Statistical Learning and Scalability of Additive Models with Total Variation Regularization

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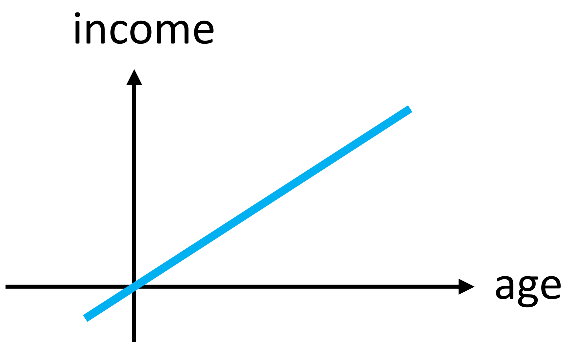
New In ML 2019

The First Group Session for Newcomers to Machine Learning

Motivation

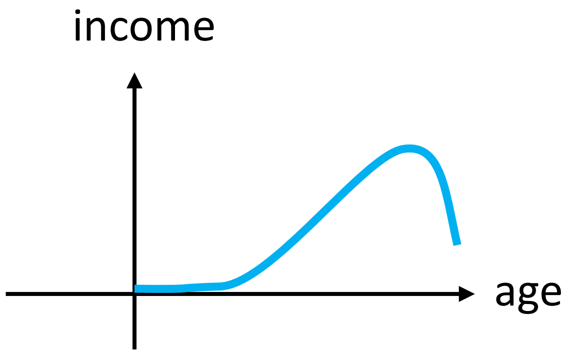
- Given dataset $(\mathbf{x}_i, y_i)_{i=1..m}, \mathbf{x}_i \in \mathbb{R}^p$
- Linear models

$$f(\mathbf{x}) = \sum_j w_j x_j$$



- **Additive models**

$$f(\mathbf{x}) = \sum_j f_j(x_j)$$



Deep knowledge discovery with more accurate predictors!

Existing methods

- Based on regularized empirical risk minimization

$$\underset{(f_j)_j}{\text{minimize}} \;\; L(f) + \lambda \sum_j \boxed{R(f_j)}$$

where L is data- and task-dependent and $R(f_j)$ is wiggleness of f_j:

$$\boxed{R(f_j)} = \int \left(\frac{d^2}{d\xi^2} f_j(\xi) \right)^2 d\xi$$

- Boils down to multiple kernel learning (MKL)

