Bilevel Optimization of Hyperparameters: Application to Structure Discovery

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slides & more available at jordan-frecon.com

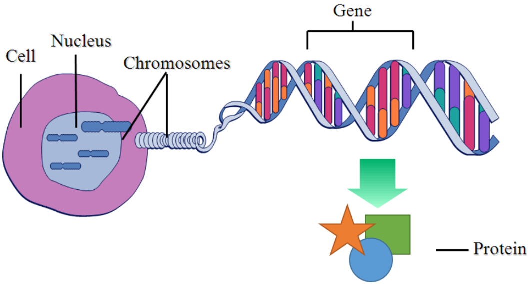
Example 1: Structured linear regression

Setting presented in
[Frecon et al. "Bilevel learning of the group Lasso structure". NeurIPS (2018)]

Motivation: genes expression analysis

Goal : Predict the function of proteins from regulatory patterns

Collaboration with Giorgio Valentini (Universita degli Studi di Milano)



Gene = long sequence with regulatory patterns (dictate gene expression)

Proteins perform various functions (transport, redox, binding ...)

Regulatory patterns

	R_1	R_2	R_3	...	R_P
	CTGAC	GGATC	GCAAG	...	ATCAG
Gene 1	1	1	0	...	0

neuron =

Protein sub-functions (Gene Ontology)

Go_1	Go_2	Go_3	...	Go_T
transport	redox	binding		
1	0	0	...	1

Sequences R_1 and R_2 are present in Gene 1

Gene 1 produces neurons

Neurons perform transport of electrons

Motivation: genes expression analysis

Regulatory patterns

	R_1	R_2	R_3	...	R_P
	CTGAC	GGATC	GCAAG	...	ATCAG
Gene 1	1	1	0	...	0
Gene 2	1	1	1	...	0

Protein sub-functions (Gene Ontology)

	Go_1	Go_2	Go_3	...	Go_T
	transport	redox	binding		
neuron	1	0	0	...	1
hormone	1	1	0	...	0

Sequences R_1, R_2 and R_3 are present in Gene 2

Gene 2 produces hormones

Hormones perform transport of particles and reduction–oxidation

Regulatory patterns

	R_1 CTGAC	R_2 GGATC	R_3 GCAAG	...	R_P ATCAG
Gene 1	1	1	0	...	0
Gene 2	1	1	1	...	0
Gene 3	0	0	0	...	1

Protein sub-functions (Gene Ontology)

	Go_1 transport	Go_2 redox	Go_3 binding	...	Go_T
neuron	1	0	0	...	1
hormone	1	1	0	...	0
antibody	0	0	1	...	0

Sequence R_P is present in Gene 3

Gene 3 produces antibodies

Antibodies perform binding of particles

Motivation: genes expression analysis

Regulatory patterns

	R_1	R_2	R_3	...	R_P
	CTGAC	GGATC	GCAAG	...	ATCAG
Gene 1	1	1	0	...	0
Gene 2	1	1	1	...	0
Gene 3	0	0	0	...	1
	⋮	⋮	⋮	⋮	⋮
Gene N	1	1	0	...	1

$X \in \{0,1\}^{N \times P}$

neuron

hormone

antibody

Protein sub-functions (Gene Ontology)

Go_1	Go_2	Go_3	...	Go_T
transport	redox	binding		
1	0	0	...	1
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0	0	1	...	0
⋮	⋮	⋮	⋮	⋮
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$y = [y_1 \cdots y_T] \in \{0,1\}^{N \times T}$

Motivation: genes expression analysis

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Gene 2	1	1	1	...	0
Gene 3	0	0	0	...	1
	⋮	⋮	⋮	⋮	⋮
Gene N	1	1	0	...	1

$X \in \{0,1\}^{N \times P}$

neuron

hormone

antibody

Protein sub-functions (Gene Ontology)

Go_1 transport	Go_2 redox	Go_3 binding	...	Go_T
1	0	0	...	1
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0	0	1	...	0
⋮	⋮	⋮	⋮	⋮
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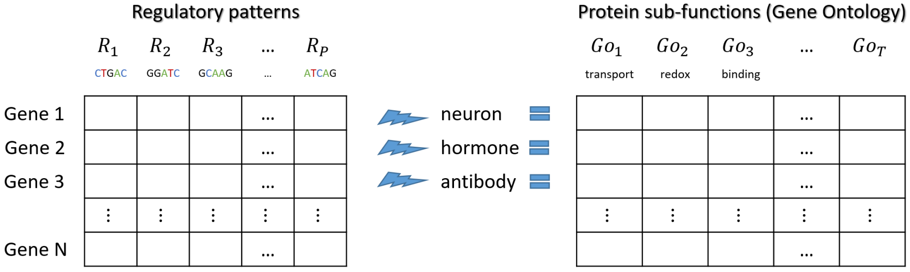
$y = [y_1 \cdots y_T] \in \{0,1\}^{N \times T}$

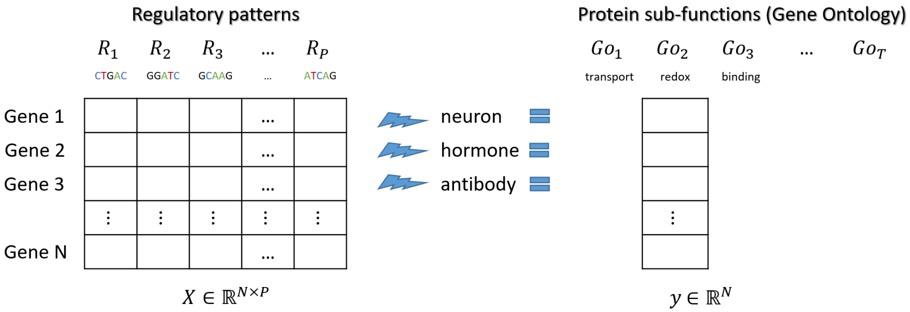
Goal 1: Predict each y_t from X



$X \in \mathbb{R}^{N \times P}$ $\quad$ $y = [y_1 \cdots y_T] \in \mathbb{R}^{N \times T}$

Goal 1: Predict each y_t from X

$\rightarrow$ to generalize: X and y are not only made of 0's and 1's



Goal 1: Predict y from X

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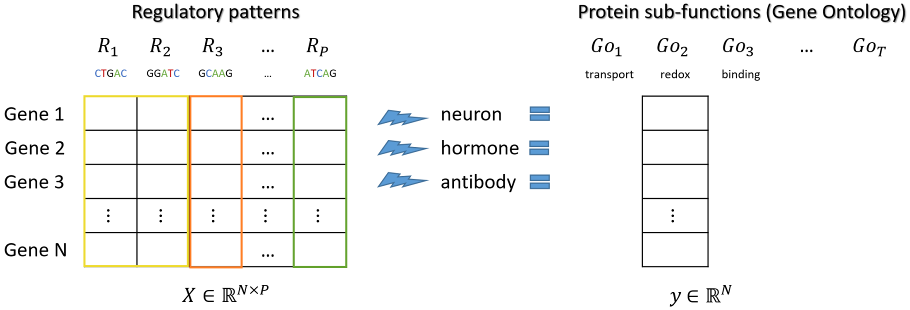
$\rightarrow$ to simplify: we first assume that $T = 1$ and omit the index t



Goal 1: Predict y from X

→ to generalize: X and y are not only made of 0's and 1's
→ to simplify: we first assume that $T = 1$ and omit the index t

Goal 2: Discover if there exist some groups in X
ex: R_1 and R_2 are both equally relevant to predict y

