

Minwise hashing for large-scale regression and classification with sparse data

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Large-scale sparse regression

Prediction problems with large-scale sparse predictors:

- 1 **Medical risk prediction/drug surveillance** (OMOP project).
 $n \approx 100,000$ patients with $p \approx 30,000$ indicator variables about medication history and symptoms.
With interactions of second order, $p \approx 450$ million.
With third order $p \approx 4.5$ trillion.
- 2 **Text data regression or classification.** Binary word indicator variables for approximately $p \approx 20,000$ words. Bi-grams and N-grams of higher order lead to hundreds of millions of variables.
- 3 **URL reputation scoring** (Ma et al, 2009). Information about a URL comprises > 3 million variables which include word-stem presence and geographical information for example.

Min-wise hashing (Broder, 1997; Broder *et al.*, 1998)

Suppose we have sets $\mathbf{z}_1, \dots, \mathbf{z}_n \subseteq \{1, \dots, p\}$. Min-wise hashing gives estimates of the Jaccard index of every pair of sets $\mathbf{z}_i, \mathbf{z}_j$, given by

$$J(\mathbf{z}_i, \mathbf{z}_j) = \frac{|\mathbf{z}_i \cap \mathbf{z}_j|}{|\mathbf{z}_i \cup \mathbf{z}_j|}.$$

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- Let π_1, \dots, π_L be random permutations of $\{1, \dots, p\}$ (in practice all random functions implemented by hash functions).
- Let the $n \times L$ matrix \mathbf{M} be given by $M_{il} = \min \pi_l(\mathbf{z}_i)$.

Then for each i, j, l , $\mathbb{P}(M_{il} = M_{jl}) = J(\mathbf{z}_i, \mathbf{z}_j)$.

Min-wise hashing matrix \mathbf{M}

$$\mathbf{X} = \begin{matrix} & \pi & 3 & 1 & 2 & 4 \\ \begin{pmatrix} * & & & * \\ & & * & * \\ * & & * & \\ & * & * \\ * & * \end{pmatrix} & \Rightarrow & \mathbf{M} = \begin{pmatrix} 1 \\ 2 \\ 2 \\ 1 \\ 1 \end{pmatrix} \end{matrix}$$

One column of \mathbf{M} generated by the random permutation π of the variables.

Min-wise hashing matrix \mathbf{M}

Can repeat L times to build \mathbf{M} with repeated (pseudo-) random permutations π .

$$\mathbf{X} = \begin{matrix} & \pi & 2 & 4 & 1 & 3 \\ \begin{pmatrix} & * & & & * \\ & & & * & * \\ * & & & * & \\ & * & & * & \\ & & * & * & \\ * & * & & & \end{pmatrix} & \Rightarrow & \mathbf{M} = \begin{pmatrix} 1 & 3 \\ 2 & 1 \\ 2 & 1 \\ 1 & 1 \\ 1 & 2 \end{pmatrix} \end{matrix}$$

Work with \mathbf{M} instead of sparse \mathbf{X} . Encode all levels in a column as dummy variables ?

b -bit min-wise hashing (Li and König, 2011)

b -bit min-wise hashing stores only the lowest b bits of each entry of \mathbf{M} when expressed in binary (i.e. the residue mod 2), so for $b = 1$,

$$M_{ij}^{(1)} \equiv M_{ij} \pmod{2}.$$

Perform regression using binary $n \times L$ matrix $\mathbf{M}^{(1)}$ rather than \mathbf{X} .

$$\mathbf{X} = \begin{pmatrix} & 1 & & 1 \\ & & 1 & 1 \\ 1 & & 1 & \\ & 1 & 1 & \\ 1 & 1 & & \end{pmatrix} \Rightarrow \mathbf{M} = \begin{pmatrix} 1 & 3 \\ 2 & 1 \\ 2 & 1 \\ 1 & 1 \\ 1 & 2 \end{pmatrix} \Rightarrow \mathbf{M}^{(1)} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \\ 0 & 1 \\ 1 & 1 \\ 1 & 0 \end{pmatrix}$$

When $L \ll p$ this gives large computational savings, and empirical studies report good performance (mostly for classification with SVM's).