$R(f_j)$ is counter-intuitive **Training costs $O(m^2)$**

Our Focus: TVAM

- Total variation-regularized additive models (TVAM)
- Learning additive models

$$\underset{(f_j)_j}{\text{minimize}}\ L(f) + \lambda \sum_j R(f_j)$$

where $R(f_j)$ is **total variation** of f_j

$$R(f_j) = \boxed{||f_j||_{\mathrm{TV}}}$$

More intuitive and more efficiently solvable

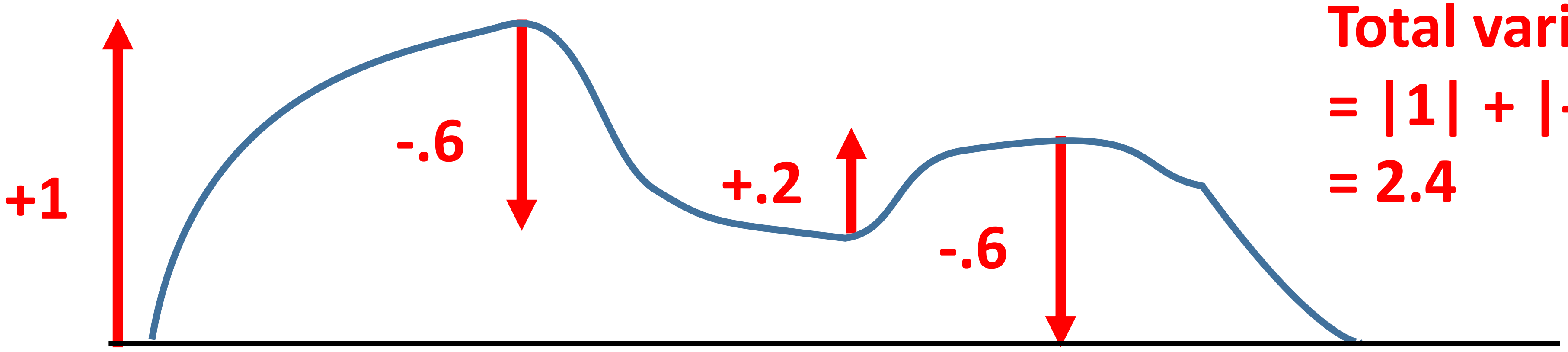
Total Variation

represents how much function value varies in total

- We assume support of each function is bounded, and function is cadlag
- Definition

$$\|f_j\|_{\mathrm{TV}} \triangleq \sup \left\{ |f_j(\xi_1)| + \sum_{i=1..n-1} |f_j(\xi_{i+1}) - f_j(\xi_i)| + |f_j(\xi_n)| \;\middle|\; \xi_1 < \xi_2 < \cdots < \xi_n, \text{ for some } n \right\}$$

- Example



Total variation
= |1| + |-.6| + |.2| +|-.6|
= 2.4

Main Questions

- We study on learning additive models based on

$$\underset{(f_j)_j}{\text{minimize}} \; L(f) + \lambda \sum_j \boxed{\|f_j\|_{\mathrm{TV}}}$$

- Algorithm
  - How to find the solution **efficiently**?
- Theory
  - **Guarantee** on the performance of the solution?

Algorithm

Parameterization

Minimization problem

$$\underset{(f_j)_j}{\text{minimize}} \quad L(f) + \lambda \sum_j \|f_j\|_{\text{TV}}$$

is boiled down to

$$\underset{(w_{jst})_{jst}}{\text{minimize}} \quad L\left(\sum_{j,s,t} w_{jst}\phi_{j,s,t}\right) + \lambda \sum_{j,s,t} |w_{jst}|$$

where

$$\phi_{j,s,t}(\mathbf{x}) = 1 \text{ if } x_{sj} \leq x_j \leq x_{tj} \text{ else } 0$$

Problem

- Minimizing

$$J(\mathbf{w}) = L\left(\sum_{j,s,t} w_{jst}\phi_{j,s,t}\right) + \lambda \sum_{j,s,t} \left|w_{jst}\right|$$

  is an L1-regularized risk minimization of linear model with a design matrix induced by $(\phi_{j,s,t})_{j,s,t}$

$$\boxed{\text{Data matrix}}_{\,j=1..p} \xrightarrow{(\phi_{j,s,t})_{j,s,t}} \boxed{\text{Design matrix}}_{\,(j,s,t)=(1,1,1)..(p,m,m)} \quad i = 1..m$$

- Design matrix is **too big** to fit in memory in a standard machine
  - We can not generate design matrix and then run standard algorithm

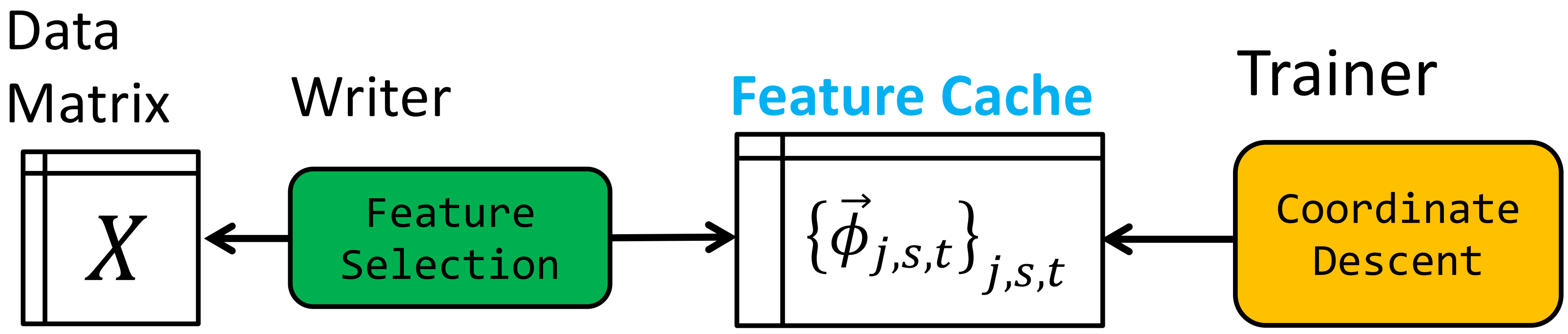
Greedy Coordinate Descent (GCD)