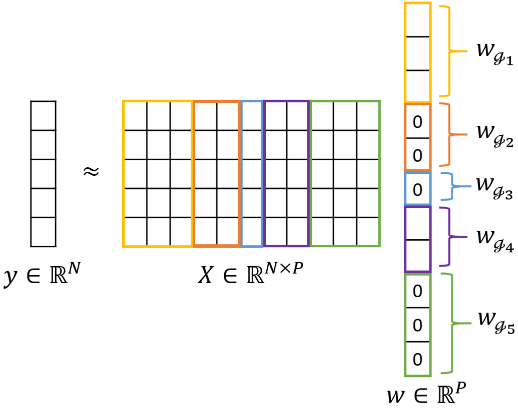
Model the observations

$\Longrightarrow$ linear model + Gaussian distribution: there exists w such that $y \sim \mathcal{N}(Xw, \sigma)$

Model the group structure

few groups of features in X are relevant to predict y

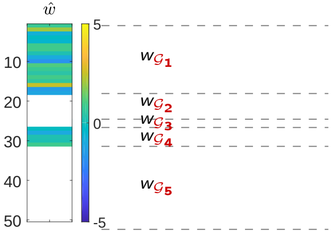
$\Longrightarrow$ group sparsity: some groups of variables in w are zero while others are non-zero



Optimization problem

Goal 1: Predict y from X Group Lasso [Yuan and Lin (2006)]

$$\hat{w}(\mathcal{G}_1, \dots, \mathcal{G}_L) = \underset{w \in \mathbb{R}^P}{\operatorname{argmin}} \underbrace{\frac{1}{2}\|y - Xw\|^2}_{\propto -\log p(y|Xw)} + \underbrace{\lambda \sum_{l=1}^{L} \|w_{\mathcal{G}_l}\|_2}_{\text{enforces structure}}$$



L partitions $\mathcal{G}_1, \dots, \mathcal{G}_L$ of P features

$$\mathcal{G}_l \subseteq \{1, \dots, P\}$$

$$\mathcal{G}_l \cap \mathcal{G}_{l'} = \emptyset \text{ if } l \neq l'$$

$$\cup_{l=1}^{L} \mathcal{G}_l = \{1, \dots, P\}$$

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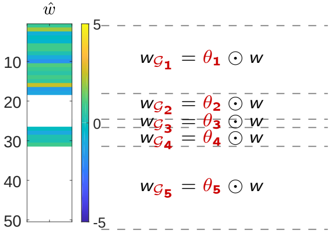
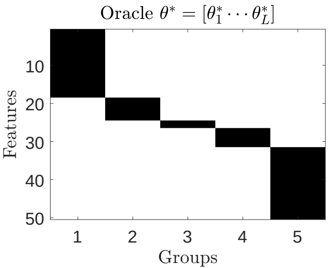


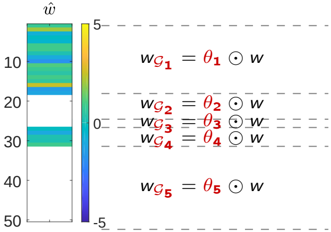


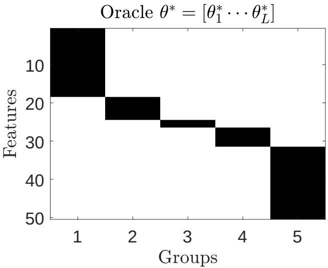
Mask $\theta_l = \{0,1\}^P$ of the l-th group

element-wise multiplication $\theta_l \odot w = [\theta_{l,1} w_1, \theta_{l,2} w_2, \ldots, \theta_{l,P} w_P]^\top$

Goal 1: Predict y from X Group Lasso [Yuan and Lin (2006)]

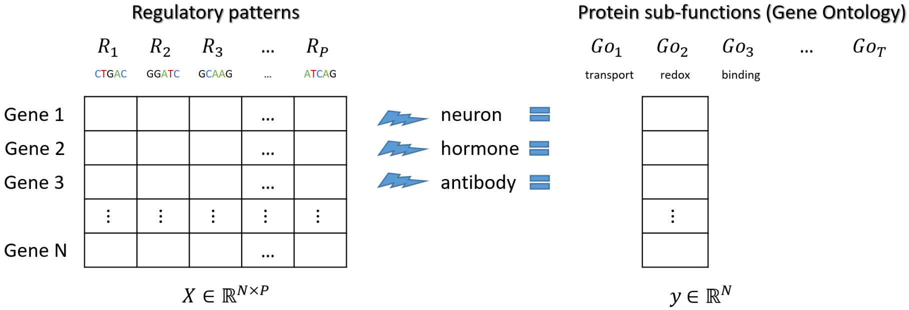
$$\hat{w}(\mathcal{G}_1, \ldots, \mathcal{G}_L) = \underset{w \in \mathbb{R}^P}{\text{argmin}} \; \underbrace{\frac{1}{2}\|y - Xw\|^2}_{\propto -\log p(y|Xw)} + \underbrace{\lambda \sum_{l=1}^{L} \|w_{\mathcal{G}_l}\|_2}_{\text{enforces structure}}$$





Goal 2: Discover the structure of X

$\Longrightarrow$ finding $\{\mathcal{G}_1, \ldots, \mathcal{G}_L\}$ $\Longleftrightarrow$ learning the hyperparameter $\theta = [\theta_1 \cdots \theta_L] \in \{0, 1\}^{P \times L}$



Goal 1: Predict y from X

$\rightarrow$ to generalize: X and y are not only made of 0's and 1's
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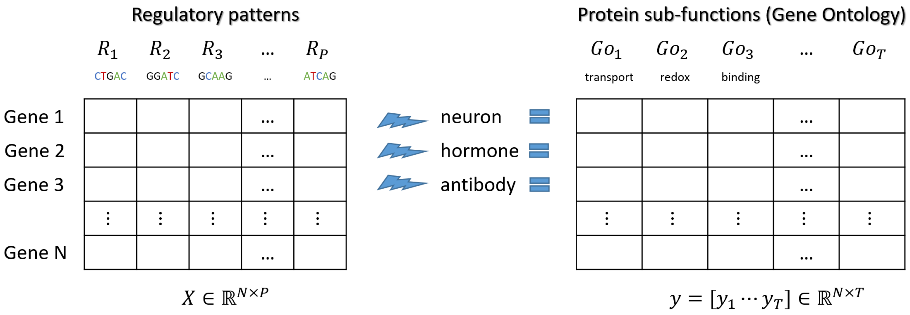
Reminder



Goal 1: Predict y from X

$\rightarrow$ to generalize: X and y are not only made of 0's and 1's

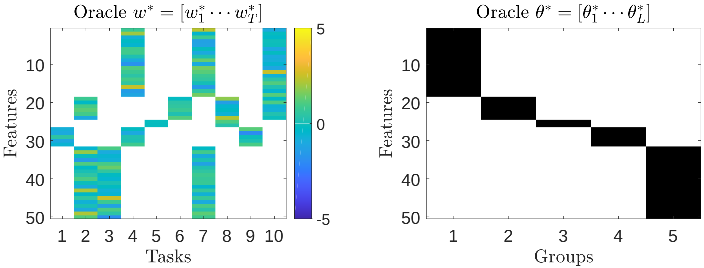
~~$\rightarrow$ to simplify: we first assume that $T = 1$ and omit the index t~~

Now we consider all T tasks

$$y \in \mathbb{R}^N \longrightarrow y \in \mathbb{R}^{N \times T}$$
$$w \in \mathbb{R}^P \longrightarrow w \in \mathbb{R}^{P \times T}$$

Multi-task setting : T tasks sharing the same group structure

$$(\forall t \in \{1, \ldots, T\}) \quad \hat{w}_t(\theta) \in \underset{w_t \in \mathbb{R}^P}{\operatorname{argmin}} \frac{1}{2}\|y_t - Xw_t\|^2 + \lambda \sum_{l=1}^{L} \|\theta_l \odot w_t\|_2,$$