Will study a variant of 1-bit min-wise hashing we call MRS-mapping (**min**-wise hash **random sign**)

- Easier to analyse and avoids choice of number of bits b to keep.
- Deals with sparse design matrices with real-valued entries
- Allows for the construction of a variable importance measure.

Downside: slightly less efficient to implement.

MRS-mapping

1-bit min-wise hashing: **keep last bit**

$$\mathbf{X} = \begin{pmatrix} & 1 & & 1 \\ & & 1 & 1 \\ 1 & & 1 & \\ & 1 & 1 & \\ 1 & 1 & & \end{pmatrix} \Rightarrow \mathbf{M} = \begin{pmatrix} 1 & 3 \\ 2 & 1 \\ 2 & 1 \\ 1 & 1 \\ 1 & 2 \end{pmatrix} \Rightarrow \mathbf{M}^{(1)} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \\ 0 & 1 \\ 1 & 1 \\ 1 & 0 \end{pmatrix}$$

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MRS-map: **random sign assignments** $\{1, \dots, p\} \mapsto \{-1, 1\}$ are chosen independently for all columns $l = 1, \dots, L$ when going from $M_{.l}$ to $S_{.l}$.

$$\mathbf{X} = \begin{pmatrix} & 1 & & 1 \\ & & 1 & 1 \\ 1 & & 1 & \\ & 1 & 1 & \\ 1 & 1 & & \end{pmatrix} \Rightarrow \mathbf{M} = \begin{pmatrix} 1 & 3 \\ 2 & 1 \\ 2 & 1 \\ 1 & 1 \\ 1 & 2 \end{pmatrix} \Rightarrow \mathbf{S} = \begin{pmatrix} 1 & 1 \\ -1 & -1 \\ -1 & -1 \\ 1 & -1 \\ 1 & 1 \end{pmatrix}$$

Equivalent to storing \mathbf{M} , we can store the “responsible” variables in \mathbf{H}

$$M_{ij} = \min \pi_I(\mathbf{z}_i)$$

$$H_{ij} = \operatorname{argmin}_{k \in \mathbf{z}_i} \pi_I(k)$$

$$\mathbf{X} = \begin{pmatrix} & 1 & & 1 \\ & & 1 & 1 \\ 1 & & 1 & \\ & 1 & 1 & \\ 1 & 1 & & \end{pmatrix} \Rightarrow \mathbf{M} = \begin{pmatrix} 1 & 3 \\ 2 & 1 \\ 2 & 1 \\ 1 & 1 \\ 1 & 2 \end{pmatrix} \Rightarrow \mathbf{S} = \begin{pmatrix} 1 & 1 \\ -1 & -1 \\ -1 & -1 \\ 1 & -1 \\ 1 & 1 \end{pmatrix}$$

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Continuous variables

Can handle continuous variables

$$\mathbf{X} = \begin{pmatrix} & 1 & & 1 \\ & & 4.2 & 1 \\ 1 & & 1 & \\ & 1 & 1 & \\ 7.1 & 1 & & \end{pmatrix} \Rightarrow \mathbf{H} = \begin{pmatrix} 2 & 4 \\ 3 & 3 \\ 3 & 3 \\ 2 & 3 \\ 2 & 1 \end{pmatrix} \Rightarrow \mathbf{S} = \begin{pmatrix} 1 & 1 \\ -4.2 & -4.2 \\ -1 & -1 \\ 1 & -1 \\ 1 & 7.1 \end{pmatrix}$$

We get $n \times L$ matrices \mathbf{H} , and \mathbf{S} given by

$$H_{il} = \operatorname{argmin}_{k \in \mathbf{z}_i} \pi_l(k)$$

$$S_{il} = \Psi_{H_{il}l} X_{iH_{il}},$$

where Ψ_{hl} is the random sign of the h -th variable in the l -th permutation.

