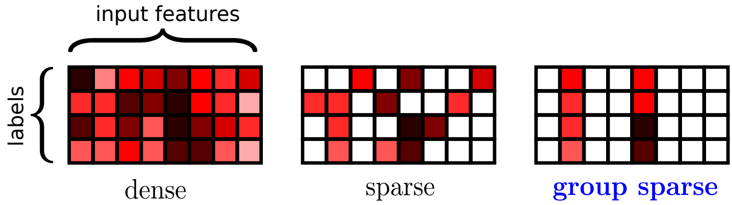

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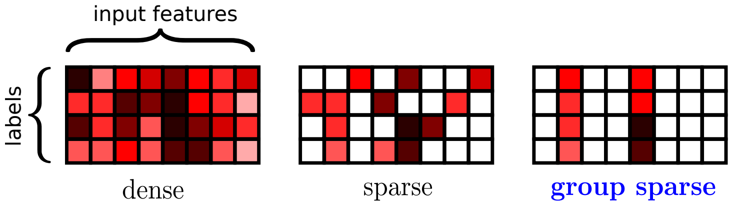

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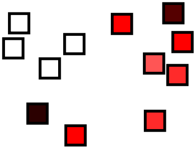
Similar structure: multi-task learning (Caruana, 1997; Obozinski et al., 2010), multiple kernel learning (Lanckriet et al., 2004)

Group Sparsity



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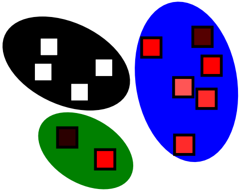

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- M groups $G_1, \ldots, G_M$, each $G_m \subseteq \{1, \ldots, D\}$
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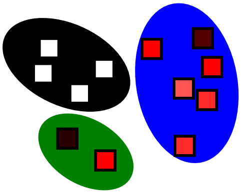

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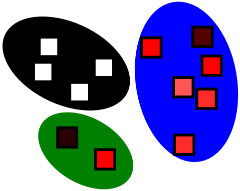

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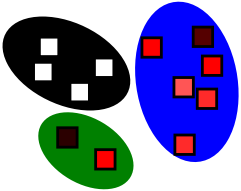

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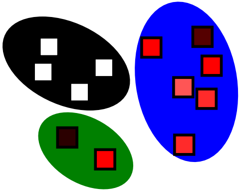

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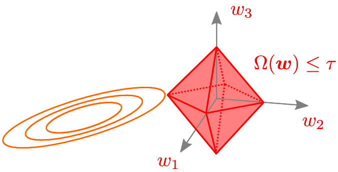
- Statisticians call these **composite absolute penalties** (Zhao et al., 2009)

Lasso versus group-Lasso



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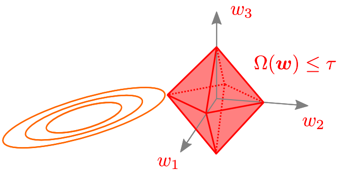

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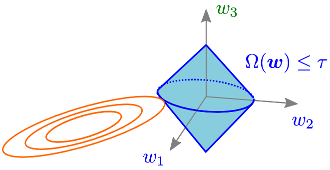

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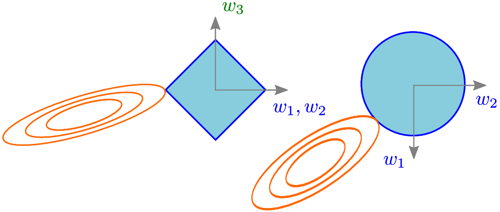

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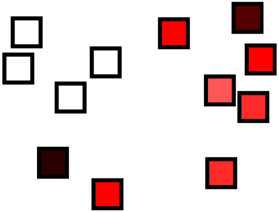
Examples of non-trivial groups:

- label-based groups (groups are columns of a matrix)
- template-based groups (next)

Example: Feature Template Selection



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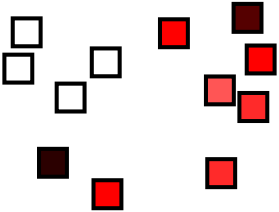

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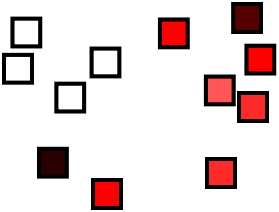

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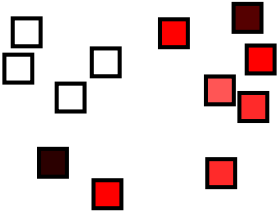

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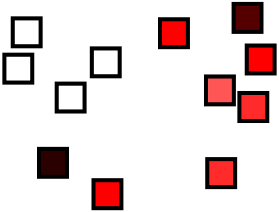

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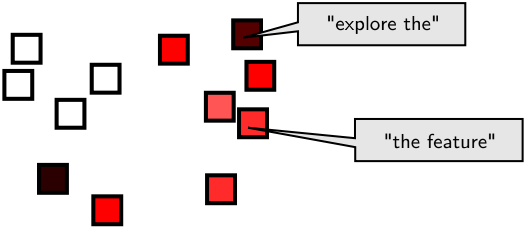

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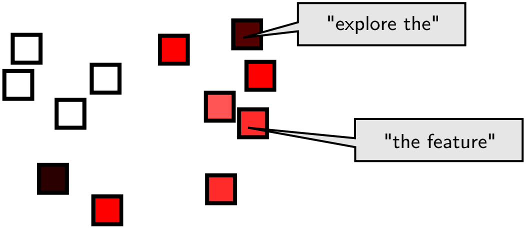

