Computationally Efficient Nyström Approximation using Fast Transforms

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Outline

- Background
- Motivation
- Fast Transforms for Nyström Approximation
  - Construct Structured Landmark Points
  - Using Fast Transforms to Speed up Kernel Value Evaluation
- Experimental Results on Fast Prediction

Background: Kernel Machines

- Popular kernel machines: training set $\{\mathbf{x}_i, y_i\}_{i=1}^n$, $\mathbf{x}_i \in \mathbb{R}^d$,
  - Kernel SVM

$$\boldsymbol{\alpha}^* \leftarrow \arg\min_{\boldsymbol{\alpha}} \frac{1}{2}\boldsymbol{\alpha}^T Q\boldsymbol{\alpha} - \mathbf{e}^T\boldsymbol{\alpha} \quad \text{s.t. } 0 \leq \boldsymbol{\alpha} \leq C,$$

  - Kernel Ridge Regression

$$\boldsymbol{\alpha}^* \leftarrow \arg\min_{\boldsymbol{\alpha}} \boldsymbol{\alpha}^T G\boldsymbol{\alpha} + \lambda\boldsymbol{\alpha}^T\boldsymbol{\alpha} - 2\boldsymbol{\alpha}^T\mathbf{y},$$

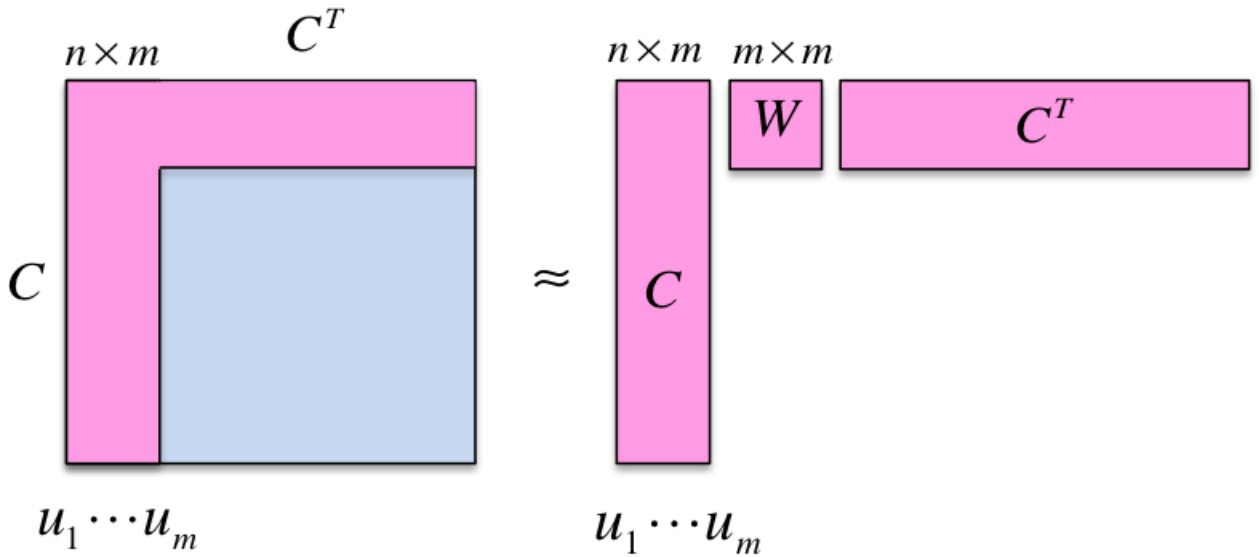
  $G \in \mathbb{R}^{n\times n}$ is the kernel matrix; $G_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$; $Q_{ij} = y_i y_j G_{ij}$.
- Slow Training:
  - $O(n^2 d)$ time to form the kernel matrix.
  - $O(n^2)$ space to store the kernel matrix.
- Slow Prediction:
  - Kernel SVM: $y = sign(\sum_{i=1}^n \alpha_i K(\mathbf{x}, \mathbf{x}_i))$; $O(d(\#SV))$.
  - Kernel Ridge Regression: $y = \sum_{i=1}^n \alpha_i K(\mathbf{x}, \mathbf{x}_i)$; $O(nd)$.

Background: Nyström Kernel Approximation

- Nyström approximation (Williams and Seeger, 2001): based on m landmark points $\mathbf{u}_1, \ldots, \mathbf{u}_m$:

$$G \approx \tilde{G} = CWC^T.$$

- Replace G with $\tilde{G}$ in the objective and train the model:



- Speed up training and prediction of kernel machines.