Approximation error

Is there a \mathbf{b}^* such that the expected value is unbiased (if averaged over the random permutations and sign assignments)?

$$\left[\begin{array}{c} \text{sparse } \mathbf{X} \in \mathbb{R}^{n \times p} \\ \left(\begin{array}{cccccccc} * & & & & * & & & \\ & & * & & & & * & \\ & * & * & & * & & & \\ & & * & & & & * & * \\ * & * & & & * & & & \\ & & & & & * & * & * \\ & & & * & & & * & * \\ * & & & & & & & \end{array} \right) \end{array} \right] \begin{array}{c} \mathbf{\beta}^* \in \mathbb{R}^p \\ \left(\begin{array}{c} * \\ * \\ * \\ * \\ * \\ * \\ * \\ * \\ * \\ * \\ * \\ * \end{array} \right) \end{array} \stackrel{?}{=} \mathbb{E}_{\pi, \psi} \left[\begin{array}{c} \mathbf{S} \in \mathbb{R}^{n \times 1} \\ \left(\begin{array}{c} * \\ * \\ * \\ * \\ * \\ * \\ * \\ * \\ * \\ * \\ * \\ * \end{array} \right) \end{array} \right] \begin{array}{c} \mathbf{b}^* \in \mathbb{R}^1 \\ \left(\begin{array}{c} * \end{array} \right) \end{array} \end{array}$$

Approximation error

Example: binary \mathbf{X} with one permutation with min-hash value H_i for $i = 1, \dots, n$ and random signs ψ_k , $k = 1, \dots, p$.

$$\mathbb{E}_{\pi, \psi} \left[\begin{array}{c} \overbrace{\left(\begin{array}{c} \psi_{H_1} \\ \psi_{H_2} \\ \dots \\ \dots \\ \dots \end{array} \right)}^{\mathbf{S} \in \mathbb{R}^{n \times 1}} \quad \overbrace{\left(q \sum_{k=1}^p \beta_k^* \psi_k \right)}{=: \mathbf{b}^* \in \mathbb{R}^1} \end{array} \right] =$$

Approximation error

Can we find a $\mathbf{b}^* \in \mathbb{R}^L$ such that $\mathbf{X}\mathbf{b}^*$ is close to $\mathbf{S}\mathbf{b}^*$ on average?

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Approximation error

Can we find a $\mathbf{b}^* \in \mathbb{R}^L$ such that $\mathbf{X}\beta^*$ is close to $\mathbf{S}\mathbf{b}^*$ on average?

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$$= \mathbf{X}\beta^* \quad (\text{..unbiased})$$

Theorem

Let $\mathbf{b}^* \in \mathbb{R}^L$ be defined by

$$b_l^* = \frac{q}{L} \sum_{k=1}^p \beta_k^* \psi_{kl} w_{\pi_l(k)},$$

where \mathbf{w} is a vector of weights. Then there is a choice of \mathbf{w} , such that:

- (i) The approximation is unbiased: $\mathbb{E}_{\pi, \psi}(\mathbf{S}\mathbf{b}^*) = \mathbf{X}\beta^*$.

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where \mathbf{w} is a vector of weights. Then there is a choice of \mathbf{w} , such that:

- (i) The approximation is unbiased: $\mathbb{E}_{\pi, \psi}(\mathbf{S}\mathbf{b}^*) = \mathbf{X}\boldsymbol{\beta}^*$.
- (ii) If $\|\mathbf{X}\|_\infty \leq 1$, then $\frac{1}{n} \mathbb{E}_{\pi, \psi}(\|\mathbf{S}\mathbf{b}^* - \mathbf{X}\boldsymbol{\beta}^*\|_2^2) \leq 2q \|\boldsymbol{\beta}^*\|_2^2 / L$.

Assume model

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta}^* + \boldsymbol{\varepsilon}.$$

Random noise $\boldsymbol{\varepsilon} \in \mathbb{R}^n$ satisfies $\mathbb{E}(\varepsilon_i) = 0$, $\mathbb{E}(\varepsilon_i^2) = \sigma^2$ and $\text{Cov}(\varepsilon_i, \varepsilon_j) = 0$ for $i \neq j$.