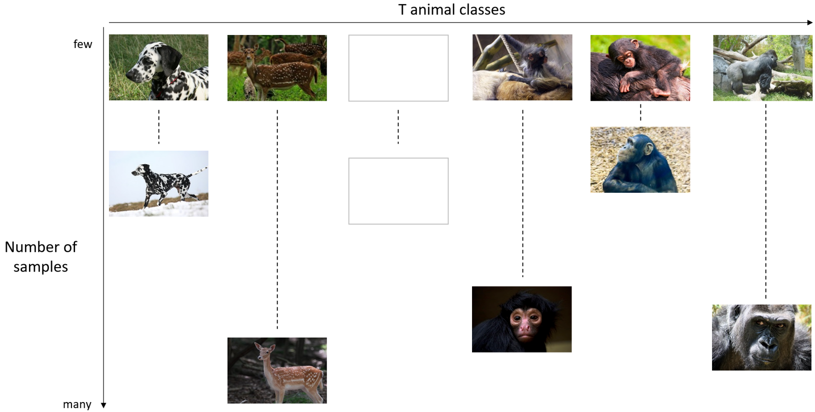
Some groups are relevant (non-zero) for some tasks and irrelevant (zero) for others

Example 2: Multi-task classification

Setting presented in

[Frecon et al. "Unveiling groups of related tasks in multi-task learning". ICPR (2020)]

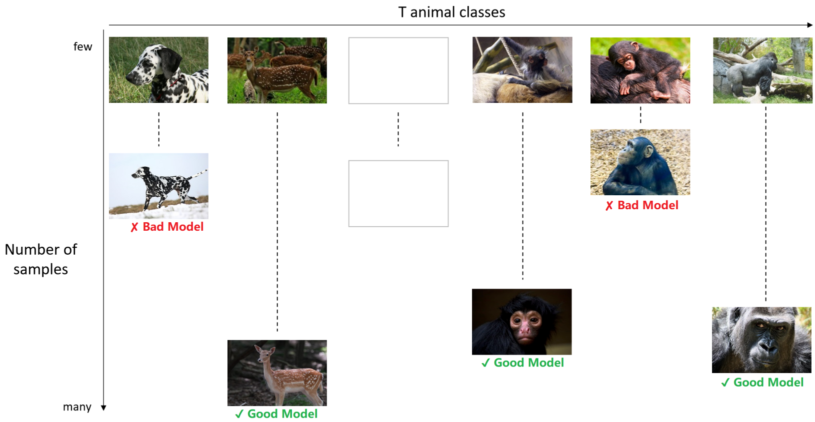
Motivation: animal recognition



$X \in \mathbb{R}^{N \times P}$ made of N vectorized image of P pixels
$y \in \mathbb{R}^{N \times T}$ such that $y_{i,t} = 1$ if X_i belongs to the t-th animal class, 0 otherwise.

Issue: some classes of animals with very few samples (e.g., dalmatians & chimpanzees)

Motivation: animal recognition

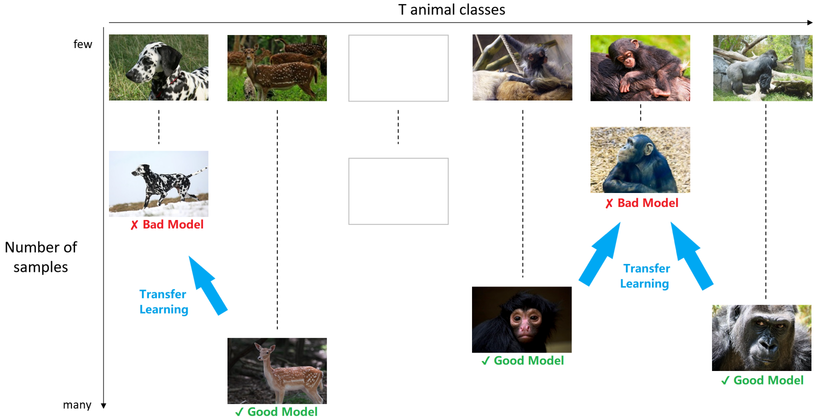


Naive idea: T binary classification tasks of one type of animal vs. all

logistic model: $(\forall t \in \{1, \dots, T\}), \exists w_t \in \mathbb{R}^P \mid y_t \sim \mathrm{Bernouilli}(p_t)$ with $p_t = \frac{1}{1+\exp(-Xw_t)}$

estimate $w_1, \dots, w_T \Rightarrow T$ independent binary logistic regressions

Motivation: animal recognition



Proposed idea: learn classifiers of similar animals jointly

logistic model: $(\forall t \in \{1, \ldots, T\}),\ \exists w_t \in \mathbb{R}^P \mid y_t \sim \mathrm{Bernouilli}(p_t)$ with $p_t = \frac{1}{1+\exp(-Xw_t)}$

estimate $w = [w_1 \cdots w_T] \Rightarrow$ Multi-task binary logistic regression

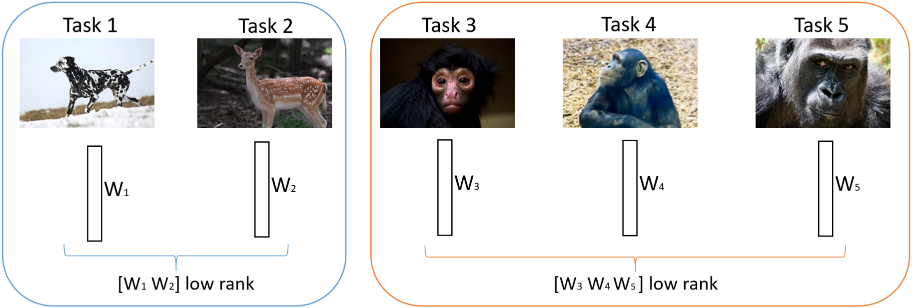
Model the observations

$$(\forall t \in \{1, \ldots, T\}),\ \exists w_t \in \mathbb{R}^P \mid y_t \sim \text{Bernouilli}(p_t) \text{ with } p_t = 1/(1 + \exp(-Xw_t))$$

Model task-relatedness

dalmatian (white + black spots) ≈ deer (brown + white spots)

$\Longrightarrow$ find $w_{\text{dalmatian}} \propto w_{\text{deer}}$ or more generally $[w_{\text{dalmatian}}\, w_{\text{deer}}]$ low-rank



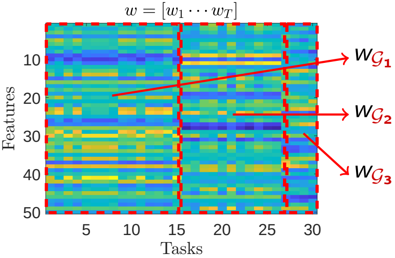
Group 1: "4 legs + spots"

Group 2: primates

Multi-task logistic regression: [Pong et al. (2010)] $\rightarrow$ here extended to L groups

$$\hat{w}(\mathcal{G}_1, \dots, \mathcal{G}_L) = \underset{w=[w_1 \cdots w_T]}{\operatorname{argmin}} \underbrace{\sum_{t=1}^{T} \log(1 - y_t \cdot X w_t)}_{\propto -\log p(y_t | X w_t)} + \lambda \underbrace{\sum_{l=1}^{L} \| w_{\mathcal{G}_l} \|_{\mathrm{tr}}}_{\text{enforces structure}}$$

Trace norm $\| \cdot \|_{\mathrm{tr}}$ = sum of singular values $\Rightarrow$ enforces low-rank



L partitions $\mathcal{G}_1, \dots, \mathcal{G}_L$ of T tasks

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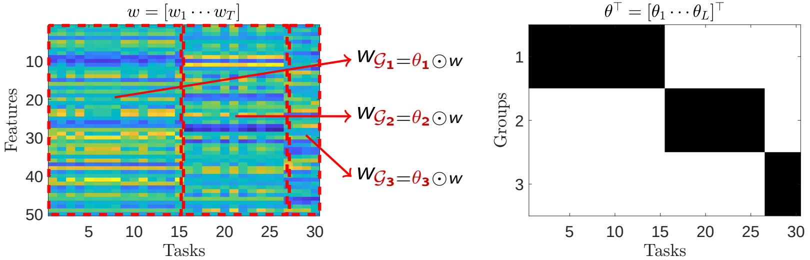

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Optimization problem

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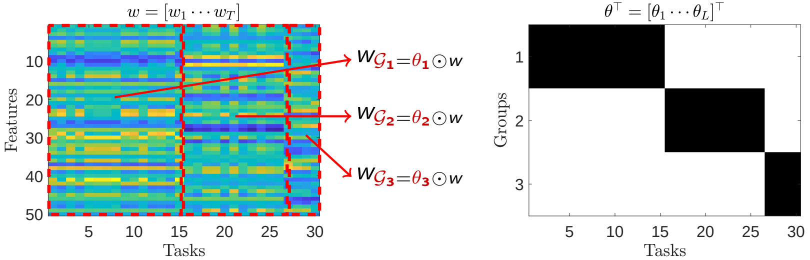

When the optimal groups are unknown

$\Longrightarrow$ find $\{\mathcal{G}_1,\dots,\mathcal{G}_L\}$ $\Longleftrightarrow$ learn the hyperparameter $\theta = [\theta_1 \cdots \theta_L] \in \{0,1\}^{T\times L}$

Disclaimer

These are **motivating** examples to introduce the optimization problems
In practice, it is more complex ...

