Approximate *l*-fold Cross-Validation with Least Squares SVM and Kernel Ridge Regression

Richard E. Edwards[1], Hao Zhang[1], Lynne E. Parker[1], Joshua R. New[2]

[1]Distributed Intelligence Lab
Department of Electrical Engineering and Computer Science
University of Tennessee, Knoxville TN, USA

[2]Whole Building and Community Integration Group
Oak Ridge National Lab
Oak Ridge TN, United States

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Outline

Applying Kernel Methods to Large Datasets

- Direct Kernel application scales poorly
  - Requires $O(n^2)$ memory
  - Model solve time increases
  - Model selection time increases
- Scaling improvements
  - Faster model solvers
  - Problem decompositions
  - Low-rank Kernel approximations
- Most scaling improvements apply to standard SVMs

Applying Kernel Methods to Large Datasets

- Least Squares Support Vector Machine (LS-SVM)
  - Naive cross-validation model calibration complexity: $O(ln^3)$
  - Best exact leave-one-out (LOO) cross-validation complexity: $O(n^2)$
  - Best approximate cross-validation complexity: $O(m^2 n)$
- We can do better!
  - Approximate cross-validation complexity: $O(n \log n)$
  - Applies to LOO as well

Outline

Previous LS-SVM Model Selection

- T. Pahikkala et al (2006) and Cawley et al. (2004) obtained $O(n^2)$ LOO cross-validation
  - utilizes matrix inverse properties
- An et al. (2007) obtained $O(m^2 n)$ l-fold cross-validation
  - uses low-rank kernel approximation
  - removes redundancy from the validation process
  - introduces a new cross-validation algorithm
- L. Ding et al. (2011) obtained $O(ln \log n)$ l-fold cross-validation
  - $O(n^2 \log n)$ LOO cross-validation

Outline

Multi-Level Matrices

- Matrices indexed by factors
- Example 3-level matrix with factors: 2x2, 4x4, 2x2
  - $|M| = (2 \times 4 \times 2) \times (2 \times 4 \times 2)$
- Level 1:

$$M = \begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix}$$

- Level 2:

$$A_{00} = \begin{bmatrix} B_{00} & B_{01} & B_{02} & B_{03} \\ B_{10} & B_{11} & B_{12} & B_{13} \\ B_{20} & B_{21} & B_{22} & B_{23} \\ B_{30} & B_{31} & B_{32} & B_{33} \end{bmatrix}$$

- Level 3:

$$B_{00} = \begin{bmatrix} 5 & 6 \\ 1 & 2 \end{bmatrix}$$

Circulant Matrices

- A special Toeplitz matrix
- Its inverse is computed in $O(n \log n)$ via Fast Fourier Transform
- Example:

$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 4 & 1 & 2 & 3 \\ 3 & 4 & 1 & 2 \\ 2 & 3 & 4 & 1 \end{bmatrix}$$

- General definition:

$$\begin{bmatrix} c_0 & c_1 & \cdots & c_n \\ c_n & c_0 & \cdots & c_{n-1} \\ \vdots & & \ddots & \vdots \\ c_1 & c_2 & \cdots & c_0 \end{bmatrix}$$

P-Level Circulant Matrices

- Combines Circulant Matrices and Multi-Level Circulant Matrices
  - Each level is a circulant matrix
  - All factors are now one diminsional
- Example 3-Level with factors 2, 4, 2:

$$M = \begin{bmatrix} A_0 & A_1 \\ A_1 & A_0 \end{bmatrix}$$

- Level 2:

$$A_0 = \begin{bmatrix} B_0 & B_1 & B_2 & B_3 \\ B_3 & B_0 & B_1 & B_2 \\ B_2 & B_3 & B_0 & B_1 \\ B_1 & B_3 & B_2 & B_0 \end{bmatrix}$$

- Level 3:

$$B_0 = \begin{bmatrix} 5 & 6 \\ 6 & 5 \end{bmatrix}$$

Outline

Overview

- We use same approximation method has L. Ding et al. (2011)
- We remove inefficienies from the cross-validation process
- Result: $n \log n$ LOO cross-validation
  - L. Ding et al.'s LOO cross-validation: $n^2 \log n$

Kernel Approximation via P-Level Circulant Matrices

- Song et al. (2010) introduced P-Level Circulant RBF Kernel approximation
  - allows $n \log n$ model solve time
  - allows fast model selection
- approximation converges as matrix level factors approach infinity
- result: $O(n + n2^p)$ complexity
  - However 2 to 3 factors work well
  - L. Ding et al. (2011) and our work
- One caveat: this approximation method only applies to RBF Kernels