We will give bounds on a mean-squared prediction error (MSPE) of the form

$$\text{MSPE}(\hat{\mathbf{b}}) := \mathbb{E}_{\boldsymbol{\varepsilon}, \boldsymbol{\pi}, \boldsymbol{\Psi}} \left(\|\mathbf{X}\boldsymbol{\beta}^* - \mathbf{S}\hat{\mathbf{b}}\|_2^2 \right) / n.$$

Theorem

Let $\hat{\mathbf{b}}$ be the least squares estimator and let $L^* = \sqrt{2qn}\|\boldsymbol{\beta}^*\|_2/\sigma$. We have

$$\text{MSPE}(\hat{\mathbf{b}}) \leq 2 \max\left\{\frac{L}{L^*}, \frac{L^*}{L}\right\} \sigma \sqrt{\frac{2q}{n}} \|\boldsymbol{\beta}^*\|_2.$$

- If the size of the signal is fixed and columns of \mathbf{X} are independent with roughly equal sparsity, then $\sqrt{q}\|\boldsymbol{\beta}^*\|_2 \leq \text{const}\sqrt{p}$ and we have $\text{MSPE}(\hat{\mathbf{b}}) \rightarrow 0$ if $p/n \rightarrow 0$.
- If the signal $\mathbf{X}\boldsymbol{\beta}^*$ is partially replicated in B groups of variables then we only need $(p/B)/n \rightarrow 0$.

Can also estimate with ridge regression. Very similar results to OLS.

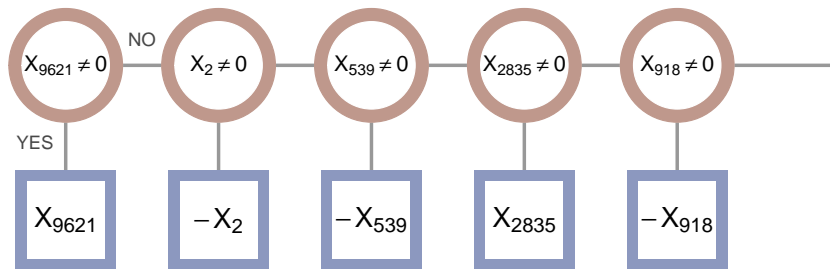
- The dimension L of the projection can be chosen arbitrarily large (from a statistical point of view).
- Ridge penalty parameter is then the relevant tuning parameter

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Similar results for logistic regression available.

Minwise hash as a tree



Can view minwise hashing operation as a tree-type operation.

Interaction models

Let $\|\mathbf{X}\|_\infty \leq 1$ and let $\mathbf{f}^* \in \mathbb{R}^n$ be given by

$$f_i^* = \sum_{k=1}^p X_{ik} \theta_k^{*,(1)} + \sum_{k,k_1=1}^p X_{ik} \mathbb{1}_{\{X_{ik_1}=0\}} \Theta_{k,k_1}^{*,(2)}, \quad i = 1, \dots, n.$$

Theorem

Define

$$\ell(\Theta^*) := \|\boldsymbol{\theta}^{*,(1)}\|_2 + 2(q \sum_{k,k_1,k_2} |\Theta_{kk_1}^{*,(2)} \Theta_{kk_2}^{*,(2)}|)^{1/2}.$$

Then there exists $\mathbf{b}^* \in \mathbb{R}^L$ such that

- (i) $\mathbb{E}_{\pi, \Psi}(\mathbf{S}\mathbf{b}^*) = \mathbf{f}^*$;
- (ii) $\mathbb{E}_{\pi, \Psi}(\|\mathbf{S}\mathbf{b}^* - \mathbf{f}^*\|_2^2)/n \leq 2q\ell^2(\Theta^*)/L.$

If there are a finite number of non-zero interaction terms with finite value, the approximation error becomes very small if $L \gg q^2$.

- Assume the linear model from before, but with $\mathbf{X}\beta^*$ replaced by \mathbf{f}^* .
- Previous results hold if $\|\beta^*\|_2$ is replaced by $\ell(\Theta^*)$.

