Dual Averaging Method for Online Graph-structured Sparsity

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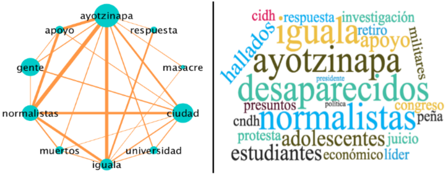
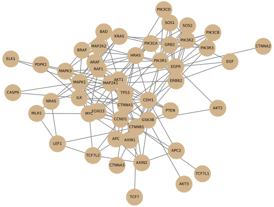
Graph data is everywhere!

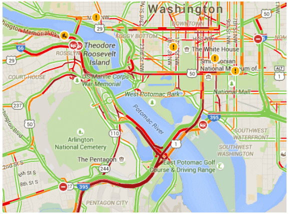
Social network



Keywords graph of social event



PPI network

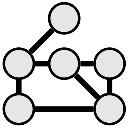


Transport network

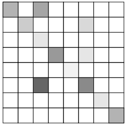
Motivation

We often encounter the following learning scenario:

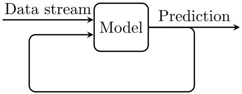
- Data samples $\{\boldsymbol{x}_t, y_t\}$ are available on the fly: at each round, the model makes a prediction based on current input sample.
- Data dimension is high, but only a small part of features is important. This small part of features is graph-structured (connectivity, density, etc) based on the graph information.



Graph-structured



Sparse



Online

Research Question

How do we learn such graph-structured sparse models under online setting ?

Problem Formulation

Under online learning setting, at each time t, the learner

1. receives question $\boldsymbol{x}_t \in \mathbb{R}^p$ and makes a prediction
2. receives a loss $f_t(\boldsymbol{w}_t, \{\boldsymbol{x}_t, y_t\})$ after true label y_t is revealed
3. updates $\boldsymbol{w}_t$

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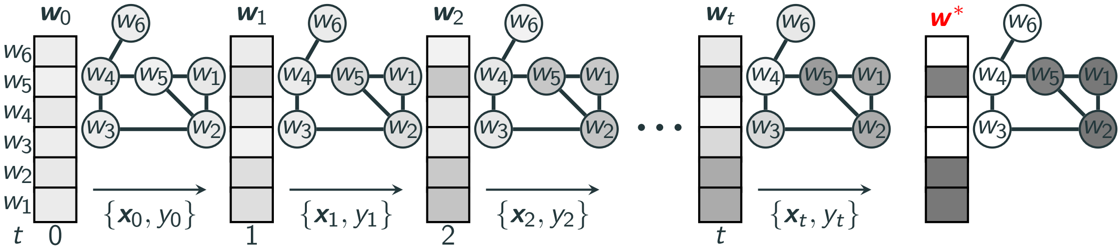

$\boldsymbol{w}^*$ is graph-structured (e.g. connectivity)!

Problem Formulation

Minimize the regret subject to a graph-structured sparsity constraint

$$R(T) := \sum_{t=1}^{T} \left\{ f_t(\boldsymbol{w}_t, \{\boldsymbol{x}_t, y_t\}) \right\} - \min_{\boldsymbol{w} \in \mathcal{M}(\mathbb{M})} \sum_{t=1}^{T} \left\{ f_t(\boldsymbol{w}, \{\boldsymbol{x}_t, y_t\}) \right\}$$

- Regret
- Accumulated Loss
- Minimum Loss in hindsight
- Graph-structured sparsity set $\mathcal{M}(\mathbb{M})$

First Try: Online Projected Gradient Descent(PGD)

The online PGD algorithm updates $\boldsymbol{w}_t$ as the following

$$\boldsymbol{w}_{t+1} = \mathrm{P}(\boldsymbol{w}_t - \eta_t \nabla f_t\left(\boldsymbol{w}_t, \{\boldsymbol{x}_t, y_t\}\right), \mathcal{M}(\mathbb{M}))$$

First Try: Online Projected Gradient Descent(PGD)

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It hardly works due to **two main drawbacks**

1. It is unable to exploit the problem structure.
2. The new information is vanishing as steps $\eta_t \to 0$.

Challenge: Can we exploit the problem structure more effectively ?

Yes: exploit the structure via the dual space

Inspired by dual avaraging [Xiao, 2010], our method updates $\boldsymbol{w}_t$ as the following

$$\boldsymbol{w}_{t+1} = \arg\min_{\boldsymbol{w} \in \mathcal{M}(\mathbb{M})} \left\{ \left\langle \frac{1}{t+1} \sum_{i=0}^{t} \boldsymbol{g}_i, \boldsymbol{w} \right\rangle + \frac{1}{2\sqrt{t}} \|\boldsymbol{w}\|^2 \right\},$$

- $\boldsymbol{g}_i \in \partial f_i(\boldsymbol{w}_i, \{\boldsymbol{x}_i, y_i\})$, each gradient is equivalently important
- $\frac{1}{t+1} \sum_{i=0}^{t} \boldsymbol{g}_i$ the average of the previous gradients — Dual Averaging
- tie-breaking rule: break ties arbitrarily

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How to solve this minimization problem ?