Kernel Approximation via P-Level Circulant Matrices

Algorithm 1 Kernel Approximation with P-level Circulant Matrix

Input: M (Kernel's size), $F = \{n_0, n_1, \ldots, n_{p-1}\}$, k (Kernel function)

1: $N \leftarrow$ {All multi-level indices defined by F}
2: $T \leftarrow zeros(M)$, $U \leftarrow zeros(M)$
3: $H_n \leftarrow \{x_0, x_1, \ldots, x_{p-1}\} \in \mathbb{R}^p$ s.t. $\forall x_i \in H_n,\ x_i > 0$
4: **for all** $j \in N$ **do**
5: $\quad T_j \leftarrow k(||jH_n||_2)$
6: **end for**
7: **for all** $j \in N$ **do**
8: $\quad D_j \leftarrow D_{j,0} \times D_{j,1} \times \cdots \times D_{j,p-1}$
9: $\quad U_j \leftarrow \sum_{l \in D_j} T_l$
10: **end for**
11: $\tilde{K} \leftarrow U$

Output: $\tilde{K}$

Efficient Cross-Validation

Theorem

Let $y^{(k)} = sign[g_k(x)]$ *denote the classifier formulated by leaving the* k*th group out and let* $\beta_{k,i} = y_{k,i} - g_k(x_{k,i})$. *Then* $\beta_{(k)} = C_{kk}^{-1}\alpha_{(k)}$.

- proven by An et al. (2007)
- Take aways:
  - Allows computing a single Kernel matrix inverse for all folds
  - Perform smaller inverses to compute the hold out result

Efficient Cross-Validation

Algorithm 2 Efficient Cross-Validation

Input: K (Kernel matrix), l (Number folds), y (response)

$K_\gamma^{-1} \leftarrow inv(K + \frac{1}{\gamma} I), \quad d \leftarrow 1_n^\mathsf{T} K_\gamma^{-1} 1_n$

$C \leftarrow K_\gamma^{-1} + \frac{1}{d} K_\gamma^{-1} 1_n 1_n^\mathsf{T} K_\gamma^{-1}$

$\alpha \leftarrow K_\gamma^{-1} y + \frac{1}{d} K_\gamma^{-1} 1_n 1_n^\mathsf{T} K_\gamma^{-1} y$

$n_k \leftarrow size(y)/l, \quad y^{(k)} \leftarrow zeros(l, n_k)$

for $k \leftarrow 1$, $k \leq l$ **do**

    Solve $C_{kk} \beta_{(k)} = \alpha_{(k)}$

    $y^{(k)} \leftarrow \text{sign}[y_{(k)} - \beta_{(k)}]$

    $k \leftarrow k + 1$

end for

$error \leftarrow \frac{1}{2} \sum_{k=1}^{l} \sum_{i=1}^{n_k} |y_i - y^{(k,i)}|$

Output: *error*

Approximate *l*-fold Cross-Validation

Theorem

If K is a p-level circulant matrix with factorization $n = n_0 n_1 \dots n_{p-1}$ and $l = n_0 n_1 \dots n_s$ s.t. $s \leq p - 1$, then the computational complexity for An et al.'s Cross-Validation Algorithm is $O(n \log n)$

- Take aways:
  - This combination produces an $O(n \log n)$ runtime
  - Works for any *l*-fold, provided the factorizations allign

Extension to Kernel Ridge Regression

- An et al.'s changes to their algorithm:
  - Change C's value to K_γ^{-1}
  - Change α's value to $K_\gamma^{-1} y$
- Our theorm still holds under these settings