See the work of practitioners:

- Gene expressions [Higuera et al., (2015)]
- Animals images [Lambert et al. (2009)]
- Brain signals [Sabbagh et al. (2019)]

Proposed Framework

Groupwise regularized optimization problem

In both examples, the prediction phase requires to solve

$$\hat{w}(\theta_1, \ldots, \theta_L) = \underset{w}{\operatorname{argmin}} \left\{ \mathcal{L}(w;\theta) \triangleq \underbrace{\ell(y, \langle X, w\rangle)}_{\substack{\text{enforces model} \\ \propto -\log p(y|Xw)}} + \underbrace{\sum_{l=1}^{L} \rho_l(\theta_l \odot w)}_{\text{enforces structure}} \right\}$$

The structure is :

- encapsulated into $\theta = [\theta_1 \cdots \theta_L]$
- applied by the bilinear mapping $\odot$
- enforced by the **norms** ρ_l

Given the parameter matrix $w \in \mathbb{R}^{P\times T}$ made of P features and T tasks

- Grouping features (1st example) $\theta_l \in \{0,1\}^P$ and $\sum_{l=1}^{L} \theta_l = \mathbb{1}_P$
- Grouping tasks (2nd example) $\theta_l \in \{0,1\}^T$ and $\sum_{l=1}^{L} \theta_l = \mathbb{1}_T$

Learning the group structure θ

In many scenarios, the group structure θ is unknown or partly known

$$\Downarrow$$

Learning θ to improve results

Issue: difficult combinatorial problem
the number of possible partitions grows exponentially with the dimension
$\Rightarrow$ trying them all is out of reach

Idea: relax and optimize

indicators/masks $\theta = [\theta_1 \dots \theta_L]$ $\xrightarrow{\text{relaxation}}$ **probabilities** $\theta = [\theta_1 \dots \theta_L] \in \Theta$ simplex

θ_l mask of group l — θ_l probability to belong to group l

$\theta_{l,i} \in \{0, 1\}$ — $\theta_{l,i} \in [0, 1]$

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θ_l mask of group l		θ_l probability to belong to group l
$\theta_{l,i} \in \{0, 1\}$		$\theta_{l,i} \in [0, 1]$

Optimizing the probabilities θ

We would like to find the groups $\theta \in \Theta$ such that the structured predictor

$$\hat{w}(\theta) = \operatorname*{argmin}_{w} \left\{ \mathcal{L}(w;\theta) \triangleq \ell(y, \langle X, w\rangle) + \sum_{l=1}^{L} \rho_l(\theta_l \odot w) \right\}$$

generalizes well to unseen data

Idea: Find θ such that $\hat{w}(\theta)$ minimizes the validation error $\mathcal{E}(\hat{w}(\theta)) = \ell(y^{\mathrm{val}}, \langle X^{\mathrm{val}}, \hat{w}(\theta)\rangle)$
$\Rightarrow$ type of continuous cross-validation

Bilevel Problem

$$\min_{\theta \in \Theta} \mathcal{E}(\hat{w}(\theta)) \qquad \text{s.t.} \qquad \hat{w}(\theta) = \operatorname*{argmin}_{w} \mathcal{L}(w;\theta)$$

Optimizing the probabilities θ

We would like to find the groups $\theta \in \Theta$ such that the structured predictor

$$\hat{w}(\theta) = \operatorname*{argmin}_{w} \Big\{ \mathcal{L}(w;\theta) \triangleq \underbrace{\ell(y, \langle X, w \rangle)}_{\text{training error}} + \sum_{l=1}^{L} \rho_l(\theta_l \odot w) \Big\}$$

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Bilevel Problem

$$\min_{\theta \in \Theta} \mathcal{E}(\hat{w}(\theta)) \qquad \text{s.t.} \qquad \hat{w}(\theta) = \operatorname*{argmin}_{w} \mathcal{L}(w;\theta)$$

Exact Problem

$$\min_{\theta\in\Theta} \left\{\mathcal{U}(\theta) \triangleq \mathcal{E}(\hat{w}(\theta))\right\}$$

$$\text{s.t.} \quad \hat{w}(\theta) = \operatorname*{argmin}_{w} \mathcal{L}(w;\theta)$$

$\hat{w}(\theta)$ without closed form

Bilevel Framework

Exact Problem

$$\min_{\theta \in \Theta} \left\{ \mathcal{U}(\theta) \triangleq \mathcal{E}(\hat{w}(\theta)) \right\}$$

$$\text{s.t.} \quad \hat{w}(\theta) = \operatorname*{argmin}_{w} \mathcal{L}(w; \theta)$$

$\hat{w}(\theta)$ without closed form

Approximate Problem

$$\min_{\theta \in \Theta} \left\{ \mathcal{U}^{(k)}(\theta) \triangleq \mathcal{E}(w^{(k)}(\theta)) \right\}$$

$$\text{s.t.} \quad \begin{array}{l} w^{(0)}(\theta) \text{ chosen arbitrarily} \\ \text{for } i = 0, \dots, k-1 \\ \lfloor \; w^{(i+1)}(\theta) = \mathcal{A}(w^{(i)}(\theta)) \\ w^{(k)}(\theta) \to \hat{w}(\theta) \end{array}$$

$\mathcal{U}^{(k)}$ smooth if $\mathcal{A}$ smooth

$\Downarrow$

choice of $\mathcal{A}$ discussed next

Exact Problem

$$\min_{\theta\in\Theta} \left\{\mathcal{U}(\theta) \triangleq \mathcal{E}(\hat{w}(\theta))\right\}$$

$$\text{s.t.} \quad \hat{w}(\theta) = \operatorname*{argmin}_{w} \mathcal{L}(w;\theta)$$

$\hat{w}(\theta)$ without closed form

Approximate Problem

$$\min_{\theta\in\Theta} \left\{\mathcal{U}^{(k)}(\theta) \triangleq \mathcal{E}(w^{(k)}(\theta))\right\}$$

s.t.
- $w^{(0)}(\theta)$ chosen arbitrarily
- for $i = 0, \dots, k-1$
  - $w^{(i+1)}(\theta) = \mathcal{A}(w^{(i)}(\theta))$
- $w^{(k)}(\theta) \to \hat{w}(\theta)$

$\mathcal{U}^{(k)}$ smooth if $\mathcal{A}$ smooth

$\theta^{(0)}$ chosen arbitrarily
for $n = 0, 1, \dots$
- $w^{(0)}(\theta^{(n)})$ chosen arbitrarily
- for $i = 0, \dots, k-1$ (inner algorithm)
  - $w^{(i+1)}(\theta^{(n)}) = \mathcal{A}(w^{(i)}(\theta^{(n)}))$
- $\theta^{(n+1)} = \mathrm{Proj}_\Theta(\theta^{(n)} - \gamma\nabla\mathcal{U}^{(k)}(\theta^{(n)}))$ where $\mathcal{U}^{(k)}(\theta^{(n)}) = \mathcal{E}(w^{(k)}(\theta^{(n)}))$