Main Theorem

Our method updates $\boldsymbol{w}_t$ as the following

$$\boldsymbol{w}_{t+1} = \operatorname*{arg\,min}_{\boldsymbol{w}\in\mathcal{M}(\mathbb{M})} \left\{ \left\langle \frac{1}{t+1}\sum_{i=0}^{t} \boldsymbol{g}_i, \boldsymbol{w} \right\rangle + \frac{1}{2\sqrt{t}}\|\boldsymbol{w}\|^2 \right\}.$$

Denote the dual averaging $\bar{\boldsymbol{s}}_{t+1} = \frac{1}{t+1}\sum_{i=0}^{t} \boldsymbol{g}_i$, it can be expressed two equivalent problems:

$$\textbf{Problem 1}: \min_{S\in\mathbb{M}} \| -\sqrt{t}\bar{\boldsymbol{s}}_{t+1} - P(-\sqrt{t}\bar{\boldsymbol{s}}_{t+1}, S)\|^2.$$

$$\textbf{Problem 2}: \max_{S\in\mathbb{M}} \|P(-\sqrt{t}\bar{\boldsymbol{s}}_{t+1}, S)\|^2$$

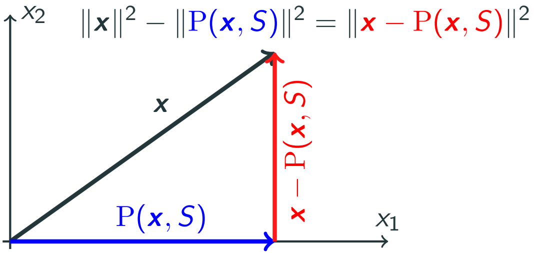
Theorem Insight: Problem 1

The original minimization problem can be equivalently expressed as

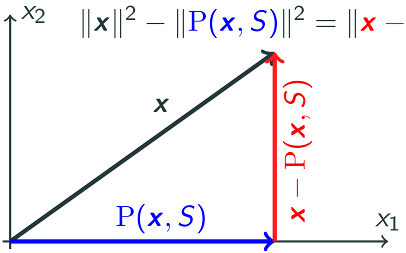
$$\begin{aligned}\boldsymbol{w}_{t+1} &= \arg\min_{\boldsymbol{w}\in\mathcal{M}(\mathbb{M})} \left\{ \langle \bar{\boldsymbol{s}}_{t+1}, \boldsymbol{w} \rangle + \frac{1}{2\sqrt{t}} \|\boldsymbol{w}\|^2 \right\} \\ &= \arg\min_{\boldsymbol{w}\in\mathcal{M}(\mathbb{M})} \left\| \boldsymbol{w} - \left(-\sqrt{t}\bar{\boldsymbol{s}}_{t+1} \right) \right\|^2,\end{aligned}$$

Each step is essentially a projection !

Theorem Insight: Problem 2



Theorem Insight: Problem 2



Step 1: Let $\boldsymbol{x} := -\sqrt{t}\bar{\boldsymbol{s}}_{t+1}$ and add min to both sides

$$\min_{S \in \mathbb{M}} \left\{ \|\boldsymbol{x}\|^2 - \|\mathrm{P}(\boldsymbol{x}, S)\|^2 \right\} = \min_{S \in \mathbb{M}} \|\boldsymbol{x} - \mathrm{P}(\boldsymbol{x}, S)\|^2.$$

Step 2: Move min into the negative term

$$\|\boldsymbol{x}\|^2 + \max_{S \in \mathbb{M}} \|\mathrm{P}(\boldsymbol{x}, S)\|^2 = \min_{S \in \mathbb{M}} \|\boldsymbol{x} - \mathrm{P}(\boldsymbol{x}, S)\|^2.$$

Online Graph Dual Averaging Algorithm

GraphDA

Input: $\mathbb{M}$

$\bar{\boldsymbol{s}}_0 = \boldsymbol{0}, \boldsymbol{w}_0 = \boldsymbol{0}$

for $t = 0, 1, 2, \ldots$ **do**

  receive $\{\boldsymbol{x}_t, y_t\}$ and make prediction

  compute $\boldsymbol{g}_t = \nabla f_t(\boldsymbol{w}_t, \{\boldsymbol{x}_t, y_t\})$