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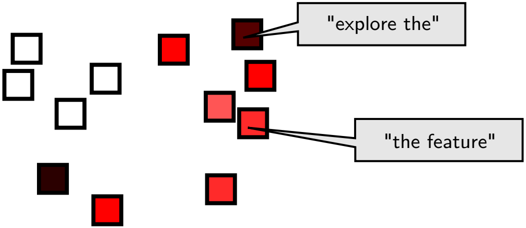

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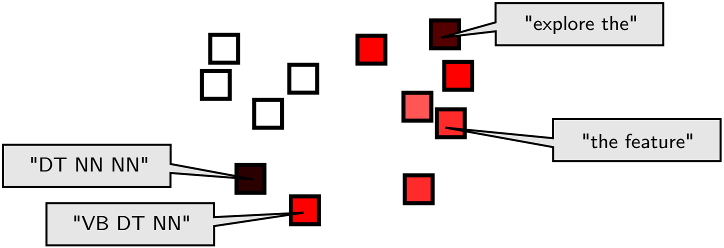

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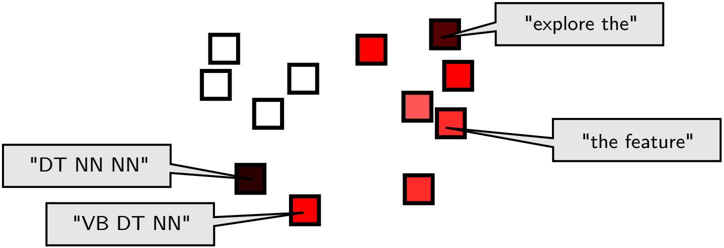

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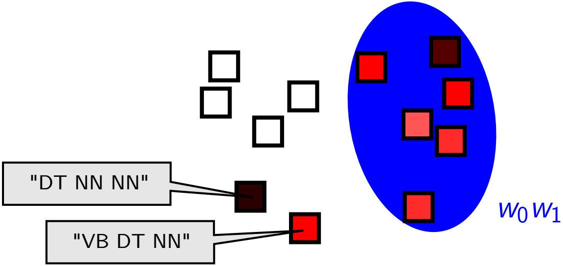

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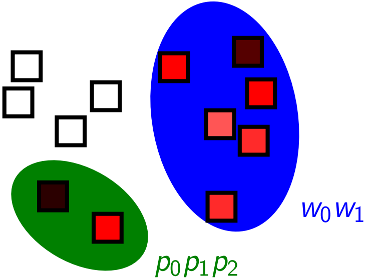

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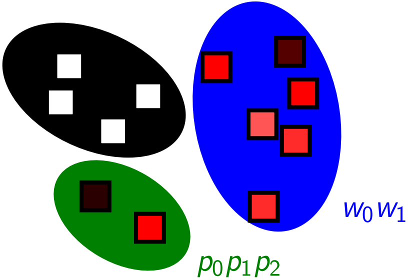

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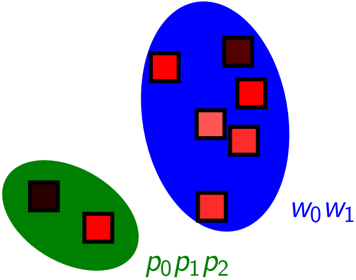

Three Scenarios

- Non-overlapping groups
- Tree-structured groups
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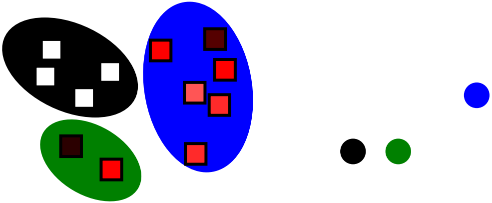

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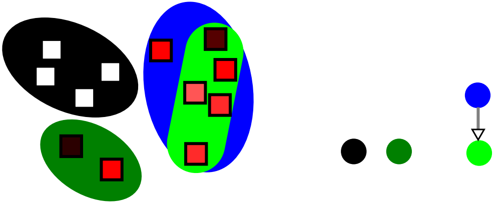

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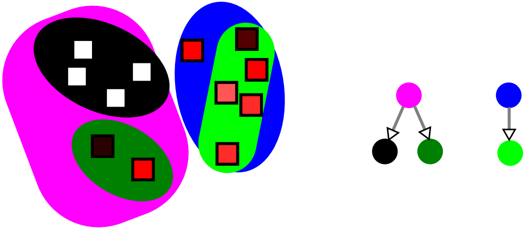

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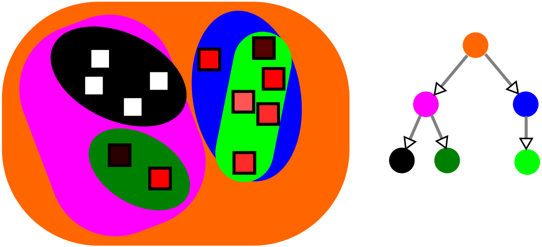

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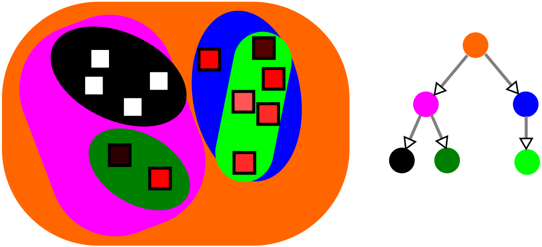