Algorithmic Solution

Optimization problem

$$\underset{w\in\mathbb{R}^P}{\text{minimize}} \;\; \underbrace{\frac{1}{2}\|y - Xw\|_2^2}_{f(w)\text{ differentiable}} + \underbrace{\lambda \sum_{l=1}^{L} \|\theta_l \odot w\|_2}_{g(A_\theta w)\text{ non differentiable}}$$

where $A_\theta : w \in \mathbb{R}^P \mapsto (\theta_1 \odot w, \ldots, \theta_L \odot w) \in \mathbb{R}^{P\times L}$

Forward-backward algorithm [Combettes and Wajs (2005)]

$$\left\{\begin{array}{l} \text{for } i = 0, \ldots, k-1 \\ \left\lfloor \; w^{(i+1)}(\theta) = \operatorname{prox}_{\beta g \circ A_\theta}\left(w^{(i)}(\theta) - \beta \nabla f(w^{(i)}(\theta))\right) \right. \end{array}\right.$$

proximity operator (prox) *?* $\longrightarrow$ *see next slide*

Group Lasso solver $\mathcal{A}$

Optimization problem

$$\underset{w\in\mathbb{R}^P}{\text{minimize}} \quad \underbrace{\frac{1}{2}\|y - Xw\|_2^2}_{f(w)\ \text{differentiable}} + \underbrace{\lambda\sum_{l=1}^{L}\|\theta_l \odot w\|_2}_{g(A_\theta w)\ \text{non differentiable}}$$

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proximity operator (prox) *?* $\longrightarrow$ *see next slide*

Proximity operator

In the 1960s, [Moreau (1962)] proposed an extension of the notion of projection operator to any convex function h, leading to the so-called proximity operator

$$\begin{aligned}\mathrm{Proj}_{\mathcal{C}}(v) &= \operatorname*{argmin}_{w \in \mathcal{C}} \frac{1}{2}\|w - v\|_2^2 \\ &= \operatorname*{argmin}_{w \in \mathbb{R}^P} \imath_{\mathcal{C}}(w) + \frac{1}{2}\|w - v\|_2^2 \quad \text{where} \quad \imath_{\mathcal{C}}(w) = \begin{cases} 0 & \text{if } w \in \mathcal{C} \\ +\infty & \text{otherwise} \end{cases}\end{aligned}$$

$$\mathrm{prox}_h(v) = \operatorname*{argmin}_{w \in \mathbb{R}^P} h(w) + \frac{1}{2}\|w - v\|_2^2$$

Group Lasso solver $\mathcal{A}$

Optimization problem

$$\underset{w \in \mathbb{R}^P}{\text{minimize}} \; \underbrace{\frac{1}{2}\|y - Xw\|_2^2}_{f(w)\text{ differentiable}} + \underbrace{\lambda \sum_{l=1}^{L} \|\theta_l \odot w\|_2}_{g(A_\theta w)\text{ non differentiable}}$$

where $A_\theta : w \in \mathbb{R}^P \mapsto (\theta_1 \odot w, \ldots, \theta_L \odot w) \in \mathbb{R}^{P \times L}$

Forward-backward algorithm [Combettes and Wajs (2005)]

$$\left\{ \begin{array}{l} \text{for } i = 0, \ldots, k-1 \\ \left\lfloor \; w^{(i+1)}(\theta) = \mathrm{prox}_{\beta g \circ A_\theta}\left(w^{(i)}(\theta) - \beta \nabla f(w^{(i)}(\theta))\right) \right. \end{array} \right.$$

generalization of projected gradient descent

projection $\longrightarrow$ proximity operator

$\mathrm{prox}_{\beta g \circ A_\theta}(v) = \underset{w \in \mathbb{R}^P}{\mathrm{argmin}} \; \beta g(A_\theta w) + \frac{1}{2}\|w - v\|_2^2$ ⚠ without closed form

Optimization problem

$$\underset{w \in \mathbb{R}^P}{\text{minimize}} \; \underbrace{\frac{1}{2}\|y - Xw\|_2^2}_{f(w) \text{ differentiable}} + \underbrace{\lambda \sum_{l=1}^{L} \|\theta_l \odot w\|_2}_{g(A_\theta w) \text{ non differentiable}}$$

where $A_\theta : w \in \mathbb{R}^P \mapsto (\theta_1 \odot w, \dots, \theta_L \odot w) \in \mathbb{R}^{P \times L}$

Forward-backward algorithm [Combettes and Wajs (2005)]

$$\left\{ \begin{array}{l} \text{for } i = 0, \dots, k-1 \\ \quad w^{(i+1)}(\theta) = \operatorname{prox}_{\beta g \circ A_\theta}\left(w^{(i)}(\theta) - \beta \nabla f(w^{(i)}(\theta))\right) \end{array} \right.$$

generalization of projected gradient descent

projection $\longrightarrow$ *proximity operator*

$$\operatorname{prox}_{\beta g \circ A_\theta}(v) = \underset{w \in \mathbb{R}^P}{\operatorname{argmin}} \; \beta g(A_\theta w) + \frac{1}{2}\|w - v\|_2^2$$ ⚠ without closed form

Duality in convex optimization

The ideas of duality and transforms are ubiquitous in mathematics

- Harmonics analysis $\to$ Fourier transform
- Convex analysis $\to$ Fenchel conjugate: $h^*(x) = \sup_w \langle w, x\rangle - h(w)$

[Rockafellar (1970)]

Example: $h\colon w \mapsto \|w\|_2 \implies h^*\colon x \mapsto \imath_{\mathcal{B}(1)}(x) = \begin{cases} 0 & \text{if } \|x\|_2 \leq 1 \\ +\infty & \text{otherwise} \end{cases}$

Duality in convex optimization

The ideas of duality and transforms are ubiquitous in mathematics

- Harmonics analysis $\rightarrow$ Fourier transform
- Convex analysis $\rightarrow$ Fenchel conjugate: $h^*(x) = \sup_w \langle w, x \rangle - h(w)$

[Rockafellar (1970)]

Example: $h\colon w \mapsto \lambda \|w\|_2 \quad \Rightarrow \quad h^*: x \mapsto \imath_{\mathcal{B}(\lambda)}(x) = \begin{cases} 0 & \text{if } \|x\|_2 \leq \lambda \\ +\infty & \text{otherwise} \end{cases}$

The ideas of duality and transforms are ubiquitous in mathematics

- Harmonics analysis $\rightarrow$ Fourier transform
- Convex analysis $\rightarrow$ Fenchel conjugate: $h^*(x) = \sup_w \langle w, x\rangle - h(w)$

[Rockafellar (1970)]

Primal problem $\longleftrightarrow$ **Dual problem**

$$\underset{w\in\mathbb{R}^P}{\text{minimize}}\ f(w) + g(A_\theta w)$$

$$A_\theta : \mathbb{R}^P \rightarrow \mathbb{R}^{P\times L}$$

$$g(v_1 \ldots v_L) = \sum_{l=1}^{L} \underbrace{\lambda\|v_l\|_2}_{\text{norm}}$$

$$\underset{u\in\mathbb{R}^{P\times L}}{\text{minimize}}\ f^*(-A_\theta^\top u) + g^*(u)$$

$$A_\theta^\top : \mathbb{R}^{P\times L} \rightarrow \mathbb{R}^P$$

$$g^*(u_1 \ldots u_L) = \sum_{l=1}^{L} \underbrace{\imath_{\mathcal{B}(\lambda)}(u_l)}_{\substack{\text{indicator}\\ \text{dual norm ball}}}$$

Link

$$w = \nabla f^*(-A_\theta^\top u)$$

$\mathrm{prox}_{g\circ A_\theta}$ without closed form $\Rightarrow$ solve dual problem to move A_θ in smooth part