  $\bar{\boldsymbol{s}}_{t+1} = \bar{\boldsymbol{s}}_t + \boldsymbol{g}_t$

  $\boldsymbol{b}_{t+1} = \mathrm{P}(\bar{\boldsymbol{s}}_{t+1}, \mathbb{M})$

  $\boldsymbol{w}_{t+1} = \mathrm{P}(-\sqrt{t}\boldsymbol{b}_{t+1}, \mathbb{M})$

end for

Online Graph Dual Averaging Algorithm

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>
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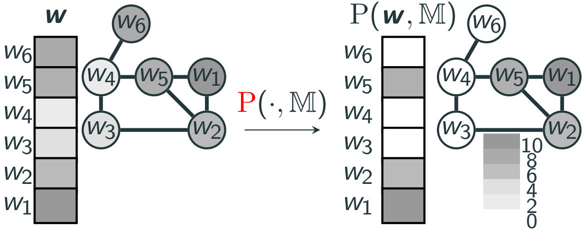
>
> $\boldsymbol{w}_{t+1} = \mathrm{P}(-\sqrt{t}\boldsymbol{b}_{t+1}, \mathbb{M})$
>
> **end for**

Let $\mathbb{M} = \{S : |S| \leq 3, S \text{ is connected }\}$. Finding a connected subgraph up to 3 nodes.



Graph Projection Operator [Hegde et al., 2015]

What if the graph information is not available ?

DA-IHT

1: **Input**: $\mathbb{M}$
2: $\bar{\boldsymbol{s}}_0 = \mathbf{0}$, $\boldsymbol{w}_0 = \mathbf{0}$
3: **for** $t = 0, 1, 2, \ldots$ **do**
4: receive $\{\boldsymbol{x}_t, y_t\}$ and make a prediction
5: compute $\boldsymbol{g}_t = \nabla f_t(\boldsymbol{w}_t, \{\boldsymbol{x}_t, y_t\})$
6: $\bar{\boldsymbol{s}}_{t+1} = \bar{\boldsymbol{s}}_t + \boldsymbol{g}_t$
7: $\boldsymbol{b}_{t+1} = \mathrm{H}(\bar{\boldsymbol{s}}_{t+1}, \mathbb{M})$
8: $\boldsymbol{w}_{t+1} = \mathrm{H}(-\sqrt{t}\boldsymbol{b}_{t+1}, \mathbb{M})$
9: **end for**

What if the graph information is not available ?

DA-IHT

Input: $\mathbb{M}$
$\bar{\boldsymbol{s}}_0 = \mathbf{0}, \boldsymbol{w}_0 = \mathbf{0}$
for $t = 0, 1, 2, \ldots$ **do**
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  $\bar{\boldsymbol{s}}_{t+1} = \bar{\boldsymbol{s}}_t + \boldsymbol{g}_t$
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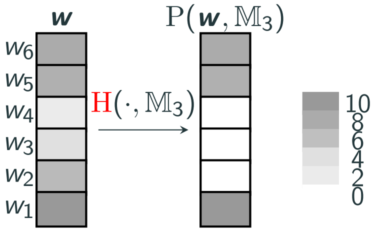
  $\boldsymbol{w}_{t+1} = \mathrm{H}(-\sqrt{t}\boldsymbol{b}_{t+1}, \mathbb{M})$
end for

Let $\mathbb{M}_3 = \{S : |S| \leq 3\}$. Sorting the magnitudes of $\boldsymbol{w}$ and thresholding entries out of top s to zero.



Hard Thresholding Operator

Time Complexity and Regret

The time complexity of GraphDA mainly depends on two projections. If we use the weighted-graph model, the per-iteration time cost could be

- non-sparse graph: $\mathcal{O}(p + |\mathbb{E}| \log^3(p))$ **Edge-dependent**
- sparse graph: $\mathcal{O}(p + p \log^3(p))$ **Nearly-linear !**

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- sparse graph: $\mathcal{O}(p + p \log^3(p))$ **Nearly-linear !**

If $\mathcal{M}(\mathbb{M})$ is a **convex set**, then

- The regret can be bounded as: $R(T, \mathcal{M}(\mathbb{M})) = C \cdot \mathcal{O}(\sqrt{T})$, where C is a constant.
- If we assume further that the loss is strongly convex, then $\|\boldsymbol{w}_T - \boldsymbol{w}^*\|_2^2 = \mathcal{O}(\frac{\ln T}{T})$.

If $\mathcal{M}(\mathbb{M})$ is a **nonconvex set**, can we still obtain a non-regret bound ?

Experimental setup

We compare GraphDA with baseline methods by using three datasets.

Method	Proposed in
Adam	Kingma and Ba [2014]
ℓ_1-RDA	Xiao [2010]
DA-GL	Yang et al. [2010]
DA-SGL	Yang et al. [2010]
AdaGrad	Duchi et al. [2011]
StoIHT	Nguyen et al. [2017]
GraphStoIHT	Zhou et al. [2019]
DA-IHT	**This paper**
GraphDA	**This paper**

Dataset	$\lvert\mathbb{V}\rvert$	$\lvert\mathbb{E}\rvert$
Benchmark	1,089	2,112
MNIST	786	1,516
KEGG	5,372	78,545

- non-sparse
- sparse: convex-based
- sparse: nonconvex-based

Two questions

Compared with baseline methods, we aim to answer the following two questions:

- **Q1:** Can GraphDA achieve better classification performance ?
- **Q2:** Can GraphDA learn a stronger interpretable model by capturing meaningful graph-structured features ?