Outline

Experimental Setup

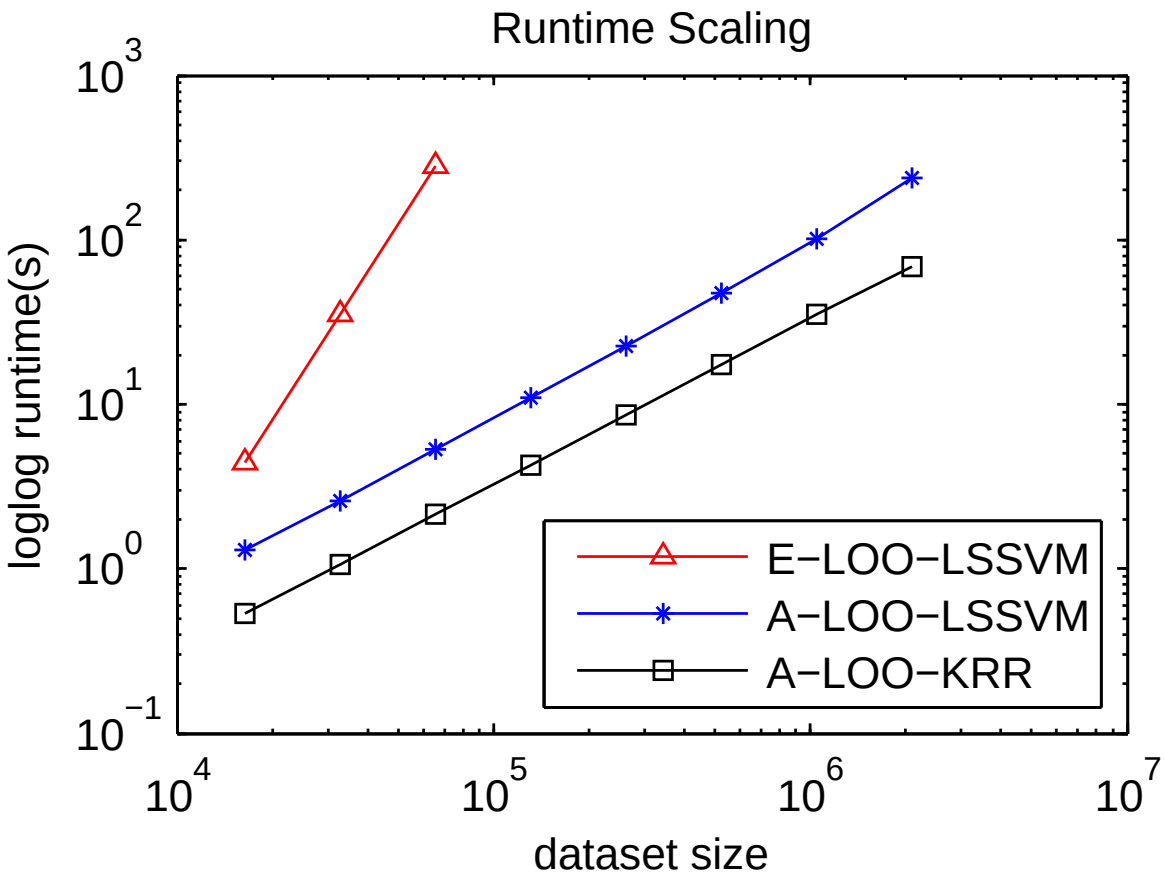
- Scaling
  - measured with randomly generated data
  - dataset sizes range from 2^{13} to 2^{20} samples
- Approximation Quality
  - measured on benchmark datasets
- Hyperparameter Selection Quality
  - Test exact models on real-world datasets

Single CPU Scaling Test

# Examples	2^{13}	2^{14}	2^{15}	2^{16}	2^{17}
E-LOO	4.43s	35.25s	281.11s	–	–
A-LOO-LSSVM	1.3s	2.6s	5.32s	10.88s	22.45s
A-LOO-KRR	0.54s	1.06s	2.14s	4.3s	8.55s