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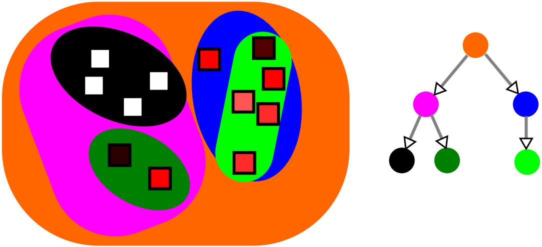

- What is the **sparsity pattern**?
- **If a group is discarded, all its descendants are also discarded**

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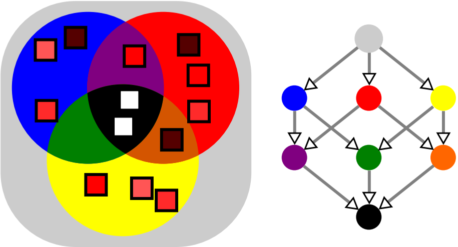
Arbitrary Groups

In general: groups can be represented as a **directed acyclic graph**

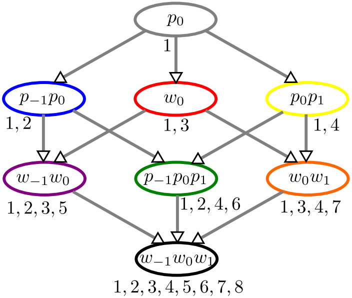


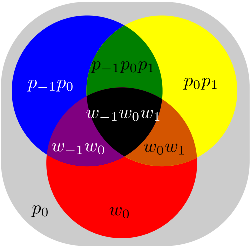
- set inclusion induces a **partial order** on groups (Jenatton et al., 2009)
- feature space becomes a **poset**
- **sparsity patterns**: given by this poset

Example: Coarse-to-Fine Regularization

1. Define a partial order between basic feature templates (e.g., $p_0 \preceq w_0$)
2. Extend this partial order to all templates by lexicographic closure: $p_0 \preceq p_0 p_1 \preceq w_0 w_1$

Goal: only include *finer* features if *coarser* ones are also in the model





Things to Keep in Mind

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- **Choice of groups:** problem dependent, opportunity to use prior knowledge to favour certain structural patterns
- **Next:** algorithms
- We'll see that optimization is easier with non-overlapping or tree-structured groups than with arbitrary overlaps

Outline

Learning the Model

Recall that learning involves solving

$$\min_{\mathbf{w}} \quad \underbrace{\Omega(\mathbf{w})}_{\text{regularizer}} + \underbrace{\frac{1}{N}\sum_{i=1}^{N} L(\mathbf{w}, x_i, y_i)}_{\text{total loss}},$$

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We'll focus on proximal gradient algorithms (both batch and online)

A Key Ingredient: Proximity Operator

The **Ω-proximity operator** is the following $\mathbb{R}^D \to \mathbb{R}^D$ map:

$$\boxed{\mathbf{w} \mapsto \mathrm{prox}_{\Omega}(\mathbf{w}) = \arg\min_{\mathbf{u}} \frac{1}{2}\|\mathbf{u} - \mathbf{w}\|^2 + \Omega(\mathbf{u})}$$

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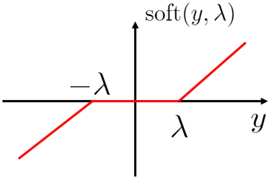
- ℓ_1 regularization $\boxed{\Omega(\mathbf{w}) = \lambda\|\mathbf{w}\|_1}$ $\Rightarrow$ **soft-thresholding**:

$$[\mathrm{prox}_{\Omega}(\mathbf{w})]_d = \begin{cases} w_d - \lambda & \text{if } w_d > \lambda \\ 0 & \text{if } |w_d| \leq \lambda \\ w_d + \lambda & \text{if } w_d < -\lambda. \end{cases}$$



Proximity Operators for Structured Sparsity

$$\boxed{\Omega(\mathbf{w}) = \sum_{m=1}^{M} \lambda_m \|\mathbf{w}_m\|_2}$$

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  The problem can be sidestepped with sequential proximity steps (Martins et al., 2011a) (more later).

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- expectation-maximization (EM) (Figueiredo and Nowak, 2003);
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Convergence: requires $O(1/\epsilon)$ iterations for ϵ-accurate objective.

Other Proximal-Gradient Variants

SpaRSA (Wright et al., 2009): the same IST update scheme, but setting η_t to mimic a Newton step (Barzilai and Borwein, 1988):

$$\eta_t^{-1}\mathbf{I} \approx \mathbf{H}(\mathbf{w}_t) \quad \text{(Hessian)}$$

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$$\boxed{\begin{array}{lcl} b_{t+1} & = & \frac{1+\sqrt{1+4\,b_t^2}}{2} \\ \mathbf{z} & = & \mathbf{w}_t + \frac{b_t-1}{b_{t+1}}(\mathbf{w}_t - \mathbf{w}_{t-1}) \\ \mathbf{w}_{t+1} & = & \mathrm{prox}_{\eta\Omega}(\mathbf{z} - \eta\nabla\Lambda(\mathbf{z})) \end{array}}$$

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- **Iteration bound:** $O(1/\sqrt{\epsilon})$ as opposed to $O(1/\epsilon)$.