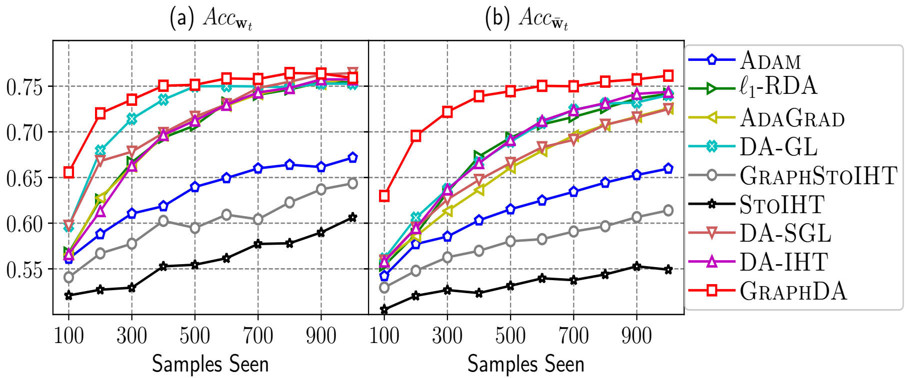
Application 1: event classification on Benchmark dataset

Given the training dataset $\{\boldsymbol{x}_i \in \mathbb{R}^p, y_i \in \{\pm 1\}\}_{i=1}^{t}$ on the fly

- $y_t = -1$: no event ("business-as-usual");
- $y_t = +1$: event: disease outbreak/computer virus etc.

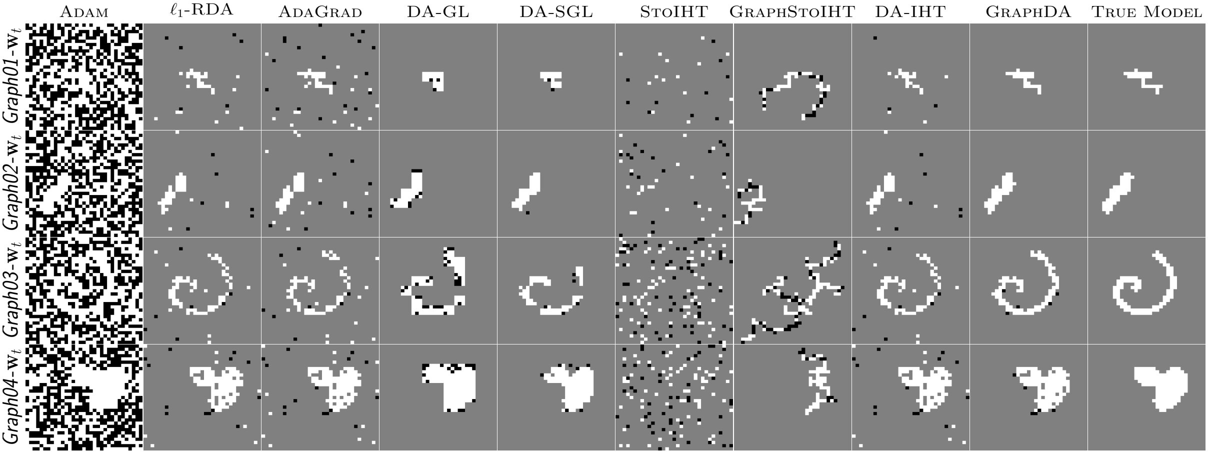
Task: To classify these samples online and at the same time to find the hidden structure on these events!

GraphDA has higher classification accuracy



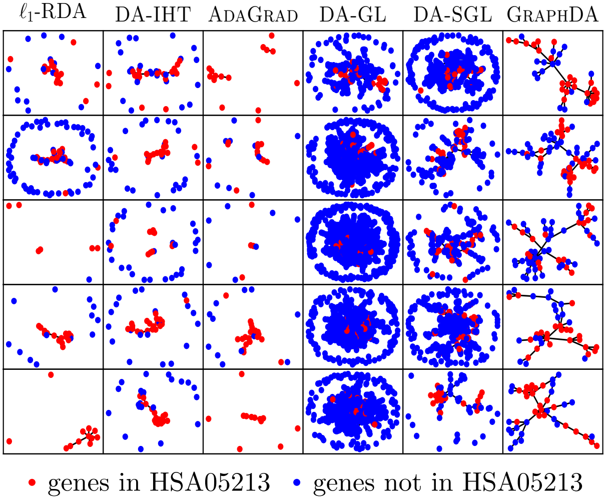
- Online PGD-based: StoIHT and GraphStoIHT **do not work!**
- Online DA-based: ℓ_1-RDA,DA-GL,DA-SGL and DA-IHT work well.
- GraphDA outperforms other DA-based with the help of graph priors.