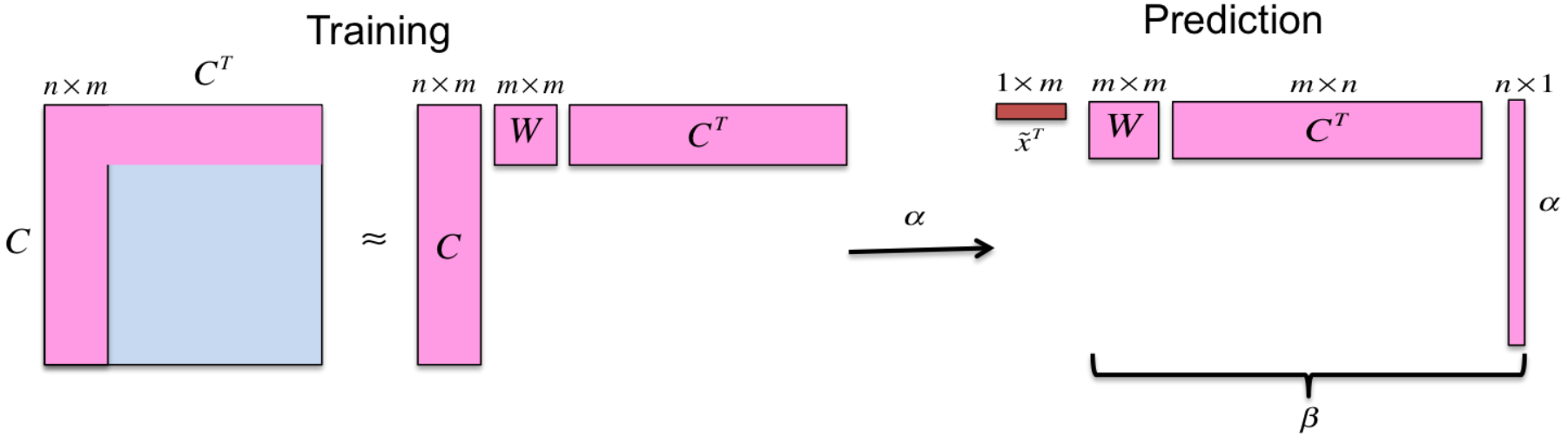
Background: Prediction Using Nyström Approximation

- Perform prediction on a new point $\mathbf{x}$ given the model $\boldsymbol{\alpha}$:

$$\sum_{i=1}^{n} \alpha_i \tilde{K}(\mathbf{x}, \mathbf{x}_i) = \tilde{\mathbf{x}}^T W C^T \boldsymbol{\alpha} = \tilde{\mathbf{x}}^T \boldsymbol{\beta}$$

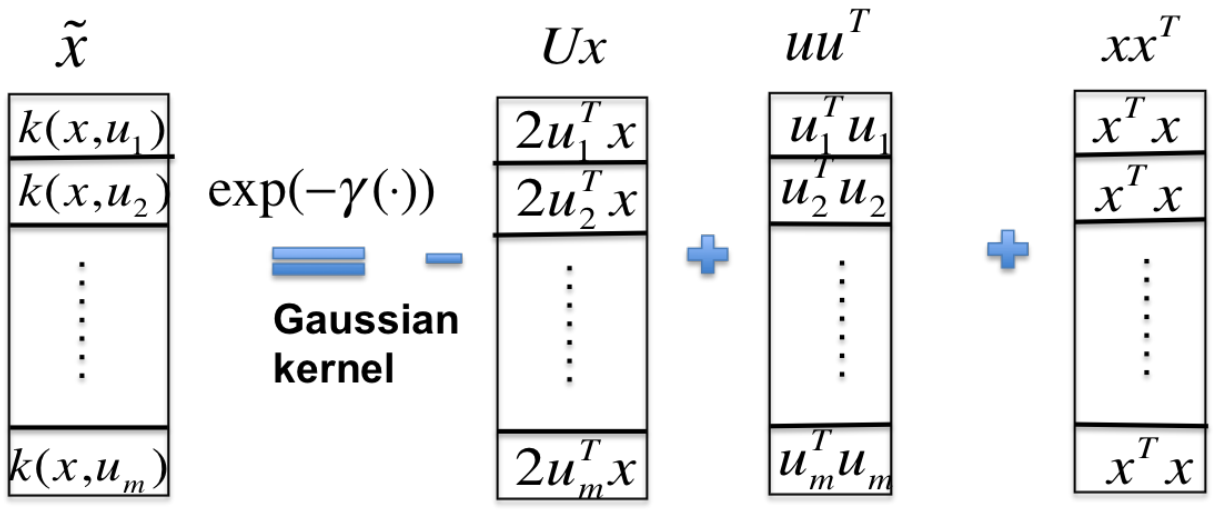
$$\text{where} \quad \tilde{\mathbf{x}} = [K(\mathbf{x}, \mathbf{u}_1), \ldots, K(\mathbf{x}, \mathbf{u}_m)]^T.$$

- Compute $\tilde{\mathbf{x}} = [k(\mathbf{x}, \mathbf{u}_1), \cdots, k(\mathbf{x}, \mathbf{u}_m)]^T$: $O(md)$.
- Compute $\tilde{\mathbf{x}}^T \beta$: $O(d)$.
- Time complexity for prediction: $O(nd) \rightarrow O(md) (n \gg m)$.



Motivation

- Consider the kernel form: $K(\mathbf{x}_i, \mathbf{x}_j) = f(\mathbf{x}_i) f(\mathbf{x}_j) g(\mathbf{x}_i^T \mathbf{x}_j)$.
- Gaussian kernel: $f(\mathbf{x}) = e^{-\|\mathbf{x}\|^2}, g(z) = e^{2z}$.



$$\exp(-\gamma \|x-u\|^2) = \exp(-\gamma(\underbrace{-2u^T x}_{} \quad \underbrace{+u^T u}_{} \quad \underbrace{+x^T x}_{}))$$

- On mnist dataset, with $n = 60K, m = 160$
  total time is 11.15 seconds and $T_{U\mathbf{x}}$ takes 10.81 seconds.
  The dominant term is $T_{U\mathbf{x}}$– usually takes $O(md)$.