Many Other Batch Algorithms

- coordinate descent (Shevade and Keerthi, 2003; Genkin et al., 2007; Krishnapuram et al., 2005; Tseng and Yun, 2009)
- Least Angle Regression (LARS) and homotopy/continuation methods (Efron et al., 2004; Osborne et al., 2000; Figueiredo et al., 2007)
- shooting method (Fu, 1998)
- grafting (Perkins et al., 2003) and grafting-light (Zhu et al., 2010)
- orthant-wise limited-memory quasi-Newton (OWL-QN) (Andrew and Gao, 2007; Gao et al., 2007)
- alternating direction method of multipliers (ADMM) (Afonso et al., 2010; Figueiredo and Bioucas-Dias, 2011).

...several more; this is an active research area!

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3. Faster to approach a near-optimal region
4. Slower convergence, but this is fine in machine learning ("the tradeoffs of large scale learning" by Bottou and Bousquet (2007))

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$$\min_{\mathbf{w}} \ \Omega(\mathbf{w}) + \frac{1}{N}\sum_{i=1}^{N} L(\mathbf{w}, x_i, y_i),$$

initialize $\mathbf{w} = \mathbf{0}$
for $t = 1, 2, \ldots$ **do**
  take training pair (x_t, y_t)
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Plain Stochastic (Sub-)Gradient Descent

$$\min_{\mathbf{w}} \; \Omega(\mathbf{w}) + \frac{1}{N}\sum_{i=1}^{N} L(\mathbf{w}, x_i, y_i),$$

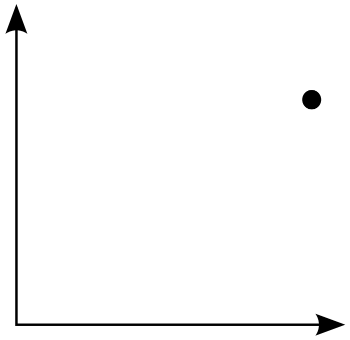
```
initialize w = 0
for t = 1, 2, ... do
    take training pair (x_t, y_t)
    (sub-)gradient step: w ← w − η_t (∇̃Ω(w) + ∇̃L(w; x_t, y_t))
end for
```

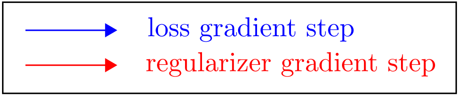
- ℓ_1-regularization $\boxed{\Omega(\mathbf{w}) = \lambda\|\mathbf{w}\|_1} \Longrightarrow \tilde{\nabla}\Omega(\mathbf{w}) = \lambda \mathrm{sign}(\mathbf{w})$

$$\mathbf{w} \leftarrow \underbrace{\mathbf{w} - \eta_t \lambda \mathrm{sign}(\mathbf{w})}_{\text{constant penalty}} - \eta_t \tilde{\nabla} L(\mathbf{w}; x_t, y_t)$$

- **Problem: iterates are never sparse!**

Plain SGD with ℓ_1-regularization





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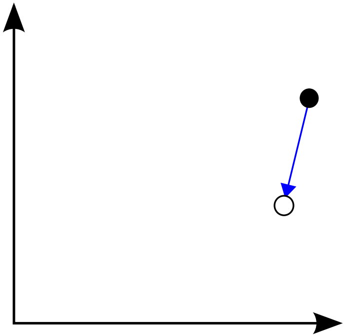

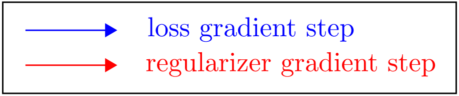

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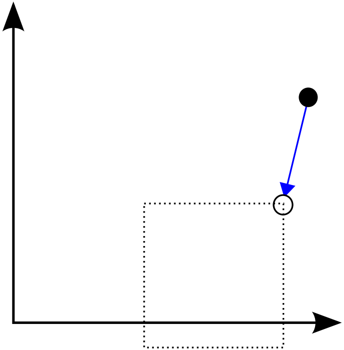

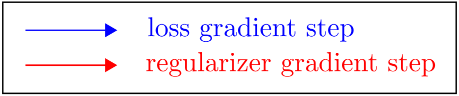

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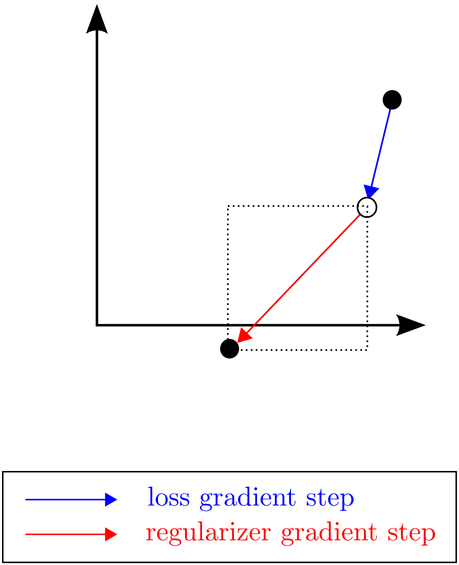

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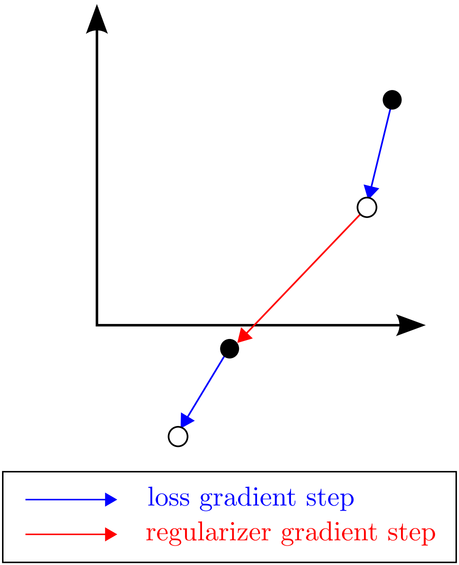