For example:

Theorem

Let $\hat{\mathbf{b}}$ be the least squares estimator and let $L^* = \sqrt{2qn} \ell(\Theta^*) / \sigma$. We have

$$\text{MSPE}(\hat{\mathbf{b}}) \leq 2 \max\left\{\frac{L}{L^*}, \frac{L^*}{L}\right\} \sigma \sqrt{\frac{2q}{n}} \ell(\Theta^*).$$

Advantages

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- requires only fit of a linear model
- does not require interactions to be created explicitly
- has a complexity saving factor of $(q/p)^2$ over the brute force approach.

Does require a larger number L of minwise hashing operations than fitting main effect models.

Variable importance

Predicted values are

$$\hat{\mathbf{f}} = \mathbf{S}\hat{\mathbf{b}}$$

Let $\hat{\mathbf{f}}^{-(k)}$ be the predictions obtained when setting $\mathbf{X}_k = \mathbf{0}$.

If the underlying model contains only main effects, $\hat{\mathbf{f}} - \hat{\mathbf{f}}^{-(k)} \approx \mathbf{X}_k\beta_k^*$.

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Store $n \times L$ matrices \mathbf{S} , $\tilde{\mathbf{S}}$ and \mathbf{H} . Then

$$\hat{\mathbf{f}}^{-(k)} = (\mathbf{S} \circ \mathbb{1}_{\{\mathbf{H} \neq k\}} + \tilde{\mathbf{S}} \circ \mathbb{1}_{\{\mathbf{H} = k\}})\hat{\mathbf{b}}.$$

Some observations from numerical simulations:

- Scheme becomes more competitive when repeating many times and aggregating.

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- Scheme becomes more competitive when repeating many times and aggregating.
- Predictive accuracy can decrease if we make L too large.
- In the absence of interactions: similar performance to ridge/random projections
- With interactions: performance between linear model (with ridge penalty or random projections) and Random Forest (Breiman, 01).

Volatility prediction

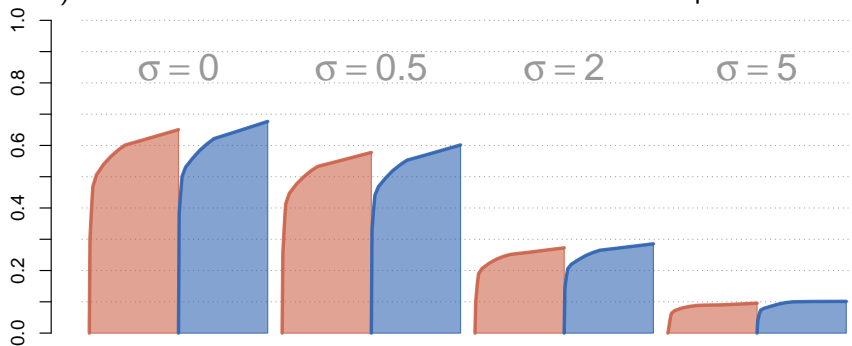
Forecast financial volatility of stocks based on 10-K report filings (Kogan, 2009).

Have $p = 4,272,227$ predictor variables for $n = 16,087$ observations.

Use various targets (volatility after release; a linear model; a non-linear model) and compare prediction accuracy with regression on random projections.

Volatility prediction

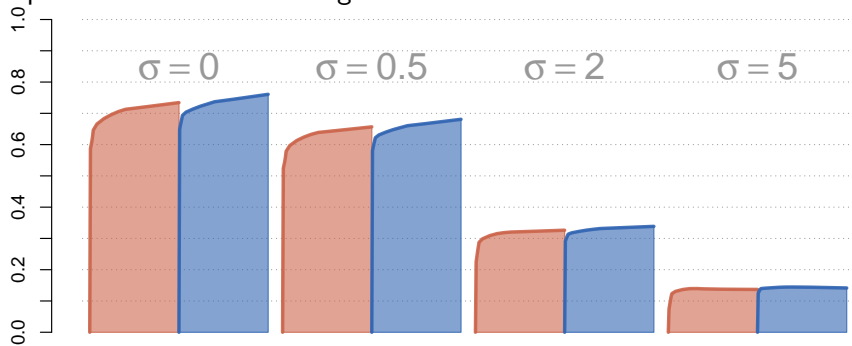
Correlation between prediction and response (volatility in year after release of text). Added additional noise with variance σ^2 to the response.