Construct Landmark Points

- How to speed up $U\mathbf{x}$?
  Our solution: construct structured landmark points based on fast transforms.
- The form of landmark points U:

$$U = [H_d V_1, H_d V_2, \ldots, H_d V_m].$$

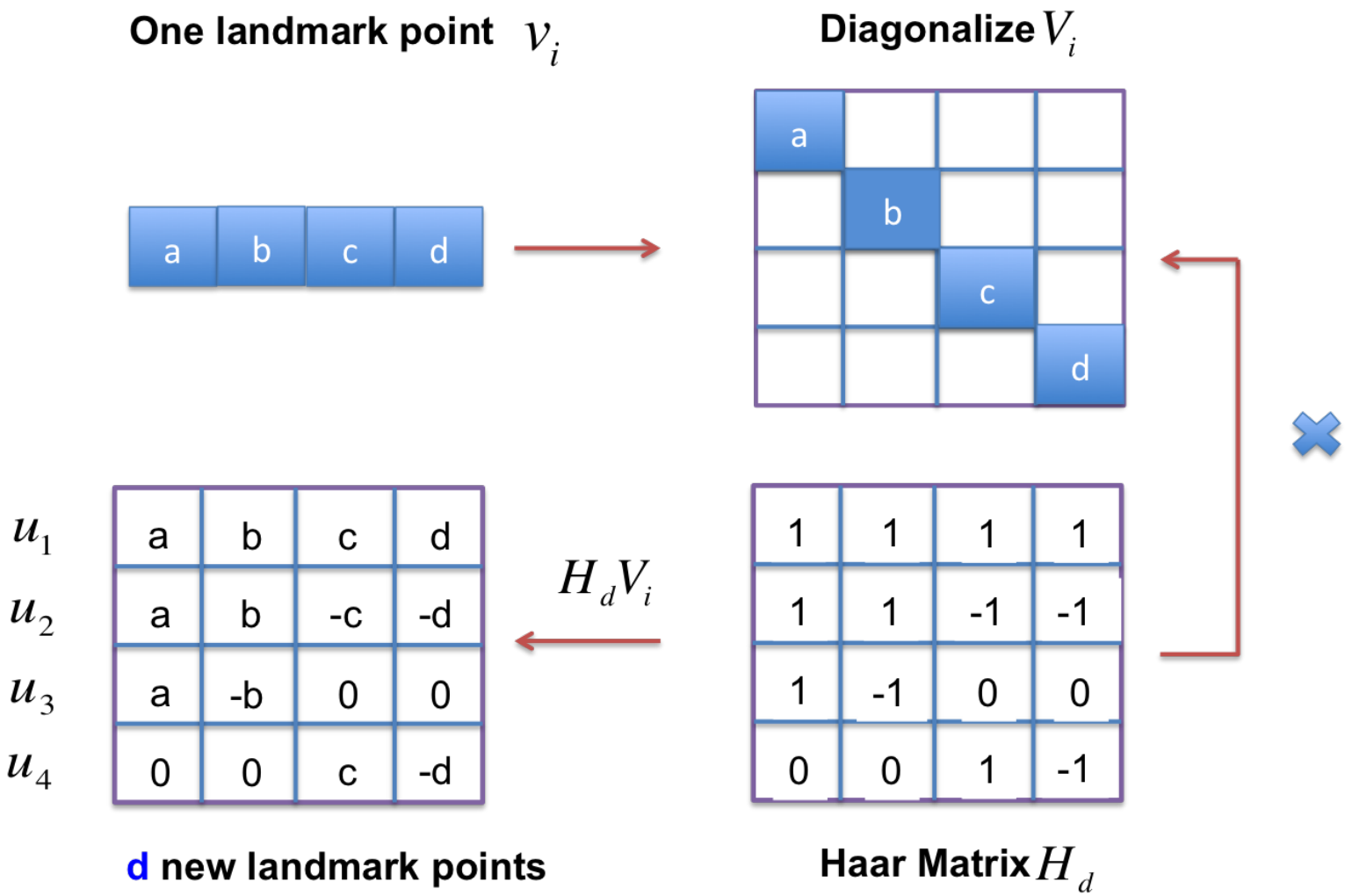
  - Given initial landmark point v_i, V_i is a diagonal matrix:

$$V_i = diag(v_{i1}, \cdots, v_{id}).$$

  - H_d contains the sign pattern of the Haar or Hadamard matrix:

$$H_{haar} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 \end{pmatrix}, \; H_{hadamard} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}.$$