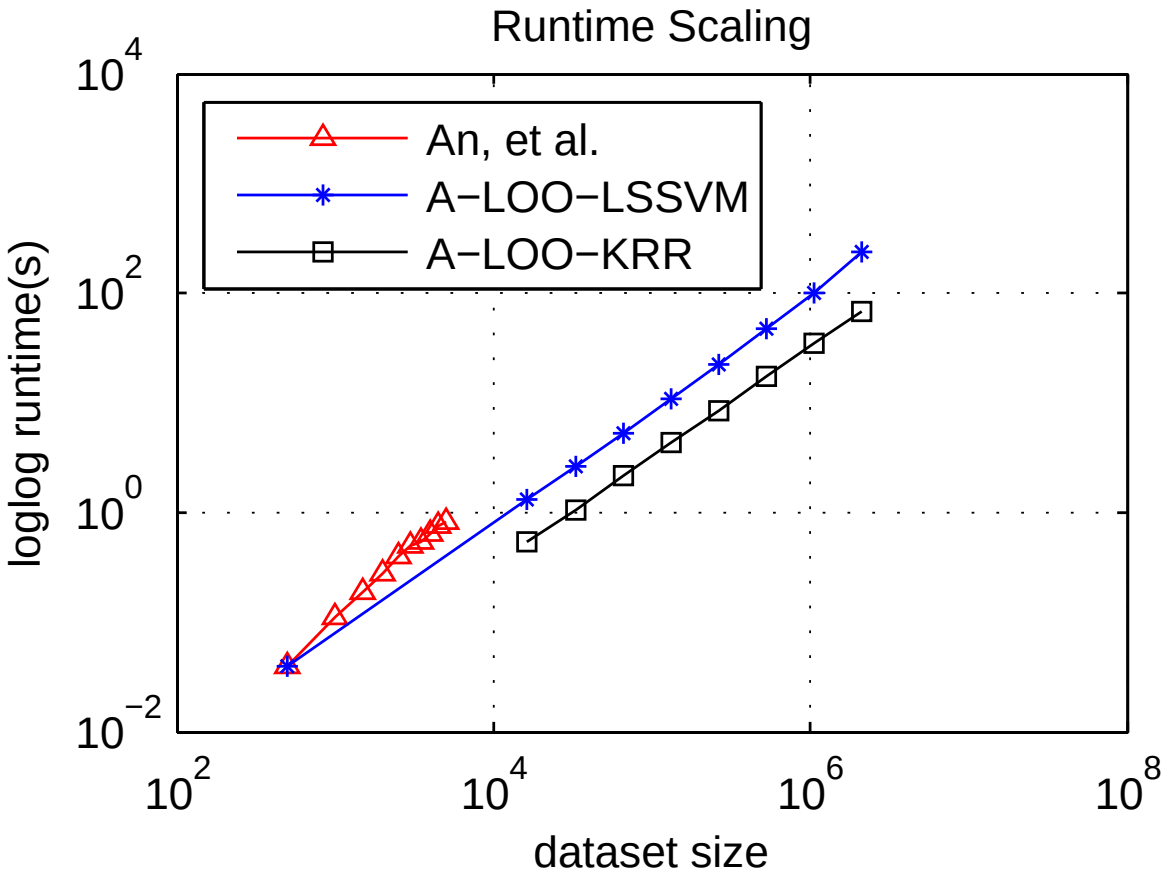
# Examples	2^{18}	2^{19}	2^{20}
E-LOO	–	–	–
A-LOO-LSSVM	47.41s	101.36s	235.83s
A-LOO-KRR	17.28s	35.39s	68.22s

Runtime Scaling Comparison



- A-LOO scales the same for LSSVM and KRR (same slopes)

Runtime Scaling Comparison



- We scale no worse than An et al's low-rank approximation
- We are assumption free, An et al. requires $m << n$

Benchmark Dataset Performance

Data set	#Train	#Test	A-Error(L. Ding, et al.)	A-Error $H_n \in (1, 2)$	A-Error $H_n \in (10, 11)$	E-Error
1) Titanic	150	2051	22.897±1.427	23.82±1.44	22.80±0.68	22.92±0.43
2) B. Cancer	200	77	27.831±5.569	29.87±5.59	26.75±5.92	25.97±4.40
3) Diabetes	468	300	26.386±4.501	25.67±1.13	25.27±2.07	23.00±1.27
4) F. Solar	666	400	36.440±2.752	35.65±2.78	36.65±2.47	33.75±1.44
5) Banana	400	4900	11.283±0.992	14.10±1.74	18.98±1.76	10.97±0.57
6) Image	1300	1010	4.391±0.631	17.64±1.52	6.89±0.73	2.47±0.53
7) Twonorm	400	7000	2.791±0.566	15.64±25.71	6.85±8.86	2.35±0.07
8) German	700	300	25.080±2.375	29.93±1.61	27.40±1.79	21.87±1.77
9) Waveform	400	4600	Not Reported	19.85±3.87	17.57±1.93	9.77±0.31
10) Thyroid	140	75	4.773±2.291	29.33±4.07	17.33±3.89	4.17±3.23

- The real values selected effect approximation quality
- Hyperparameter selection is now $\mathbb{R}^{p+2}$, rather than $\mathbb{R}^2$

Real World Dataset

Data set	CoV(%)	MAPE(%)	CoV(%)	MAPE(%)
House 1	19.6±1.69	15.3±0.47	20.1±0.81	16.1±0.85
Sensor A	1.3±0.05	1.0±0.05	–	–
Sensor B	17.2±4.89	10.8±0.25	–	–
Sensor C	12.0±2.31	7.8±0.68	–	–
Sensor D	1.4±0.09	0.9±0.03	–	–
S1	13.1±0.00	10.0±0.00	13.7±0.00	11.2±0.00
S2	3.1±0.00	4.7±0.00	6.4±0.00	4.5±0.00

- Selected hyperparameters work well with exact models

Outline

Conclusion

- The approach provides an $O(n \log n)$ l-fold cross-validation method
- The approach scales well
- The approach selects hyperparameters that perform well with the exact model
- Hyperparameter selection is now $\mathbb{R}^{p+2}$, rather than $\mathbb{R}^2$