GraphDA learns more interpretable models

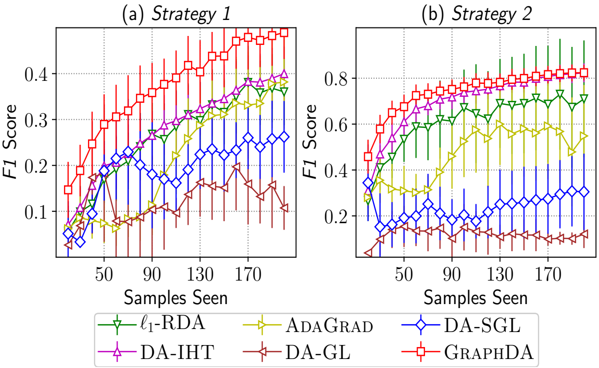


Black dots: $(\boldsymbol{w}_t)_i < 0$; Gray $(\boldsymbol{w}_t)_i = 0$; White dots $(\boldsymbol{w}_t)_i > 0$

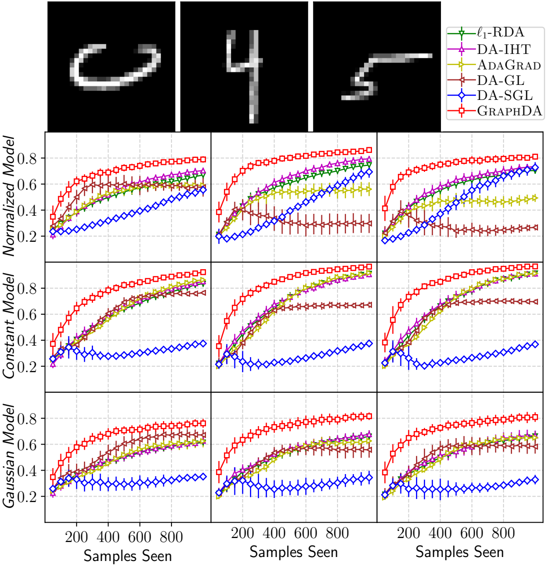
Application 2: gene identification on KEGG dataset



$$F1_{\boldsymbol{w}_t} = \frac{2|\mathrm{supp}(\boldsymbol{w}^*) \cap \mathrm{supp}(\boldsymbol{w}_t)|}{|\mathrm{supp}(\boldsymbol{w}^*)| + |\mathrm{supp}(\boldsymbol{w}_t)|}$$



GraphDA learns more cancer-related genes and more structures (edges).



Use the least square loss $f_t(\boldsymbol{w}_t, \{\boldsymbol{x}_t, y_t\}) = (y_t - \langle \boldsymbol{w}_t, \boldsymbol{x}_t \rangle)^2$.

Samples are generated by using the following linear relation: $y_t = \langle \boldsymbol{x}_t, \boldsymbol{w}^* \rangle$, where $\boldsymbol{x}_t \in \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$. We use three different strategies to obtain $\boldsymbol{w}^*$.

Task: To learn the structure of $\boldsymbol{w}^*$!

Summary

Conclusion

- We propose a dual averaging-based method, GraphDA, for online graph-structured sparsity constraint problems.
- We prove that the minimization problem in the dual averaging step can be formulated as two equivalent optimization problems.
- GraphDA achieves better classification performance and stronger interpretability.

Summary

Conclusion

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- We prove that the minimization problem in the dual averaging step can be formulated as two equivalent optimization problems.
- GraphDA achieves better classification performance and stronger interpretability.

Future work

- Does GraphDA have non-regret bound under some proper assumption ?
- What if true structure of features are time evolving ?

Thank you!

Q & A

Code and datasets: https://github.com/baojianzhou/graph-da

Install GraphDA: **pip install sparse-learn**

Roadmap

- Motivation
- Problem Formulation
- Proposed Algorithm
- Experimental Results
- Conclusion

Implementation Details

Algorithm 1 Head/Tail Projection ($\mathrm{P}(\boldsymbol{w}, \mathbb{M})$) Hegde et al. [2015]