Fast Transforms based Landmark Points



Construct Structured Landmark Points

- Initially m landmark points $v_1, \cdots, v_m$.
- The form of new landmark points U (*md* **landmark points**):

$$U = [H_d V_1,\ H_d V_2, \ldots, H_d V_m].$$

m initial landmark points ⟶ **md new landmark points**

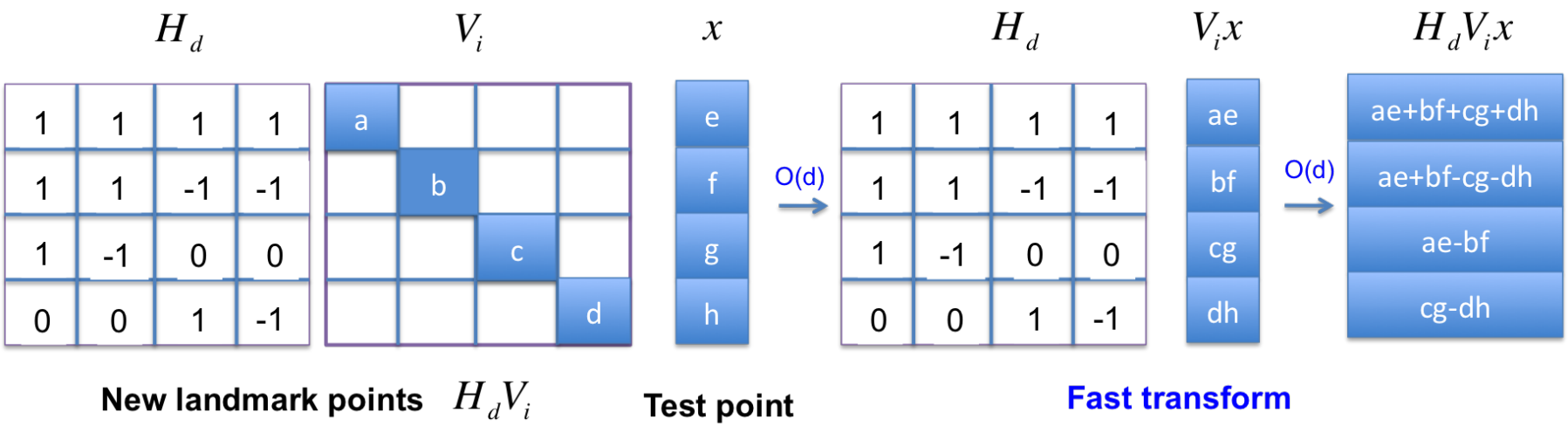
$$\{v_1,\cdots,v_m\} \to \left\{ \left[H_d \begin{pmatrix} v_{11} & 0 & \cdots & 0 \\ 0 & v_{12} & \cdots & \vdots \\ \vdots & \cdots & \ddots & 0 \\ 0 & \cdots & 0 & v_{1d} \end{pmatrix} \right], \cdots, \left[H_d \begin{pmatrix} v_{m1} & 0 & \cdots & 0 \\ 0 & v_{m2} & \cdots & \vdots \\ \vdots & \cdots & \ddots & 0 \\ 0 & \cdots & 0 & v_{md} \end{pmatrix} \right] \right\}$$

Benefit of U

- $U\mathbf{x}$ will become:

$$U\mathbf{x} = [(H_d V_1 \mathbf{x}),\ (H_d V_2 \mathbf{x}), \ldots,\ (H_d V_m \mathbf{x})].$$

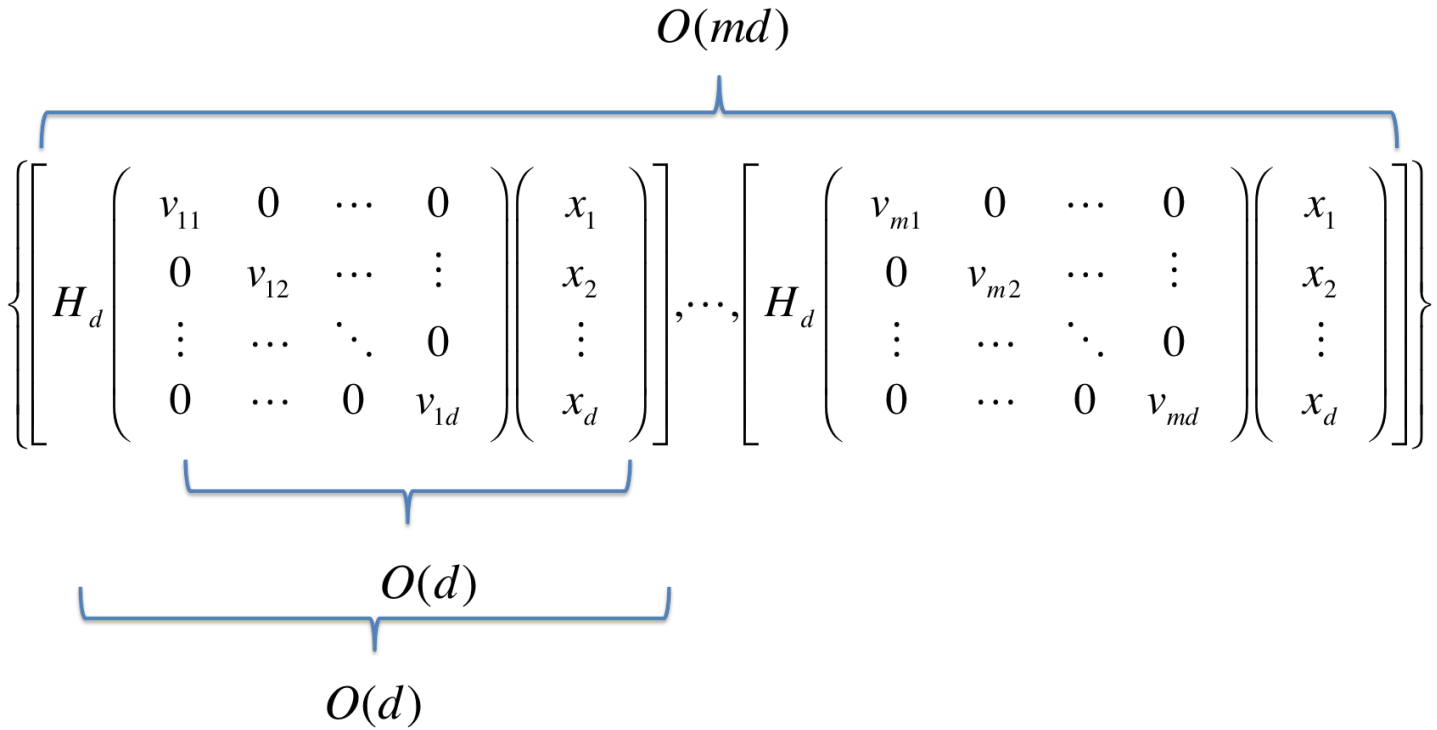
- Time for computing one block $H_d V_i \mathbf{x}$:
  - Haar landmark points: $O(d)$.
  - Hadamard landmark points: $O(dlog(d))$.