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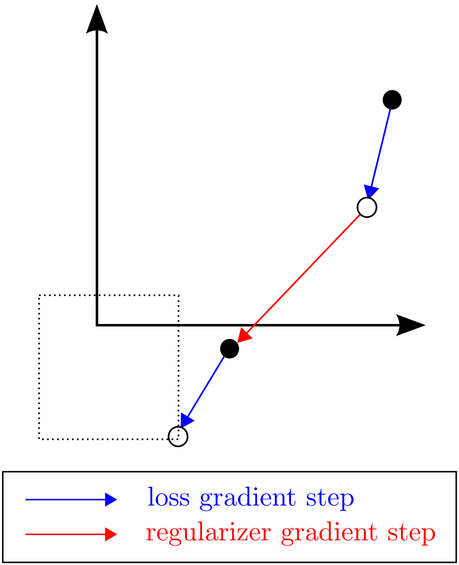

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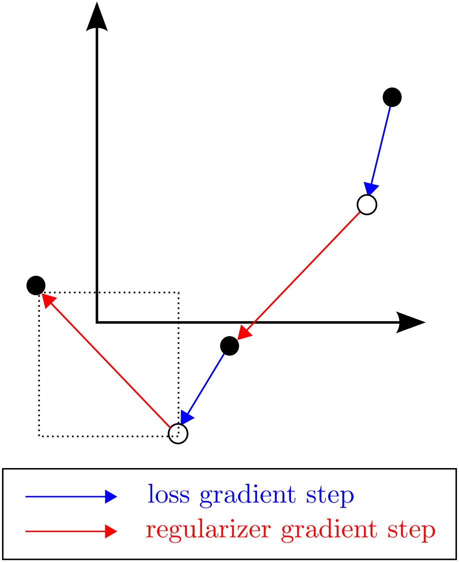

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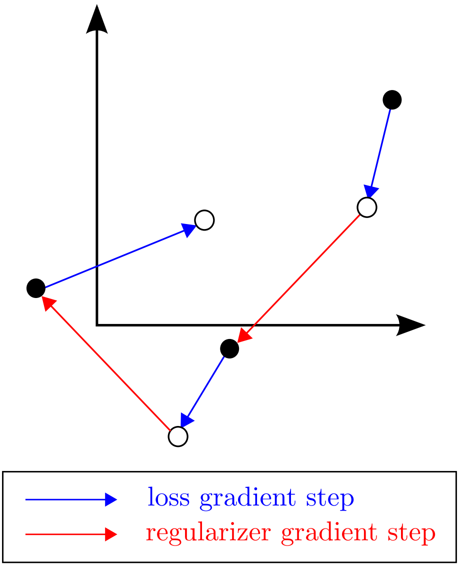

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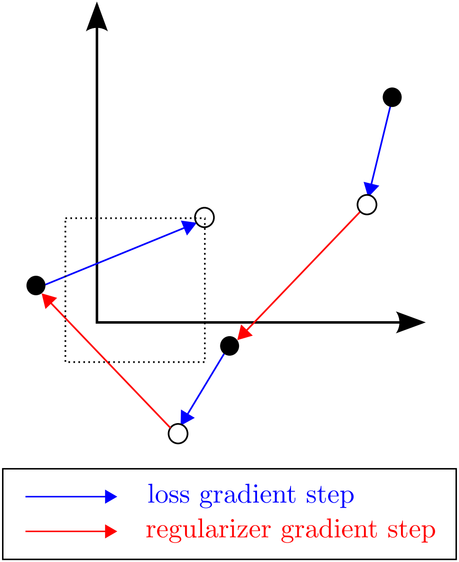

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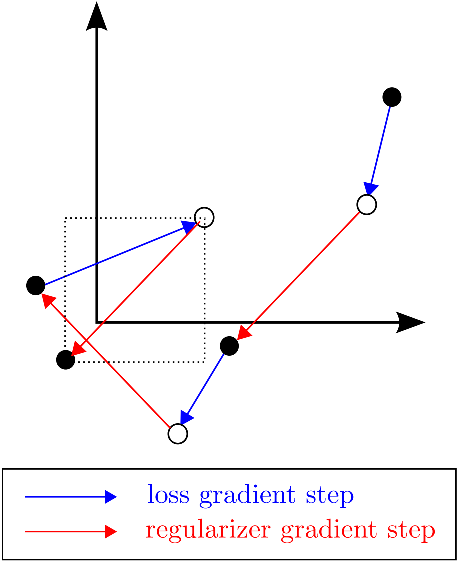
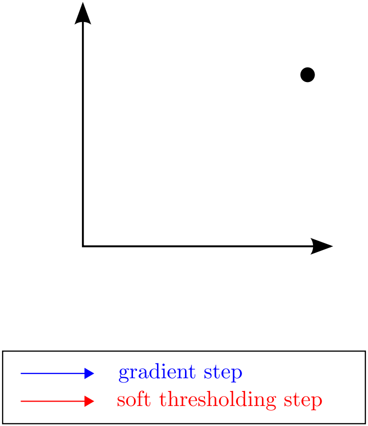