Input: $\boldsymbol{w}, max\_iter, \mathbb{M} = (\mathbb{G}(\mathbb{V}, \mathbb{E}, \boldsymbol{c}), s_l, s_h, g)$
$\boldsymbol{\pi} = \boldsymbol{w} \cdot \boldsymbol{w}$ // vector dot product, i.e., $\pi_i = w_i * w_i$
$\lambda_l = 0, \lambda_h = \max\{\pi_1, \pi_2, \ldots, \pi_p\}$, $\lambda_m = 0$, $t = 0$
repeat
    $\lambda_m = (\lambda_l + \lambda_h)/2$; $\boldsymbol{c}_m = \lambda_m \cdot \boldsymbol{c}$ // scale dot product, i.e., $(\boldsymbol{c}_m)_i = \lambda_m * c_i$
    $\mathcal{F} = \mathrm{PCST}(\mathbb{G}(\mathbb{V}, \mathbb{E}, \boldsymbol{c}_m), \boldsymbol{\pi}, g)$
    if $s_l < |\mathcal{F}| < s_h$ **then** **return** $\boldsymbol{w}_{\mathcal{F}}$;
    if $|\mathcal{F}| > s_h$ **then** $\lambda_l = \lambda_m$ **else** $\lambda_h = \lambda_m$;
    $t = t + 1$
until $t >$ max_iter
$\boldsymbol{c}_h = \lambda_h \cdot \boldsymbol{c}$; $\mathcal{F} = \mathrm{PCST}(\mathbb{G}(\mathbb{V}, \mathbb{E}, \boldsymbol{c}_h), \boldsymbol{\pi}, g)$;
return $\boldsymbol{w}_{\mathcal{F}}$

The code is written in C language with the standard C11.

How to choose the sparsity

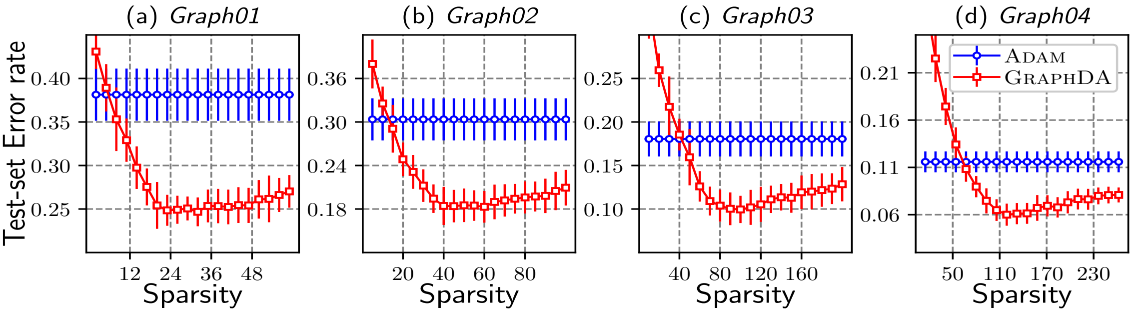


Figure: Test dataset error rates as a function of sparsity s

Parameter Tuning

- ℓ_1-RDA
  - regularization: $\lambda \in \{0.0001, 0.0005, 0.001, 0.005, 0.01, 0.03, 0.05, 0.1, 0.3, 0.5, 1, 3, 5, 10\}$.
  - learning rate (implicit): $\gamma \in \{1, 5, 1e1, 5e1, 1e2, 5e2, 1e3, 5e3, 1e4\}$
  - sparsity-enhancing:
    $\rho \in \{0.0, 0.00001, 0.00005, 0.0001, 0.0005, 0.001, 0.005, 0.01, 0.05, 0.1, 0.5, 1\}$
- Adam
  - $\beta_1 = 0.9, \beta_2 = 0.999, \epsilon = 10^{-8}$
  - $\alpha \in \{0.0001, 0.0005, 0.001, 0.005, 0.01, 0.05, 0.1, 0.5\}$.
- DA-GL/SGL
  - $\lambda \in \{0.0001, 0.0005, 0.001, 0.005, 0.01, 0.03, 0.05, 0.1, 0.3, 0.5, 1, 3, 5, 1e1\}$
  - $\gamma \in \{1, 5, 1e1, 5e1, 1e2, 5e2, 1e3, 5e3, 1e4\}$
  - 3×3 grids as groups for Benchmark dataset.
  - 2×2 grids for MNIST dataset.

Parameter Tuning

- AdaGrad
  - $\lambda \in \{0.0001, 0.0005, 0.001, 0.005, 0.01, 0.03, 0.05, 0.1, 0.3, 0.5, 1, 3, 5, 1e1\}$
  - $\eta \in \{0.0001, 0.0005, 0.001, 0.005, 0.01, 0.05, 0.1, 0.5, 1.0, 5.0, 1e1, 5e1, 1e2, 5e2, 1e3, 5e3\}$.
- StoIHT
  - sparsity $s \in \{5, 10, \ldots, 150\}$
  - $\gamma \in \{1, 5, 1e1, 5e1, 1e2, 5e2, 1e3, 5e3, 1e4\}$
- GraphStoIHT/GraphDA
  - sparsity $s \in \{5, 10, \ldots, 150\}$
  - $\gamma \in \{1, 5, 1e1, 5e1, 1e2, 5e2, 1e3, 5e3, 1e4\}$