Prediction Cost

$$U\mathbf{x} = [(H_d V_1 \mathbf{x}),\ (H_d V_2 \mathbf{x}), \ldots,\ (H_d V_m \mathbf{x})]$$

- Time complexity analysis (*U* **has** *md* **landmark points**):



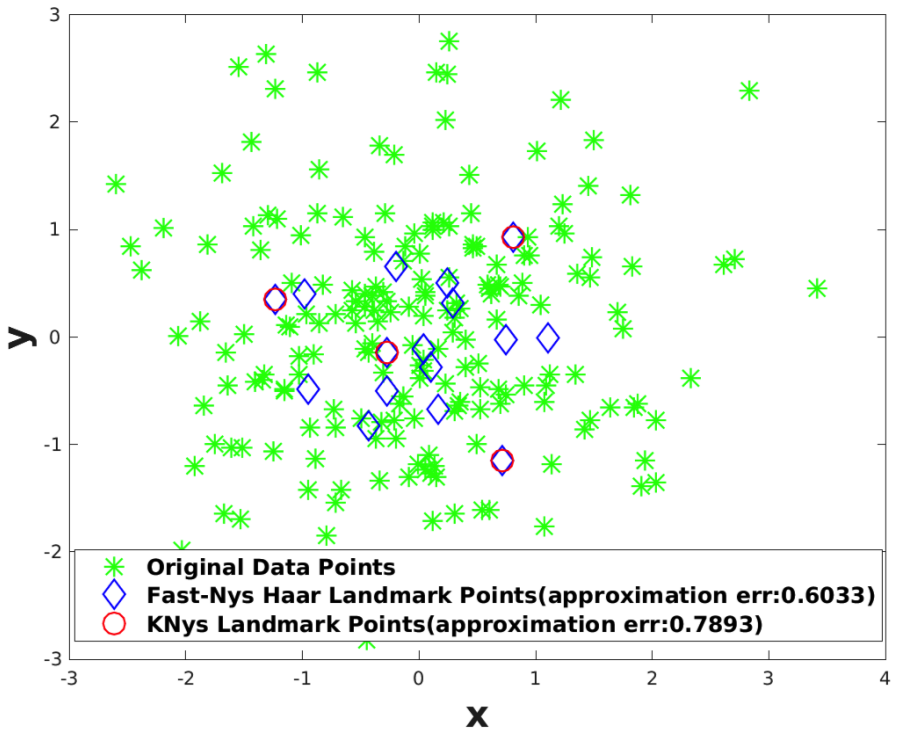
- Prediction time for *md* landmark points:
  - Haar landmark points: $O(md)$.
  - Hadamard landmark points: $O(mdlog(d))$.

Time Complexity Analysis

Table : Time complexity analysis. d is the dimension of the instance.

	# of initial landmark points	# of new landmark points	Prediction time
Standard Nyström	m	0	$O(md)$
Haar landmark points	m	md	$O(md)$
Hadamard landmark points	m	md	$O(md \log d)$

- $d = 4$; $m = 4$; initial landmark points are kmeans centroids



Setting:
4 dimensional data points
4 initial landmark points
16 new landmark points

Results:
Fast-Nys App. Error: 0.6033
Kmeans-Nys App. Error: 0.7893

Learning the Structure

- How to learn U automatically?
  - Satisfy the structural constraints $U = [H_d V_1,\ H_d V_2, \ldots, H_d V_m]$.
  - Minimize the upper bound of the kernel approximation error.

$$\arg\min_{U \in S} \sum_{i=1}^{n} \left(\min_{t(i)} \left\| x_i - u_{t(i)} \right\|^2 \right)$$

Structural constraints ↑ ↓ **Kmeans objective** ↑

$$U = [H_d V_1, \cdots, H_d V_m]$$

- How to do optimization? Kmeans-like way
  - Update indicator $t(i)$: the landmark point $\mathbf{u}_{t(i)}$ that $\mathbf{x}_i$ is closest to.
  - Update landmark points U: recompute the new centroids under structural constraints.
- Details are in the paper.