“Sparse” Online Algorithms

- Truncated Gradient (Langford et al., 2009)
- Online Forward-Backward Splitting (Duchi and Singer, 2009)
- Regularized Dual Averaging (Xiao, 2010)
- Online Proximal Gradient (Martins et al., 2011a)

Truncated Gradient (Langford et al., 2009)

- take gradients-step **only with respect to the loss**
- apply soft-thresholding
- **converges to ϵ-accurate objective after $O(1/\epsilon^2)$ iterations**



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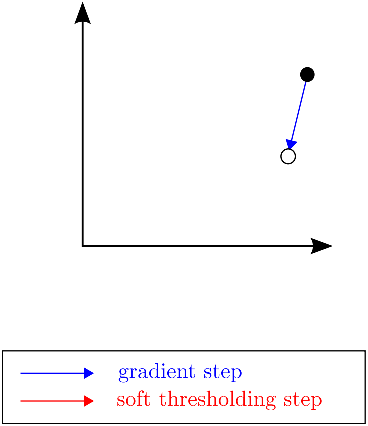

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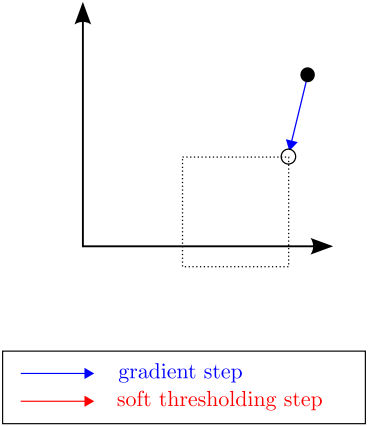

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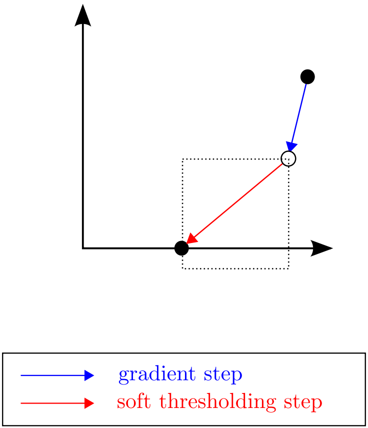

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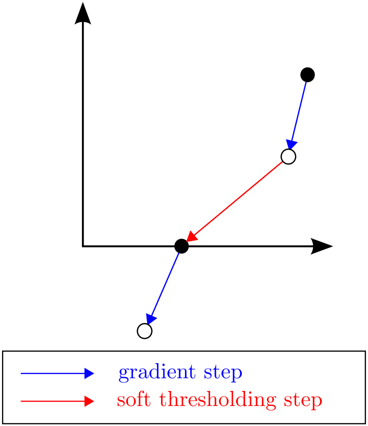

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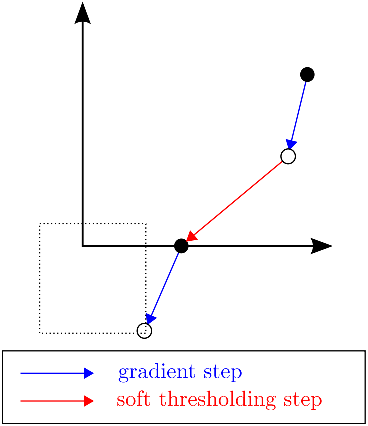

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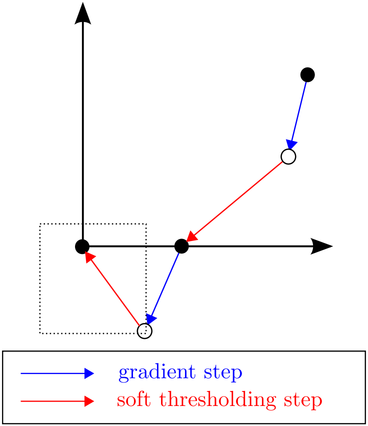

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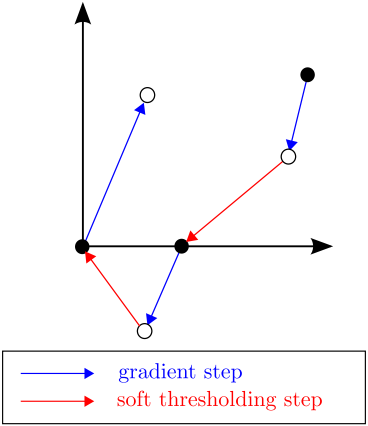

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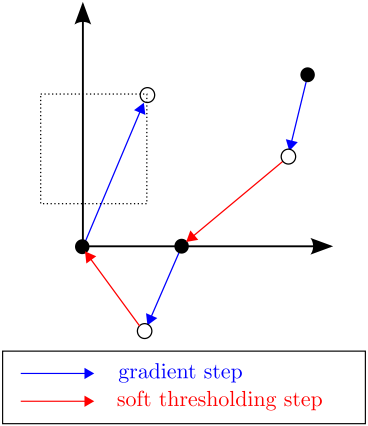

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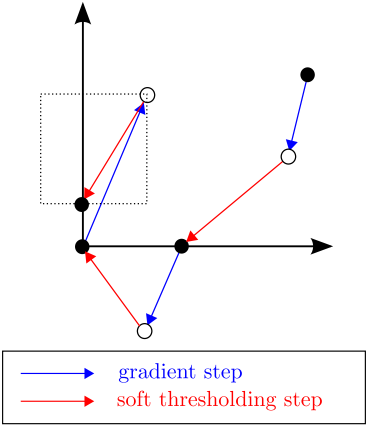