Dual problem

$$\underset{u\in\mathbb{R}^{P\times L}}{\text{minimize}} \; \underbrace{f^*(-A_\theta^\top u)}_{\text{differentiable}} + \underbrace{g^*(u)}_{\text{non differentiable}}$$

Dual forward-backward algorithm

$$\begin{cases} \text{for } i = 0, \ldots, k-1 \\ \quad \big\lfloor \; u^{(i+1)}(\theta) = \mathrm{prox}_{\beta g^*}\left(u^{(i)}(\theta) + \beta A_\theta \nabla f^*(-A_\theta^\top u^{(i)}(\theta))\right) \\ w^{(k)}(\theta) = \nabla f^*(-A_\theta^* u^{(k)}(\theta)) \qquad \textbf{(link)} \end{cases}$$

Dual problem

$$\underset{u\in\mathbb{R}^{P\times L}}{\text{minimize}}\ \underbrace{f^*(-A_\theta^\top u)}_{\text{differentiable}} + \underbrace{g^*(u)}_{\text{non differentiable}}$$

Dual forward-backward algorithm

$$\begin{cases} \text{for } i = 0,\ldots,k-1 \\ \quad \left\lfloor\ u^{(i+1)}(\theta) = \operatorname{prox}_{\beta g^*}\left(u^{(i)}(\theta) + \beta A_\theta \nabla f^*(-A_\theta^\top u^{(i)}(\theta))\right) \right. \\ w^{(k)}(\theta) = \nabla f^*(-A_\theta^* u^{(k)}(\theta)) \qquad \textbf{(link)} \end{cases}$$

where the proximal operator reads:

$$\begin{aligned} \operatorname{prox}_{\beta g^*}(v) &= \underset{u\in\mathbb{R}^{P\times L}}{\operatorname{argmin}}\ \beta g^*(u) + \frac{1}{2}\|u-v\|^2 \\ &= \underset{u\in\mathbb{R}^{P\times L}}{\operatorname{argmin}}\ \beta \sum_{l=1}^{L} \imath_{\mathcal{B}(\lambda)}(u_l) + \frac{1}{2}\|u-v\|^2 \\ &= \operatorname{Proj}_{\mathcal{B}(\lambda)^L}(v) \end{aligned}$$

⚠ not differentiable

$\theta^{(0)}$ chosen arbitrarily
for $n = 0, 1, \ldots$
  $w^{(0)}(\theta^{(n)})$ chosen arbitrarily
  for $i = 0, \ldots, k-1$ (inner algorithm = dual forward-backward)
    $w^{(i+1)}(\theta^{(n)}) = \mathcal{A}(w^{(i)}(\theta^{(n)}))$
  $\theta^{(n+1)} = \mathrm{Proj}_\Theta(\theta^{(n)} - \gamma \nabla \mathcal{U}^{(k)}(\theta^{(n)}))$ where $\mathcal{U}^{(k)}(\theta^{(n)}) = \mathcal{E}(w^{(k)}(\theta^{(n)}))$

We want a differentiable dual forward-backward algorithm
because it inside a bilevel algorithm !

Group Lasso solver $\mathcal{A}$: dual approach

Dual forward-backward algorithm

$$\begin{cases} \text{for } i = 0, \ldots, k-1 \\ \quad \left\lfloor \; u^{(i+1)}(\theta) = \mathrm{prox}_{\beta g^*}\big(\quad u^{(i)}(\theta) \; + \beta A_\theta \nabla f^*(-A_\theta^\top u^{(i)}(\theta))\big) \right. \\ w^{(k)}(\theta) = \nabla f^*(-A_\theta u^{(k)}(\theta)). \end{cases}$$

where

$$\begin{aligned} \mathrm{prox}_{\beta g^*}(v) &= \underset{u \in \mathbb{R}^{P \times L}}{\mathrm{argmin}}\, \beta g^*(u) + \frac{1}{2}\|u - v\|^2 \\ &= \underset{u \in \mathbb{R}^{P \times L}}{\mathrm{argmin}}\, \beta g^*(u) + \frac{1}{2}\|u\|^2 - \langle u, v \rangle + \mathrm{cst} \end{aligned}$$

Group Lasso solver $\mathcal{A}$: dual approach

Dual forward-backward algorithm

$$\begin{cases} \text{for } i = 0, \ldots, k-1 \\ \quad \left\lfloor \; u^{(i+1)}(\theta) = \operatorname{prox}_{\beta g^*}\left(\quad u^{(i)}(\theta) \;\; + \beta A_\theta \nabla f^*(-A_\theta^\top u^{(i)}(\theta))\right) \right. \\ w^{(k)}(\theta) = \nabla f^*(-A_\theta u^{(k)}(\theta)). \end{cases}$$

where

$$\operatorname{prox}_{\beta g^*}(v) = \underset{u \in \mathbb{R}^{P \times L}}{\operatorname{argmin}} \, \beta g^*(u) + \frac{1}{2}\|u\|^2 - \langle u, v \rangle + \text{cst}$$

Dual forward-backward algorithm with Bregman distances [Bauschke et al. (2016)]

$$\begin{cases} \text{for } i = 0, \dots, k-1 \\ \left\lfloor \; u^{(i+1)}(\theta) = \operatorname{prox}^{\Phi}_{\beta g^*}\big(\nabla\Phi(u^{(i)}(\theta)) + \beta A_\theta \nabla f^*(-A_\theta^\top u^{(i)}(\theta))\big) \right. \\ w^{(k)}(\theta) = \nabla f^*(-A_\theta u^{(k)}(\theta)). \end{cases}$$

where the Bregman proximal operator associated to Φ :

$$\operatorname{prox}^{\Phi}_{\beta g^*}(v) = \underset{u \in \mathbb{R}^{P \times L}}{\operatorname{argmin}}\, \beta g^*(u) + \Phi(u) - \langle u, v \rangle$$

Choice of Φ to smooth the updates

Dual forward-backward algorithm with Bregman distances

$$\left\{\begin{array}{l} \text{for } i = 0, \ldots, k-1 \\ \left\lfloor \; u^{(i+1)}(\theta) = \mathrm{prox}^{\Phi}_{\beta g^*}\big(\nabla\Phi(u^{(i)}(\theta)) + \beta A_\theta \nabla f^*(-A_\theta^\top u^{(i)}(\theta))\big) \right. \\ w^{(k)}(\theta) = \nabla f^*(-A_\theta u^{(k)}(\theta)). \end{array}\right.$$

where

$$\mathrm{prox}^{\Phi}_{\beta g^*}(v) = \underset{u\in\mathbb{R}^{P\times L}}{\mathrm{argmin}}\, \beta g^*(u) + \Phi(u) - \langle u, v\rangle$$

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where

$$\mathrm{prox}^{\Phi}_{\beta g^*}(v) = \underset{u\in\mathbb{R}^{P\times L}}{\mathrm{argmin}} \sum_{l=1}^{L} \imath_{\mathcal{B}(\lambda)}(u_l) + \Phi(u) - \langle u, v\rangle$$