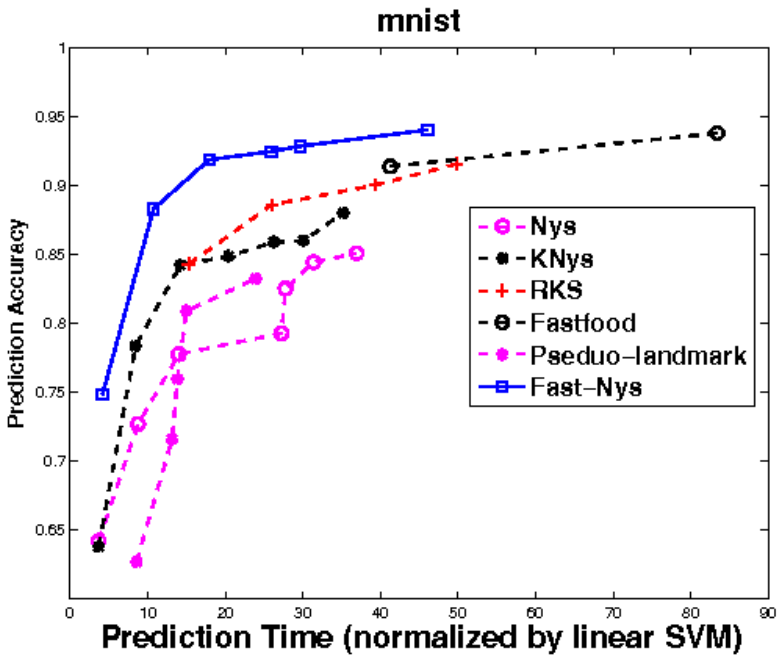
The Experimental Setting

- Methods compared in the experiments:
  1. The standard Nyström method(Nys)(Williams and Seeger, 2001);
  2. Kmeans Nyström (KNys)(Zhang et al. 2008);
  3. Random Kitchen Sinks(RKS)(Rahimi and Recht, 2007);
  4. Fastfood with "Hadamard features"(fastfood)(Le et al. 2013);
  5. Pseudo Landmark points (Pseudo) (Hsieh et al. 2014);
  6. The Local Deep Kernel Learning method (LDKL) (Jose et al. 2013);
  7. Divide-and-Conquer based fast Prediction (DC-Pred++)(Hsieh et al. 2014);
  8. Fast transform based Nyström Approximation (**Fast-Nys**) (Si et al. 2016).
- Data set statistics (n: number of samples):

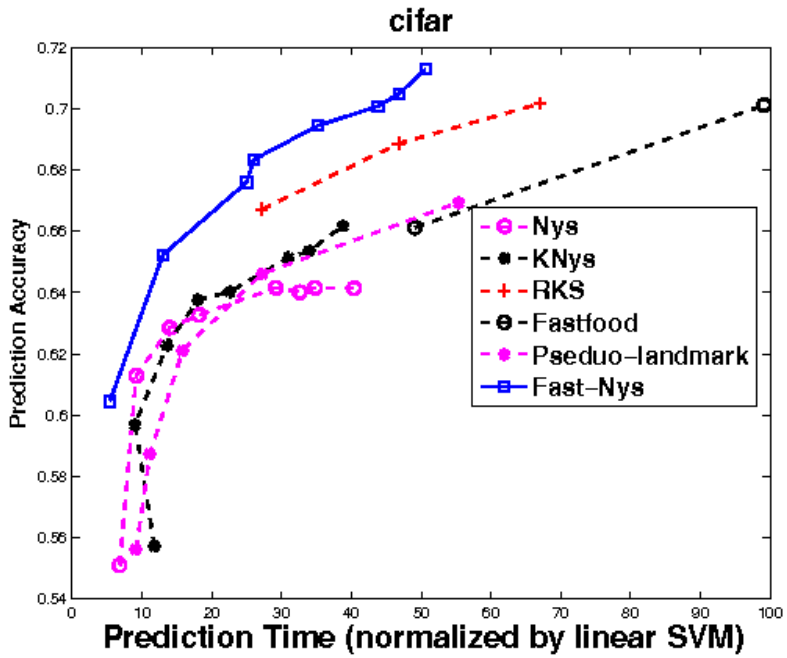
Dataset	n	d	Dataset	n	d
usps	9298	256	webspam	350,000	254
a9a	48,842	123	mnist	60,000	784
letter	18,000	16	cifar	60,000	400

Results on Fast Prediction

- Prediction Time vs. Prediction Accuracy.
- The unit of prediction time is linear SVM's prediction time.
- Both Haar and Hadamard landmark points yield similar results.



(a) mnist



(b) cifar

More Results on Fast Prediction

- Combine Fast-Nys with divide-and-conquer framework: **DC-Fast-Nys**.
- The unit in prediction time is linear SVM prediction time.
- DC-Pred++ and LDKL are two state-of-the-art fast prediction algorithms.

Dataset	Metric	**DC-Fast-Nys**	DC-Pred++	LDKL	KNys	RKS	Fastfood	Liblinear
letter	Prediction Time	**7.6x**	12.8x	29x	140x	61x	50x	1x
	Accuracy	95.4%	**95.90%**	95.78%	87.58%	89.93%	89.9%	73.08%
usps	Prediction Time	**7.31x**	14.4x	12.01x	200x	72.5x	80x	1x
	Accuracy	94.9%	95.56%	**95.96%**	92.53%	91.33%	94.39%	83.65%
webspam	Prediction Time	**11.21x**	20.5x	23x	200x	34.5x	80x	1x
	Accuracy	98.0%	**98.4%**	95.15%	95.01%	96.4%	96.7%	93.10%

Conclusions

- Observation: Computing Ux is the bottleneck.
- Fast-Nys: Fast Transforms for Nyström Approximation.
  - Construct Structured Landmark Points.
  - Using Fast Transforms to Speed up Kernel Value Evaluation.
- Experimental Results on Fast Prediction.