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Online Forward-Backward Splitting (Duchi and Singer, 2009)

initialize $\mathbf{w} = \mathbf{0}$
for $t = 1, 2, \ldots$ **do**
  take training pair (x_t, y_t)
  gradient step: $\mathbf{w} \leftarrow \mathbf{w} - \eta_t \nabla L(\mathbf{w}; x_t, y_t)$
  proximal step: $\mathbf{w} \leftarrow \mathrm{prox}_{\eta_t \Omega}(\mathbf{w})$
end for

- generalizes truncated gradient to arbitrary regularizers Ω
  - can tackle non-overlapping or hierarchical group-Lasso, but arbitrary overlaps are difficult to handle (more later)
- **converges to ϵ-accurate objective after $O(1/\epsilon^2)$ iterations**

“Sparse” Online Algorithms

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Prox-Grad with Overlaps (Martins et al., 2011a)

Key idea: decompose $\Omega(\mathbf{w}) = \sum_{j=1}^{J} \Omega_j(\mathbf{w})$, where each Ω_j is non-overlapping, and apply **sequential proximal steps**:

$$\textbf{gradient step}: \ \mathbf{w} \ \leftarrow \ \mathbf{w} - \eta_t \nabla L(\theta; x_t, y_t)$$

$$\textbf{proximal steps}: \ \mathbf{w} \ \leftarrow \ \mathrm{prox}_{\eta_t \Omega_J}\left(\mathrm{prox}_{\eta_t \Omega_{J-1}}\left(\ldots \mathrm{prox}_{\eta_t \Omega_1}(\mathbf{w})\right)\right)$$

Prox-Grad with Overlaps (Martins et al., 2011a)

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> **gradient step**: $\mathbf{w} \leftarrow \mathbf{w} - \eta_t \nabla L(\boldsymbol{\theta}; x_t, y_t)$
>
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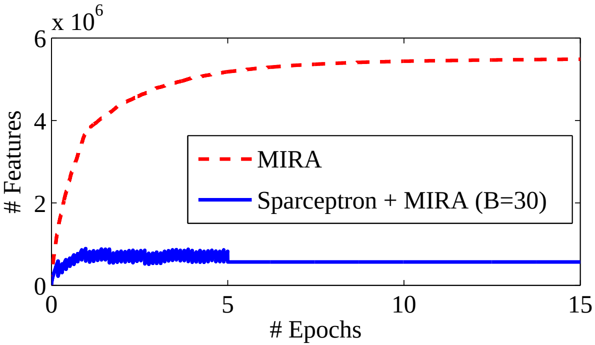
- still convergent, same $O(1/\epsilon^2)$ iteration bound
- **gradient step:** linear in # of features that fire, *independent* of D.
- **proximal steps:** linear in # of groups M.
- other implementation tricks (debiasing, budget-driven shrinkage, etc.)

Memory Footprint

- 5 epochs for identifying relevant groups, 10 epochs for debiasing



Summary of Algorithms

	Converges	Rate	Sparse	Groups	Overlaps
Coord. desc.	✓	?	✓	Maybe	No
Prox-grad	✓	$O(1/\epsilon)$	Yes/No	✓	Not easy
OWL-QN	✓	?	Yes/No	No	No
SpaRSA	✓	$O(1/\epsilon)$ or better	Yes/No	✓	Not easy
FISTA	✓	$O(1/\sqrt{\epsilon})$	Yes/No	✓	Not easy
ADMM	✓	$O(1/\epsilon)$	No	✓	✓
Online subgrad.	✓	$O(1/\epsilon^2)$	No	✓	No
Truncated grad.	✓	$O(1/\epsilon^2)$	✓	No	No
FOBOS	✓	$O(1/\epsilon^2)$	Sort of	✓	Not easy
Online prox-grad	✓	$O(1/\epsilon^2)$	✓	✓	✓

Outline

Applications of Structured Sparsity in ML

We will focus on two recent NLP applications (Martins et al., 2011b):

- Named entity recognition
- Dependency parsing

We use **feature templates** as groups.

Named Entity Recognition

Only	France	and	Britain	backed	Fischler	's	proposal	.
RB	NNP	CC	NNP	VBD	NNP	POS	NN	.

Named Entity Recognition

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	LOCATION		LOCATION		PERSON			

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- Spanish, Dutch, and English CoNLL datasets
- 452 feature templates using POS tags, words, shapes, affixes, with various context sizes