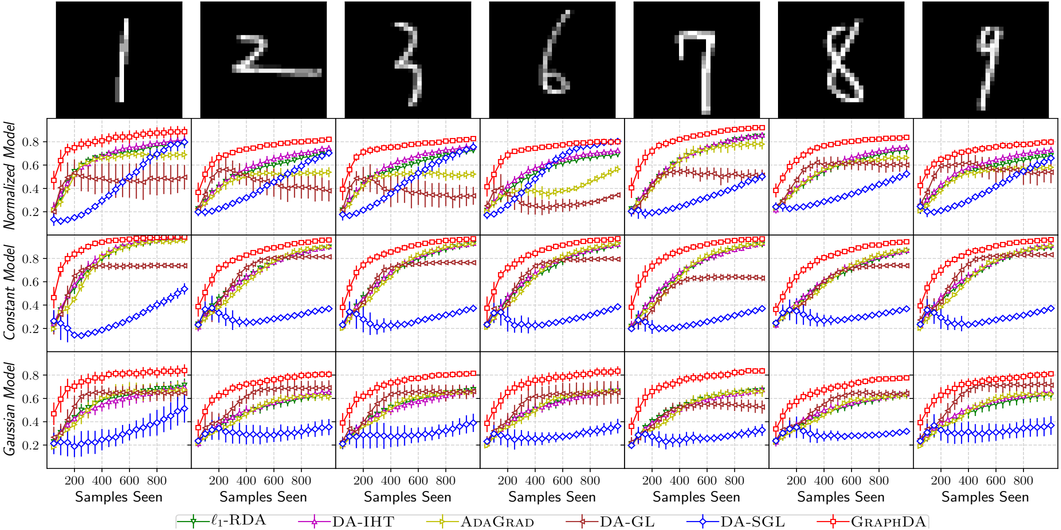
Classification Performance

$$Pre_{\boldsymbol{w}_t} = \frac{|\text{supp}(\boldsymbol{w}^*) \cap \text{supp}(\boldsymbol{w}_t)|}{|\text{supp}(\boldsymbol{w}_t)|},\ Rec_{\boldsymbol{w}_t} = \frac{|\text{supp}(\boldsymbol{w}^*) \cap \text{supp}(\boldsymbol{w}_t)|}{|\text{supp}(\boldsymbol{w}^*)|} F1_{\boldsymbol{w}_t} = \frac{2|\text{supp}(\boldsymbol{w}^*) \cap \text{supp}(\boldsymbol{w}_t)|}{|\text{supp}(\boldsymbol{w}^*)| + |\text{supp}(\boldsymbol{w}_t)|},\ \text{NR}_{\boldsymbol{w}} = \frac{|\text{supp}(\boldsymbol{w})|}{p}.$$

Method	$Pre_{\boldsymbol{w}_t}$	$Rec_{\boldsymbol{w}_t}$	$F1_{\boldsymbol{w}_t}$	$AUC_{\boldsymbol{w}_t, \bar{\boldsymbol{w}}_t}$	$Acc_{\boldsymbol{w}_t, \bar{\boldsymbol{w}}_t}$	$Miss_{\boldsymbol{w}_t, \bar{\boldsymbol{w}}_t}$	$NR_{\boldsymbol{w}_t, \bar{\boldsymbol{w}}_t}$
ADAM	0.024	**1.000**	0.047	(0.618, 0.603)	(0.619, 0.603)	(166.35, 173.10)	(100.0%, 100.0%)
ℓ_1-RDA	0.267	0.863	0.389	(0.693, 0.672)	(0.694, 0.673)	(155.30, 166.05)	(11.58%, 83.60%)
ADAGRAD	0.256	0.877	0.379	(0.696, 0.636)	(0.696, 0.637)	(156.00, 166.00)	(11.33%, 100.0%)
DA-GL	0.176	0.967	0.283	(0.735, 0.666)	(0.735, 0.667)	(142.90, 162.20)	(15.99%, 100.0%)
DA-SGL	0.523	0.854	0.506	(0.699, 0.647)	(0.699, 0.647)	(151.00, 165.50)	(25.54%, 100.0%)
STOIHT	0.057	0.150	0.072	(0.552, 0.523)	(0.553, 0.523)	(194.55, 195.25)	(7.79%, 40.62%)
GRAPHSTOIHT	0.151	0.356	0.194	(0.603, 0.570)	(0.602, 0.570)	(174.65, 181.40)	(7.84%, **22.06**%)
DA-IHT	0.507	0.744	0.566	(0.697, 0.666)	(0.697, 0.666)	(155.65, 162.85)	(4.35%, 39.50%)
GRAPHDA	**0.869**	0.906	**0.880**	(**0.749**, **0.739**)	(**0.749**, **0.739**)	(**133.45**, **136.20**)	(**2.56**%, 32.12%)