Choice of Φ to smooth the updates

Dual forward-backward algorithm with Bregman distances

$$\begin{cases} \text{for } i = 0, \ldots, k-1 \\ \left\lfloor \; u^{(i+1)}(\theta) = \mathrm{prox}^{\Phi}_{\beta g^*}\big(\nabla\Phi(u^{(i)}(\theta)) + \beta A_\theta \nabla f^*(-A_\theta^\top u^{(i)}(\theta))\big) \right. \\ w^{(k)}(\theta) = \nabla f^*(-A_\theta u^{(k)}(\theta)). \end{cases}$$

where

$$\mathrm{prox}^{\Phi}_{\beta g^*}(v) = \underset{u \in \mathbb{R}^{P \times L}}{\mathrm{argmin}} \sum_{l=1}^{L} \big(\imath_{\mathcal{B}(\lambda)}(u_l) + \phi(u_l) - \langle u_l, v_l \rangle\big)$$

for $\Phi(u) = \sum_{l=1}^{L} \phi(u_l)$

Choice of Φ to smooth the updates

Dual forward-backward algorithm with Bregman distances

$$\begin{cases} \text{for } i = 0, \ldots, k-1 \\ \lfloor \; u^{(i+1)}(\theta) = \operatorname{prox}^{\Phi}_{\beta g^*}\left(\nabla\Phi(u^{(i)}(\theta)) + \beta A_\theta \nabla f^*(-A_\theta^\top u^{(i)}(\theta))\right) \\ w^{(k)}(\theta) = \nabla f^*(-A_\theta u^{(k)}(\theta)). \end{cases}$$

where

$$\operatorname{prox}^{\Phi}_{\beta g^*}(v) = \underset{u \in \mathbb{R}^{P \times L}}{\operatorname{argmin}} \sum_{l=1}^{L} \left(\imath_{\mathcal{B}(\lambda)}(u_l) - \sqrt{\lambda^2 - \|u_l\|^2} - \langle u_l, v_l \rangle \right)$$

for $\phi(u_l) = -\sqrt{\lambda^2 - \|u_l\|^2} \Rightarrow \operatorname{dom}\phi = \mathcal{B}(\lambda)$

$\Rightarrow \imath_{\mathcal{B}(\lambda)}(u_l)$ always equal to 0 !

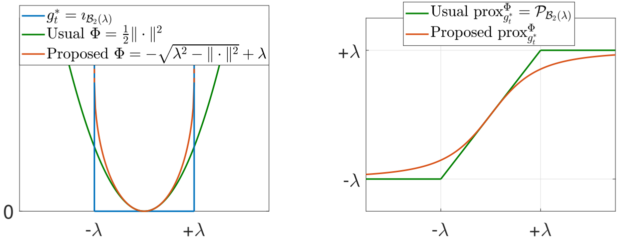
⚠ **trick for a differentiable algorithm**

Dual forward-backward algorithm with Bregman distances

$$
\begin{cases}
\text{for } i = 0, \ldots, k-1 \\
\quad \left\lfloor \; u^{(i+1)}(\theta) = \mathrm{prox}^{\Phi}_{\beta g^*}\left(\nabla\Phi(u^{(i)}(\theta)) + \beta A_\theta \nabla f^*(-A_\theta^\top u^{(i)}(\theta))\right) \right. \\
w^{(k)}(\theta) = \nabla f^*(-A_\theta u^{(k)}(\theta)).
\end{cases}
$$

where

$$
\mathrm{prox}^{\Phi}_{\beta g^*}(v) = \left(\frac{\lambda v_l}{\sqrt{1 + \|v_l\|_2^2}} \right)_{l=1,\ldots,L}
$$



Convergence $w^{(k)}(\theta) \to \hat{w}(\theta)$

Theorem 1: For every $\theta \in \Theta$, $\|w^{(k)}(\theta) - \hat{w}(\theta)\|^2 \leq \dfrac{\text{Const}}{k}$

Convergence "$\mathcal{U}^{(k)}(\theta) \to \mathcal{U}(\theta)$"

Theorem 2: Assume that Θ is a non-empty compact subset of $\mathbb{R}_+^{P\times L}$. If the iterates $\{\mathrm{w}^{(k)}(\theta)\}_{k\in\mathbb{N}}$ converge to $\hat{\mathrm{w}}(\theta)$ uniformly in Θ when $k \to +\infty$, then

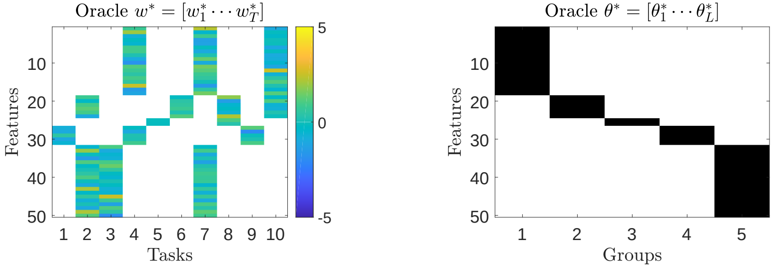
$$\inf_{\theta\in\Theta} \mathcal{U}^{(k)}(\theta) \underset{k\to+\infty}{\longrightarrow} \inf_{\theta\in\Theta} \mathcal{U}(\theta) \qquad \text{and} \qquad \underset{\theta\in\Theta}{\operatorname{argmin}}\ \mathcal{U}^{(k)}(\theta) \underset{k\to+\infty}{\longrightarrow} \underset{\theta\in\Theta}{\operatorname{argmin}}\ \mathcal{U}(\theta)$$

Reminder : $$\begin{cases} \mathcal{U}(\theta) & = \mathcal{E}(\hat{w}(\theta)) \\ \mathcal{U}^{(k)}(\theta) & = \mathcal{E}(\hat{w}^{(k)}(\theta)) \end{cases}$$

Numerical Experiments

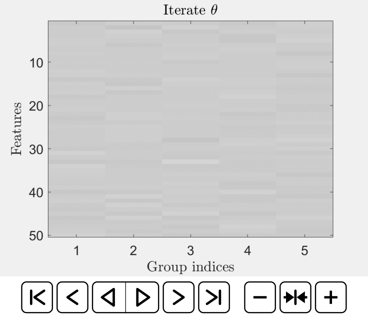
Setting: $T = 500$ tasks, $N = 25$ noisy observations, $P = 50$ parameters.

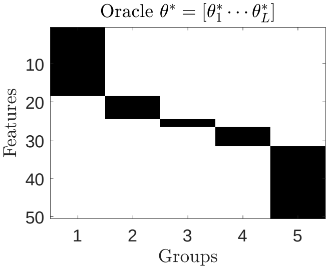
Goal: Estimate and group the parameters



$$y_t = X_t w_t^* + \epsilon_t \quad \text{where} \quad \epsilon_t \sim \mathcal{N}(0, \sigma = 0.1)$$

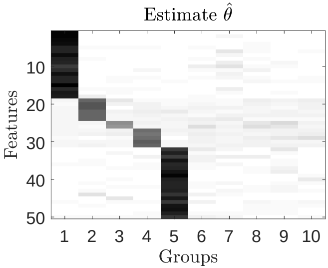
Result

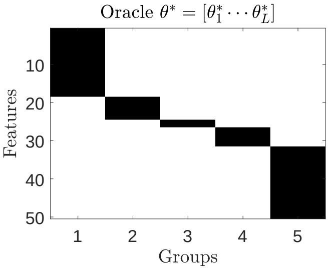




Recover the correct groups ! (just different ordering)

When the number of groups is unknown





Works even when the number of groups is unknown !

Conclusion

Conclusion

1. Define structured predictor with groups θ

$$\hat{w}(\theta) = \underset{w}{\operatorname{argmin}}\, \mathcal{L}(w; \theta)$$

2. **Ideal:** find groups θ such that $\hat{w}(\theta)$ minimizes the validation error

$$\min_{\theta \in \Theta} \mathcal{E}(\hat{w}(\theta)) \quad \text{s.t.} \quad \hat{w}(\theta) = \underset{w}{\operatorname{argmin}}\, \mathcal{L}(w; \theta)$$

3. **Practice:** solve a differentiable bilevel problem

$$\min_{\theta \in \Theta} \mathcal{E}(w^{(k)}(\theta)) \quad \text{s.t.} \quad \begin{array}{l} w^{(0)}(\theta) \text{ chosen arbitrarily} \\ \text{for } i = 0, \ldots, k-1 \\ \lfloor \; w^{(i+1)}(\theta) = \mathcal{A}(w^{(i)}(\theta)) \end{array} \qquad \text{with } \mathcal{A} \text{ differentiable}$$

What is next

1. More complex structures (overlapping, hierarchical, ...)
2. New multi-task models to transfer learning
3. Theoretical guarantees for bilevel optimization (global minima, convergence rate, ...)