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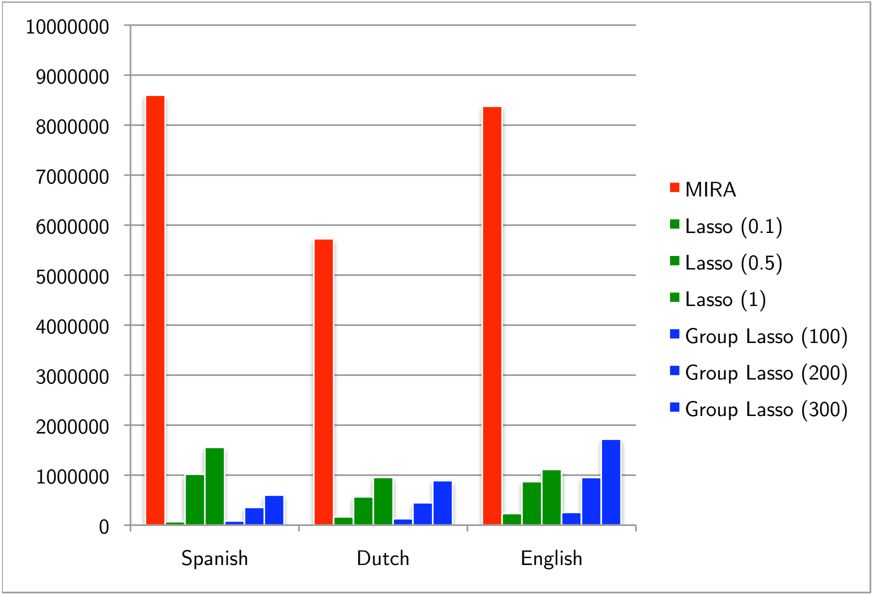
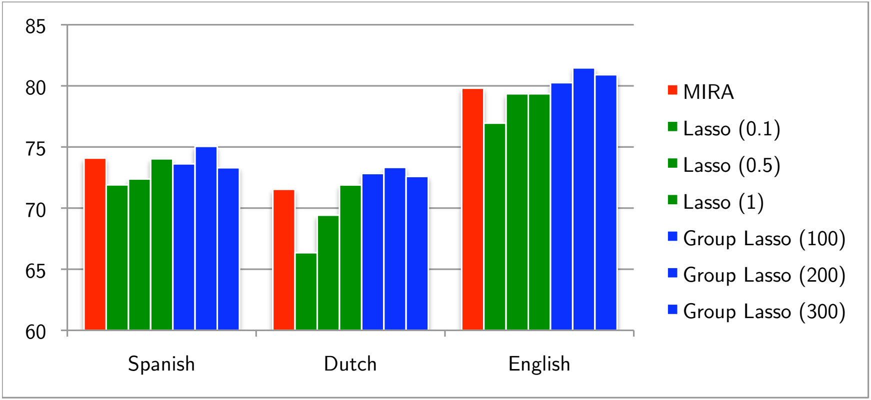
- Spanish, Dutch, and English CoNLL datasets
- 452 feature templates using POS tags, words, shapes, affixes, with various context sizes

Comparison between:

- ℓ_2-regularization (MIRA), best λ on dev-set, all features
- ℓ_1-regularization (Lasso), varying λ
- $\ell_{2,1}$-regularization (**Group Lasso**), varying the template budget

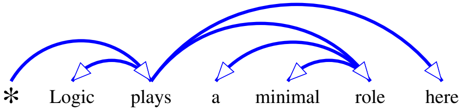


Named entity models: number of features. (Lasso $C = 1/\lambda N$.)



Named entity models: F_1 accuracy on the test set. (Lasso $C = 1/\lambda N$.)

Dependency Parsing



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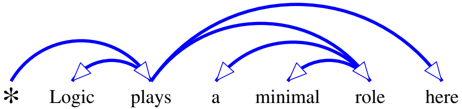

- Arabic, Danish, Dutch, Japanese, Slovene, Spanish CoNLL datasets
- 684 feature templates (using words, lemmas, POS, contextual POS, arc length and direction)

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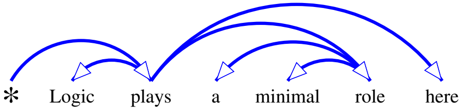
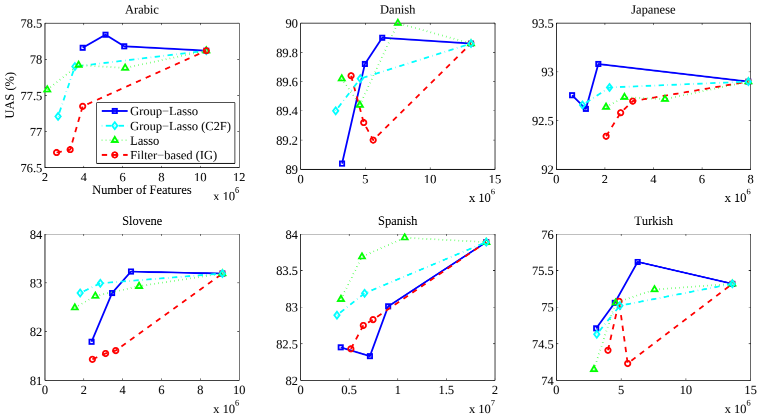


- Arabic, Danish, Dutch, Japanese, Slovene, Spanish CoNLL datasets
- 684 feature templates (using words, lemmas, POS, contextual POS, arc length and direction)

Comparison between:

- ℓ_2-regularization (MIRA), all features
- filter-based template selection (information gain)
- ℓ_1-regularization (Lasso)
- $\ell_{2,1}$-regularization (**Group Lasso**, coarse-to-fine regularization)

Dependency Parsing (c'ed)



Template-based group lasso is better at selecting feature templates than the IG criterion, and slightly better than **coarse-to-fine**.

Outline

Summary

- Sparsity is desirable in machine learning: *feature selection*, *runtime*, *memory footprint*, *interpretability*
- Beyond plain sparsity: **structured sparsity** can be promoted through group-Lasso regularization
- Choice of groups reflects prior knowledge about the desired sparsity patterns.
- Small/medium scale: many batch algorithms available, with fast convergence (IST, FISTA, SpaRSA, ...)
- Large scale: online proximal-gradient algorithms suitable to explore large feature spaces

Thank you!

- Questions?

Acknowledgments

- National Science Foundation (USA), CAREER grant IIS-1054319
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