- Repeat until the maximum value is less than λ:
  - $\boxed{\text{Find } (j,s,t) = \underset{j,s,t=(1,1,1)..(p,m,m)}{\operatorname{argmax}} \left| \frac{\partial L}{\partial w_{jst}} \right|}$ **Done by O(mp)!**
  - $\boxed{\text{Minimize } J(\mathbf{w}) \text{ w.r.t. } w_{jst}}$ **Done by O(m)!**

Each step does not require the information of the entire design matrix

Cached Loops

Run two types of threads asynchronously



- Repeat
  - Find $(j, s, t) = \operatorname*{argmax}_{j,s,t=(1,1,1)..(p,m,m)} \left| \frac{\partial L}{\partial w_{jst}} \right|$
  - Push it in **Feature Cache**
  - If small enough then break

- Repeat
  - Randomly choose (j,s,t) in **Feature Cache**
  - Minimize $J(\mathbf{w})$ w.r.t. w_{jst}
  - If w_{jst} stayed at 0, then delete it from **Feature Cache**

Theory

Solution of TVAM

$$\underset{(f_j)_j}{\text{minimize}} \sum_i \ell\left(f(\mathbf{x}_i), y_i\right) + \lambda \sum_j \|f_j\|_{\mathrm{TV}}$$

can be expressed as

$$\hat{f} = \underset{f \in \mathrm{TVAM}(C)}{\operatorname{argmin}} \frac{1}{m} \sum_i \ell\left(f(\mathbf{x}_i), y_i\right)$$

where

$$\mathrm{TVAM}(C) = \left\{ f \,\middle|\, \sum_j \|f_j\|_{\mathrm{TV}} \le C \right\}$$

Main Results

- Gap between ideal and reality
  - Ideal

$$f^* = \operatorname*{argmin}_{f \in \mathrm{TVAM}(C)} \mathbb{E}_{x,y} \ell\big(f(x), y\big)$$

  - Reality

$$\hat{f} = \operatorname*{argmin}_{f \in \mathrm{TVAM}(C)} \frac{1}{m} \sum_i \ell\Big(f(x_i), y_i\Big)$$

- Is the gap smaller when m is large?

$$\mathbb{E}_{\mathbf{x},y} \ell\Big(\hat{f}(\mathbf{x}), y\Big) - \mathbb{E}_{\mathbf{x},y} \ell\Big(f^*(\mathbf{x}), y\Big)$$

- We show **the gap converges to 0 at rate** $O(\sqrt{\log p/m})$ **with high probability**

Why?

- Complexity of TVAM is as much as complexity of linear models!
  - Rademacher complexity for $(\mathbf{x}_i, y_i)_{i=1..m}, \mathbf{x}_i \in \mathbb{R}^p$