Thank you

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What is next (theoretical guarantees)

Exact problem

$$\min_{\theta\in\Theta} \left\{\mathcal{U}(\theta) \triangleq \mathcal{E}(\hat{w}(\theta))\right\}$$

s.t. $\hat{w}(\theta) = \operatorname*{argmin}_{w\in\mathcal{W}} \mathcal{L}(w;\theta)$

Approximate problem

$$\min_{\theta\in\Theta} \left\{\mathcal{U}^{(k)}(\theta) \triangleq \mathcal{E}(w^{(k)}(\theta))\right\}$$

s.t. $w^{(0)}(\theta)$ chosen arbitrarily

for $i = 0, \ldots, k-1$

$\lfloor\; w^{(i+1)}(\theta) = \mathcal{A}(w^{(i)}(\theta))$

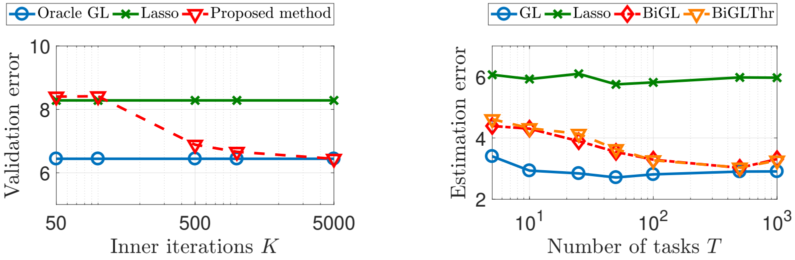
$w^{(k)}(\theta) \to \hat{w}(\theta)$

$$\theta^{(n+1)} = \mathrm{Proj}_\Theta(\theta^{(n)} - \mu\nabla\mathcal{U}^{(k)}(\theta^{(n)}))$$

- $\inf_{\theta\in\Theta} \mathcal{U}^{(k)}(\lambda) \xrightarrow[k\to+\infty]{} \inf_{\theta\in\Theta} \mathcal{U}(\lambda)$ ✓
- $\operatorname*{argmin}_{\theta\in\Theta} \mathcal{U}^{(k)}(\lambda) \xrightarrow[k\to+\infty]{} \operatorname*{argmin}_{\theta\in\Theta} \mathcal{U}(\lambda)$ ✓
- Efficient computation of $\nabla\mathcal{U}^{(k)}$ ✓

- Impact of warm-restart on $w^{(0)}$?
- $\lim_{k\to\infty} \nabla\mathcal{U}^{(k)}(\theta) \in \partial\mathcal{U}(\theta)$?
- $\lim_{n\to\infty} \theta^{(n)} \in \partial\mathcal{U}^{-1}(0)$?

Reminder : $[w_1^{(k)}(\theta) \cdots w_T^{(k)}(\theta)] \to [\hat{w}_1(\theta) \cdots \hat{w}_T(\theta)]$



(GL) group Lasso with oracle groups
(Lasso) Lasso
(BiGL) proposed method

Convergence of the upper iterates

Convergence to a stationary point

Theorem 3: For $\bar{n}$ uniformly sampled in $\{1, \ldots, n_{\max}\}$:

$$\mathbb{E}\left[\|G_\gamma(\theta^{(\bar{n})})\|^2\right] \leq \frac{\text{Const}}{n_{\max}},$$

where G_γ with step-size γ

$$G_\gamma(\theta) = \frac{1}{\gamma}\left(\theta - \mathcal{P}_\Theta(\theta - \gamma \nabla \mathcal{U}^{(k)}(\theta)\right)$$

Intuition : Without the projection, $G_\gamma(\theta) = \nabla \mathcal{U}^{(k)}(\theta)$

$$\begin{cases} u^{(0)}(\theta) \in \mathcal{H} \\ \text{for } i = 0, \dots, k-1 \\ \left\lfloor \; u^{(i+1)}(\theta) = \mathcal{A}(u^{(i)}(\theta), \theta) \right. \\ w^{(k)}(\theta) = \mathcal{B}(u^{(k)}(\theta), \theta), \end{cases} \tag{1}$$

we get

$$\nabla \mathcal{U}^{(k)}(\theta) = (u^{(k)})'(\theta)^\top \partial_1 \mathcal{B}(u^{(k)}(\theta), \theta)^\top \nabla C(w^{(k)}(\theta)) + \partial_2 \mathcal{B}(u^{(k)}(\theta), \theta)^\top \nabla C(w^{(k)}(\theta)). \tag{2}$$

Moreover, using the updating rule for $u^{(i)}(\theta)$ in (1) we have

$$(u^{(i+1)})'(\theta) = \partial_1 \mathcal{A}(u^{(i)}(\theta), \theta)(u^{(i)})'(\theta) + \partial_2 \mathcal{A}(u^{(i)}(\theta), \theta). \tag{3}$$

Setting $A_1^{(i)}(\theta) = \partial_1 \mathcal{A}(u^{(i)}(\theta), \theta)$ and $A_2^{(i)}(\theta) = \partial_2 \mathcal{A}(u^{(i)}(\theta), \theta)$, we have

$$(u^{(i+1)})'(\theta)^\top = (u^{(i)})'(\theta)^\top A_1^{(i)}(\theta)^\top + A_2^{(i)}(\theta)^\top. \tag{4}$$

Then, by combining the two equations above we have

$$\begin{aligned}
\nabla\mathcal{U}^{(k)}(\theta) &= (u^{(k)})'(\theta)^\top \partial_1\mathcal{B}(u^{(k)}(\theta),\theta)^\top \nabla C(w^{(k)}(\theta)) + \partial_2\mathcal{B}(u^{(k)}(\theta),\theta)^\top \nabla C(w^{(k)}(\theta)) \\
&= (u^{(k-1)})'(\theta)^\top A_1^{(k-1)}(\theta)^\top \underbrace{\partial_1\mathcal{B}(u^{(k)}(\theta),\theta)^\top \nabla C(w^{(k)}(\theta))}_{a_Q} \\
&\quad + A_2^{(k-1)}(\theta)^\top \underbrace{\partial_1\mathcal{B}(u^{(k)}(\theta),\theta)^\top \nabla C(w^{(k)}(\theta))}_{a_k} + \underbrace{\partial_2\mathcal{B}(u^{(k)}(\theta),\theta)^\top \nabla C(w^{(k)}(\theta))}_{b_k} \\
&= (u^{(k-1)})'(\theta)^\top \underbrace{A_1^{(k-1)}(\theta)^\top a_k}_{a_{k-1}} + \underbrace{A_2^{(k-1)}(\theta)^\top a_k + b_k}_{b_{k-1}} \\
&= (u^{(k-2)})'(\theta)^\top \underbrace{A_1^{(k-2)}(\theta)^\top a_{k-1}}_{a_{k-2}} + \underbrace{A_2^{(k-2)}(\theta)^\top a_{k-1} + b_{k-1}}_{b_{k-2}} \\
&= \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\
&= \underbrace{A_2^{(0)}(\theta)^\top a_1 + b_1}_{b_0},
\end{aligned}$$

where in the last line we used that $u^{(0)}(\theta)$ is constant.

State-of-the-art: joint optimization [Kang et al. (2011), Kshirsagar et al. (2017).]

$$(\hat{w}, \hat{\theta}) = \operatorname*{argmin}_{w,\theta\in\Theta} \left\{ \mathcal{L}(w;\theta) \triangleq \ell(y, \langle X, w\rangle) + \sum_{l=1}^{L} \rho_l(\theta_l \odot w) \right\}$$

issues: some trivial undesired minima
unclear interpretation of the solution

Proposed method: bilevel optimization [Frecon et al. (2018), Frecon et al. (2020).]

$$\min_{\theta\in\Theta} \mathcal{E}(\hat{w}(\theta)) \qquad \text{s.t.} \qquad \hat{w}(\theta) = \operatorname*{argmin}_{w} \mathcal{L}(w;\theta)$$

idea: find θ such that $\hat{w}(\theta)$ generalizes well to unseen data
$\rightarrow$ choose $\mathcal{E}$ as the validation error