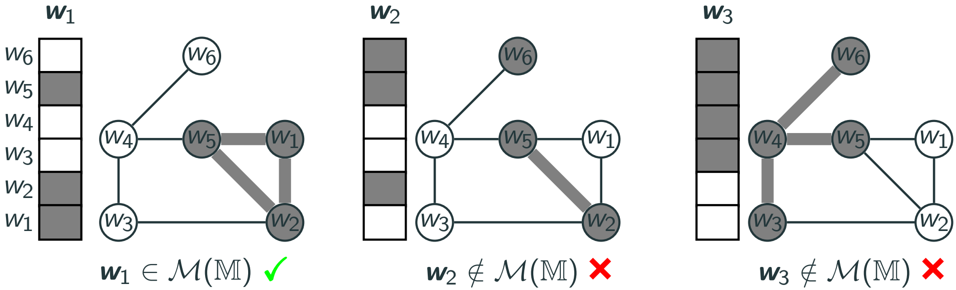
Online Graph Sparse Linear Regression

F1 score as a function of samples seen (2nd to 4th row) on seven handwritten digits.



$\mathcal{M}(\mathbb{M})$— A toy example

$\mathcal{M}(\mathbb{M}) := \{\boldsymbol{w} | \text{supp}(\boldsymbol{w}) \in \mathbb{M}\}$ where $\mathbb{M} := \{S | \mathbb{G}(S, \mathbb{E}') \text{ is connected subgraph up to size 3.}\}$



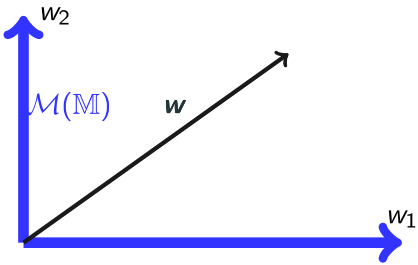
At each time t, we need $\mathbb{G}(\text{supp}(\boldsymbol{w}_t), \mathbb{E}')$ is connected and $|\text{supp}(\boldsymbol{w}_t)| \leq 3$.

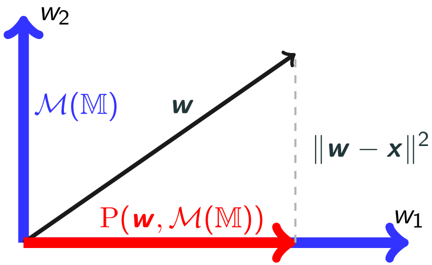
Projection explanation

How can we make sure $\boldsymbol{w}_t$ is in $\mathcal{M}(\mathbb{M})$? **Projection!**

The projection onto $\mathcal{M}(\mathbb{M})$ is defined as

$$\mathrm{P}(\boldsymbol{w}, \mathcal{M}(\mathbb{M})) = \arg\min_{\boldsymbol{x} \in \mathcal{M}(\mathbb{M})} \|\boldsymbol{w} - \boldsymbol{x}\|^2.$$





Online Mirror Descent

Algorithm 2 OMD(Online Mirror Descent [Hazan et al., 2016])

Input: η, $R(\boldsymbol{x}), B_R(\boldsymbol{x}, \boldsymbol{y}), \mathcal{K}$
let $\boldsymbol{y}_1$ be such that $\nabla R(\boldsymbol{y}_1) = 0$ and $\boldsymbol{x}_1 = \arg\min_{\boldsymbol{x}\in\mathcal{K}} B_R(\boldsymbol{x}, \boldsymbol{y}_1)$
for $t = 0, 1, 2, \ldots$ **do**
    update $\boldsymbol{y}_t$ by rule $\nabla R(\boldsymbol{y}_{t+1}) = \nabla R(\boldsymbol{y}_t) - \eta \nabla f_t(\boldsymbol{x}_t)$
    projection step $\boldsymbol{x}_{t+1} = \arg\min_{\in\mathcal{K}} B_R(\boldsymbol{x}, \boldsymbol{y}_{t+1})$
end for

- $R(\boldsymbol{x})$ is a Legendre Function (1. strictly convex; 2. has continuous first order derivatives; and 3. $\lim_{\boldsymbol{x}\to\bar{\mathcal{K}}\setminus\mathcal{K}} \|\nabla R(\boldsymbol{x}) = +\infty$).
- $B_R(\boldsymbol{x}, \boldsymbol{y}) = R(\boldsymbol{x}) - R(\boldsymbol{y}) - \langle \boldsymbol{x} - \boldsymbol{y}, \nabla F(\boldsymbol{y})\rangle$
- Online Mirror Descent is a generalized version of Online PGD.
- When $R(\boldsymbol{x}) = \frac{1}{2}\langle \boldsymbol{x}, \boldsymbol{x}\rangle$, OMD is exactly the same as Online PGD.

Regret (Continue)

Open problems: Provided the GraphDA algorithm,

- Can we obtain a non-regret bound under some condition ?
- What are the conditions ?

References

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