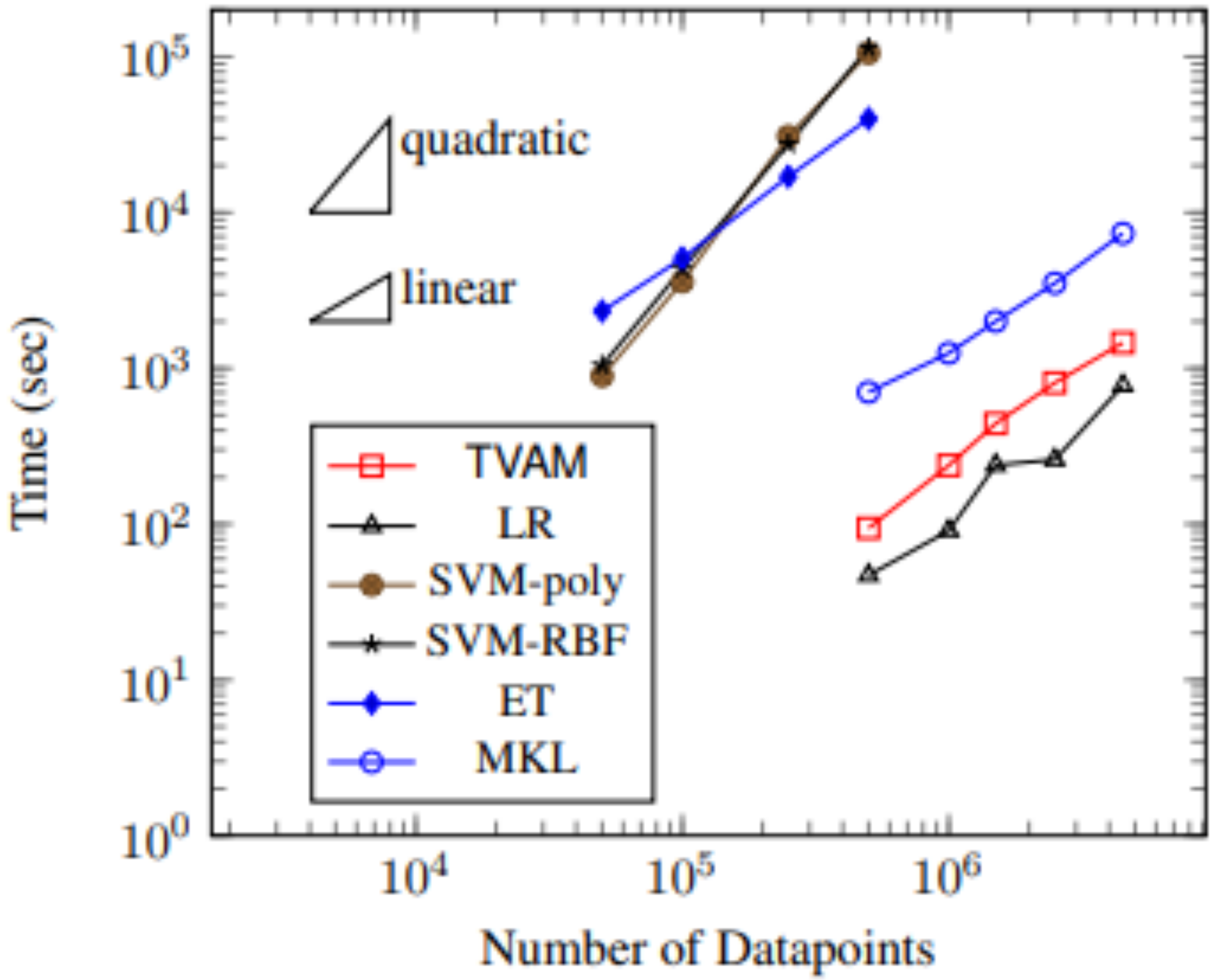
$$\mathrm{Rad}(\mathrm{TVAM}(C)) \sim \sqrt{\frac{\log p}{m}}$$

$$\mathrm{Rad}(\text{Linear model}) \sim \sqrt{\frac{\log p}{m}}$$

Experimental Results

Scalability

- Log loss for binary classification
- Exhibits **linear scalability** in experiments
- TVAM is only a few times slower than learning linear models



Predictive Performance (AUC)

- TVAM achieves **best AUC** among all additive predictors!