Our poster # 66 — Tuesday 10:00am to 1:00pm

References

[1] Williams, Christopher and Seeger, Matthias *Using the Nyström Method to Speed Up Kernel Machines.* NIPS, 2001.

[2] Hsieh, C.-J., Si, S., and Dhillon, I. S. Fast Prediction for Large-Scale Kernel Machines. NIPS, 2014.

[3] Jose, C., Goyal, P., Aggrwal, P., and Varma, M. Local deep kernel learning for efficient non-linear SVM prediction. ICML, 2013.

[4] Le, Q. V., Sarlos, T., and Smola, A. J. *Fastfood – Approximating Kernel Expansions in Loglinear Time.* ICML, 2013.

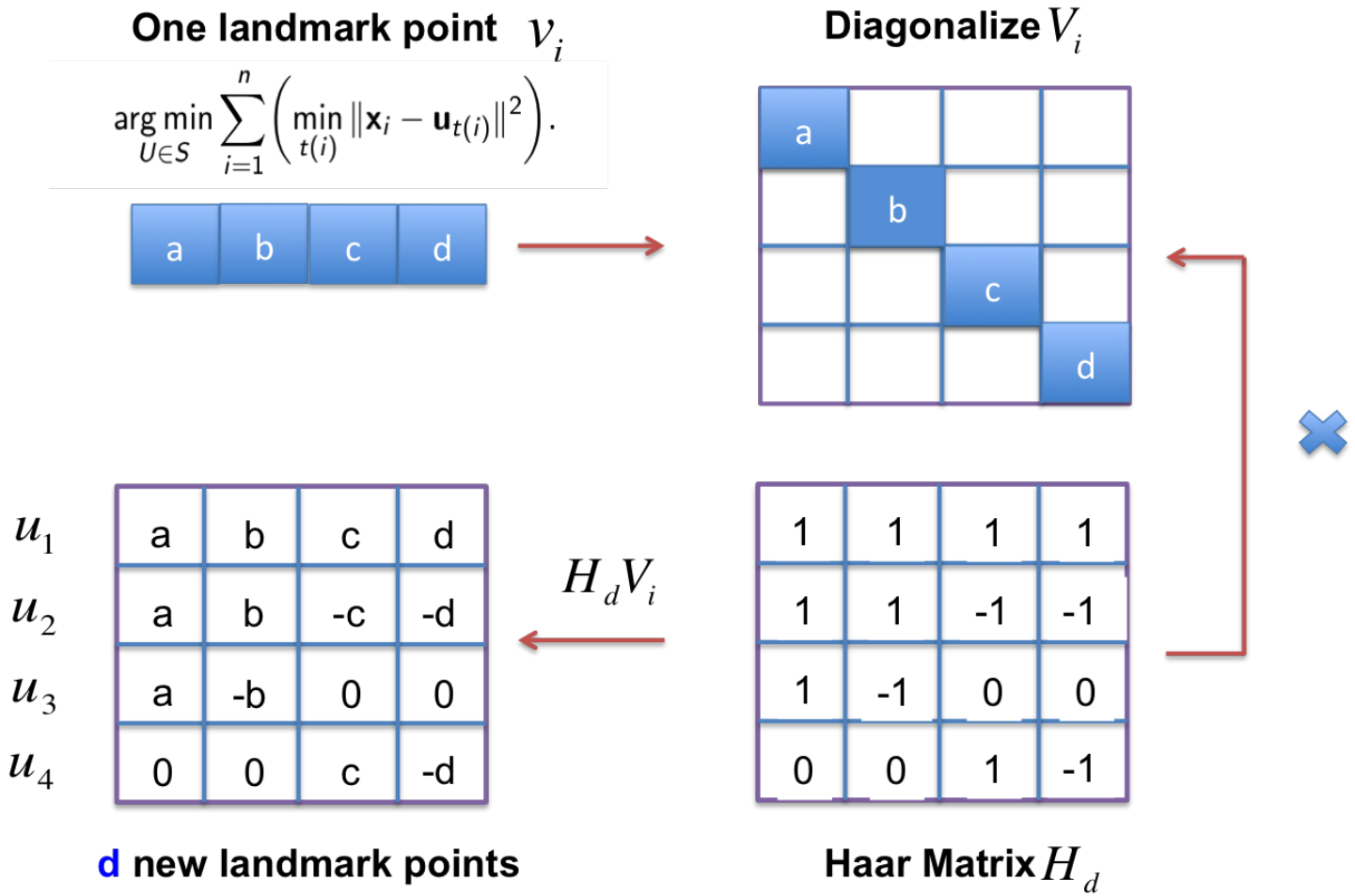
[5] Rahimi, A. and Recht, Benjamin. *Random Features for Large-scale Kernel Machines.* NIPS, 2007.

[6] Si, S., Hsieh, C.-J., and Dhillon, I. S. *Computationally Efficient Nyström Approximation using Fast Transforms.* ICML, 2016.