Red: MRS-mapping. Blue: random projections
(as functions of L up to 500)

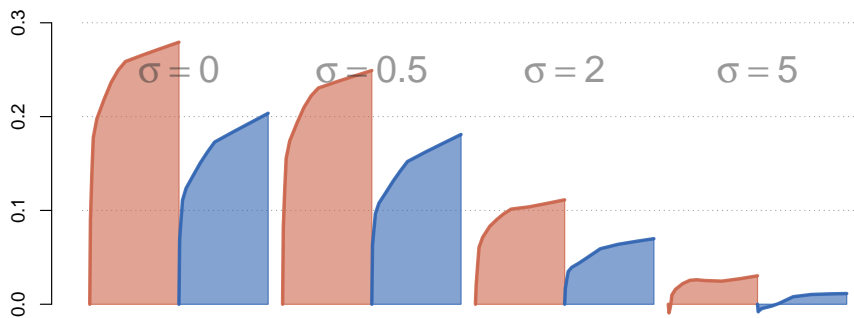
Volatility prediction

Response: linear model in original variables



Volatility prediction

Response: interaction model in original variables



URL identification

Classification of malicious URLs with

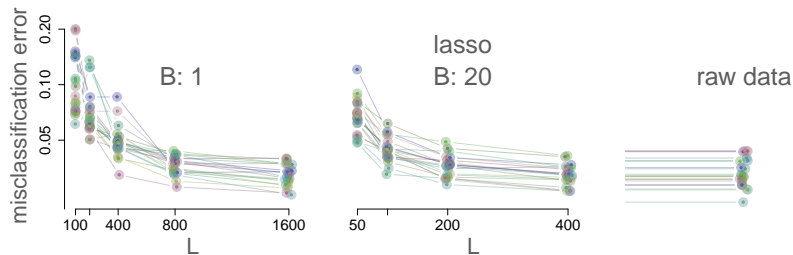
$n \approx 2$ million and $p \approx 3$ million.

Data are ordered into consecutive days.

Response $\mathbf{Y} \in \{0, 1\}^n$ is a binary vector where 1 corresponds to a malicious URL.

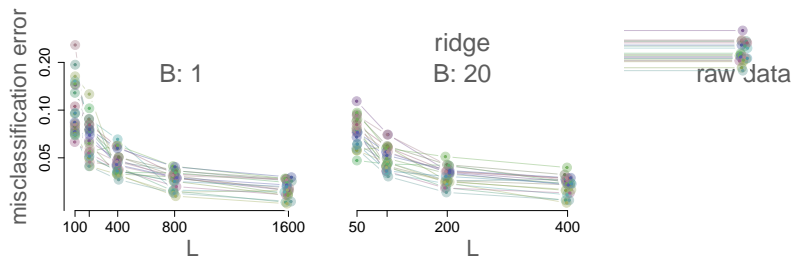
In order to compare MRS-mapping with the Lasso- and ridge-penalised logistic regression, we split the data into the separate days, training on the first half of each day and testing on the second. This gives on average $n \approx 20,000$, $p \approx 100,000$.

URL identification: Lasso regression



Lasso with and without MRS-mapping has similar performance here.

URL identification: Ridge regression



Ridge regression following MRS-mapping performs better than ridge regression applied to the original data.

B-bit minwise hashing and closely related *MRS-maps* interesting technique for dimensionality reduction for large-scale sparse design matrices.

- Prediction error can be bounded with a slow rate (in the absence of assumptions on the design except sparsity).
- Behaves similar to random projections (or ridge regression) if only linear effects are present
- Linear model in the compressed, dense, low-dimensional matrix can fit interactions among the large number of original sparse variables.