Dataset	n	d	TVAM	ET	MKL	FB	NB	LR
				additive predictors				
				nonlinear			linear	
SUSY	4,500,000	17	**87.4**	/	87.2	82.9	78.6	85.4
covtype.binary	500,000	54	**73.8**	55.7	67.6	70.3	70.3	68.5
skin-nonskin	200,000	3	**98.9**	63.6	94.4	67.4	91.2	93.3
cod-rna	59,535	8	**99.3**	99.1	93.6	79.3	81.4	98.8
ijcnn1	49,990	22	96.2	**96.6**	91.5	79.7	90.5	91.3
wilt	4,339	5	**92.3**	85.0	83.6	45.2	50.0	78.8
madelon	2,000	500	**71.3**	68.2	60.9	64.7	62.1	62.2
german.numer	1,000	24	80.8	81.3	**83.0**	80.6	82.6	82.9

Summary of Our Paper

- We learn interpretable additive models based on

$$\underset{(f_j)_j}{\text{minimize}} \; L(f) + \lambda \sum_j \boxed{\|f_j\|_{\mathrm{TV}}}$$

- Algorithm
  - Establish an efficient algorithm
- Theory
  - Statistical learning rate of $O(\sqrt{\log p/m})$
- Experiments
  - Scalability and predictive performance

END

Predictive Performance (AUC)

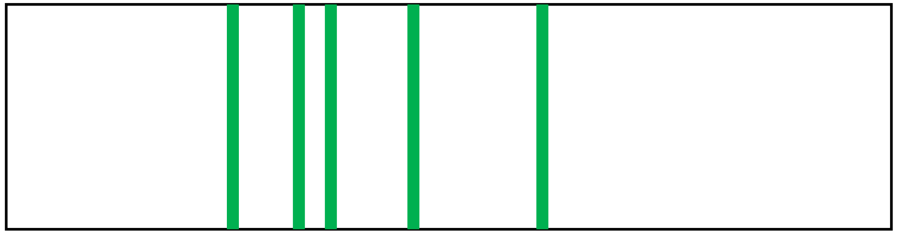
- TVAM achieves **best AUC** among all additive predictors!

Dataset	n	d	additive predictors						non-additive predictors		
				nonlinear			linear		(Kernel SVM)		
			TVAM	ET	MKL	FB	NB	LR	RBF	poly	XGB
SUSY	4,500,000	17	**87.4**	/	87.2	82.9	78.6	85.4	/	/	87.5
covtype.binary	500,000	54	**73.8**	55.7	67.6	70.3	70.3	68.5	/	/	78.4
skin-nonskin	200,000	3	**98.9**	63.6	94.4	67.4	91.2	93.3	/	/	100.0
cod-rna	59,535	8	**99.3**	99.1	93.6	79.3	81.4	98.8	99.6	98.1	99.3
ijcnn1	49,990	22	96.2	**96.6**	91.5	79.7	90.5	91.3	98.2	97.5	99.6
wilt	4,339	5	**92.3**	85.0	83.6	45.2	50.0	78.8	70.4	89.2	94.4
madelon	2,000	500	**71.3**	68.2	60.9	64.7	62.1	62.2	50.0	69.0	86.5
german.numer	1,000	24	80.8	81.3	**83.0**	80.6	82.6	82.9	81.7	80.0	79.3

END

- https://ttsreader.com/

Design matrix



$i = 1..m$

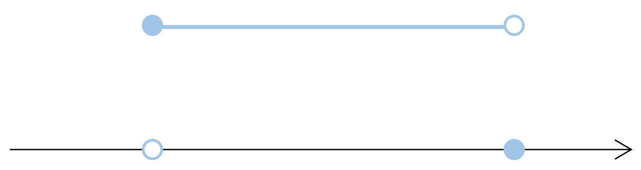
$j, s, t = (1, 1, 1)..(p, m, m)$

With probability more than 1-δ:

$$\mathbb{E}_{x,y}\ell(\hat{f}(x), y) - \ell^* \leq \rho C\sqrt{\frac{5\lceil \log d \rceil}{m}} + \frac{5C}{2}\sqrt{\frac{2\log(2/\delta)}{m}}$$

$\ell : \rho$-Lipschitz

Form of $\phi_{j,s,t}(\cdot)$

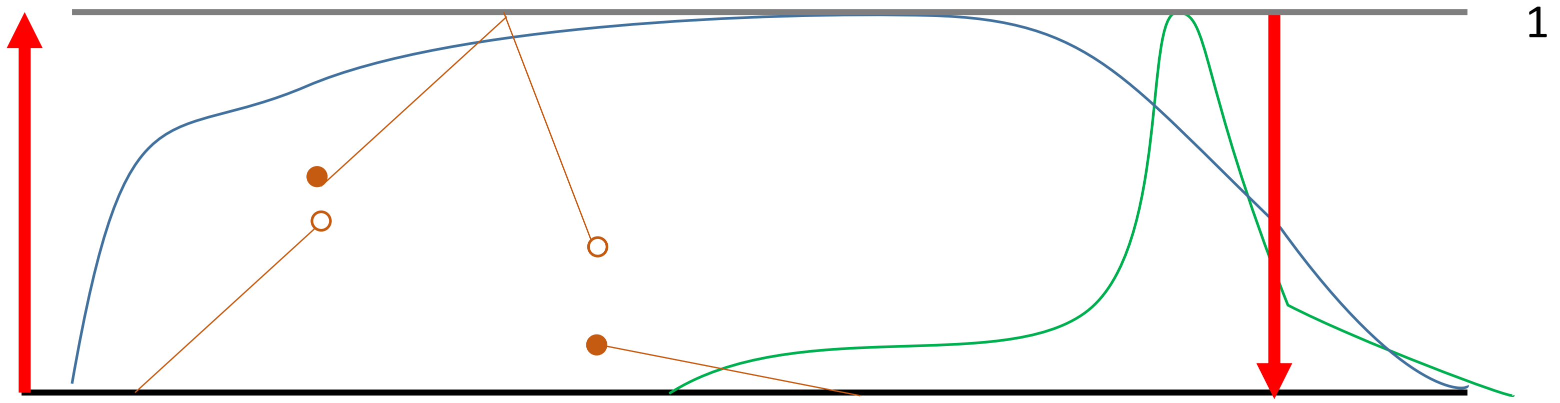


Total variation

We assume support of each function is bounded, and function is cadlag

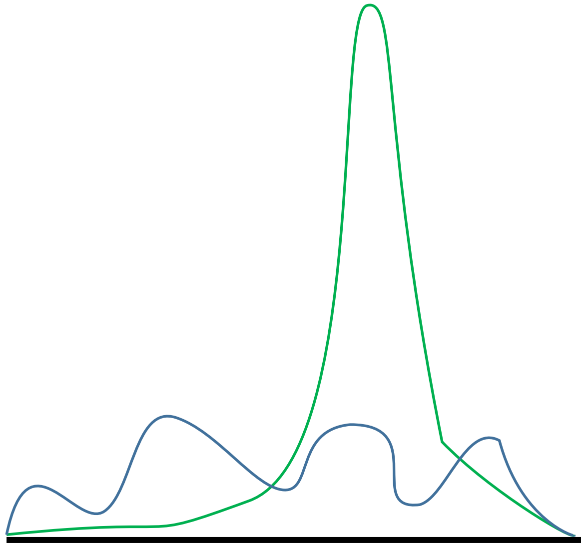
- Total variation represents how much function value varies in total
- Definition

- They all have total variation of 2

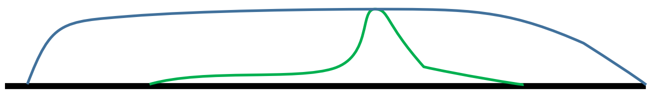


Total variation

- Large total variation



- Small total variation



- Definition