[7] Zhang, K, Tsang, I. W., and Kwok, J. T. *Improved Nyström Low Rank Approximation and Error Analysis.* ICML, 2008.

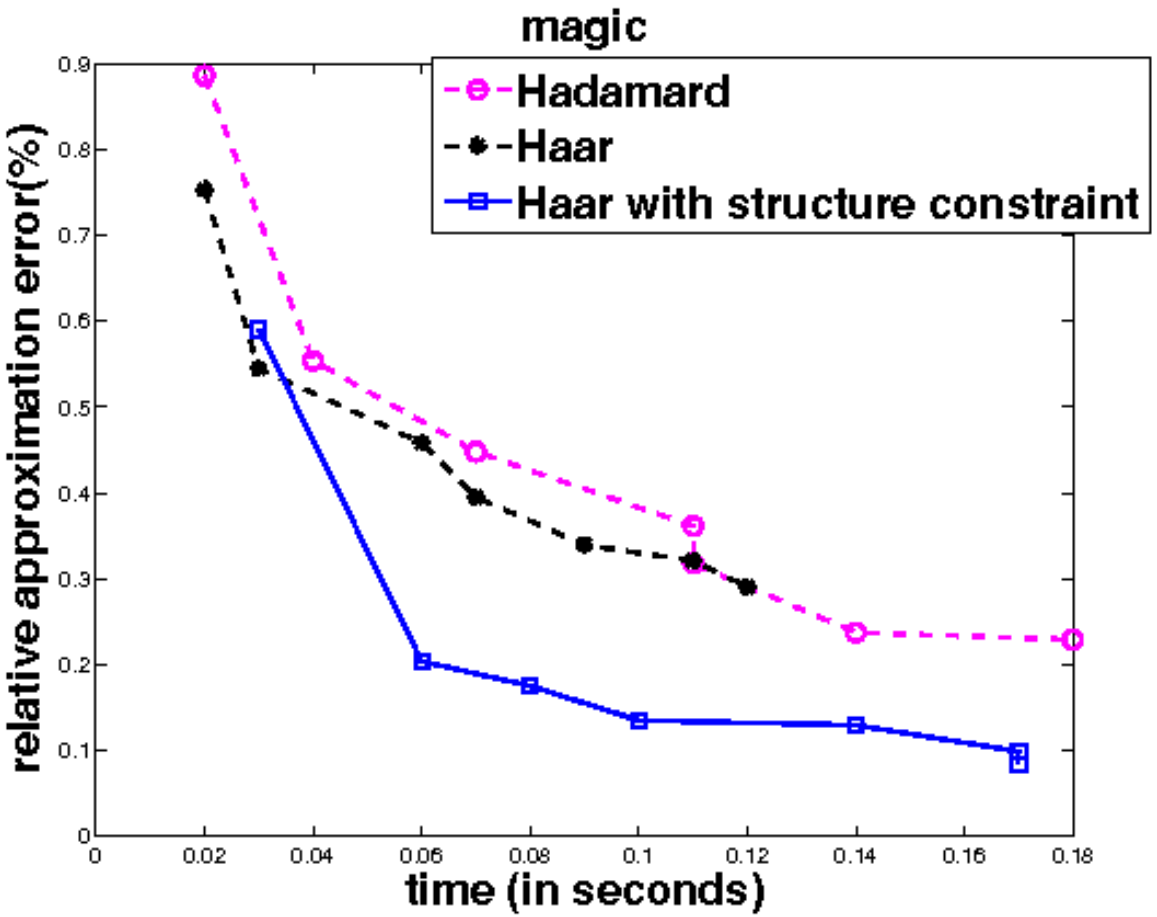
Algorithm

- Learn the initial *m* landmark points.
- Construct *md* new landmark points.
- Use *md* new landmark points during training and prediction.



Learning Structure of Landmark Points

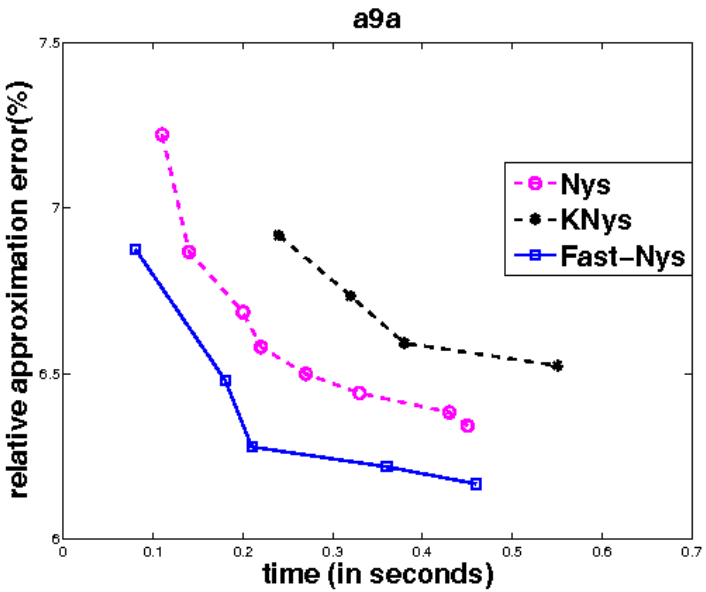
- Learning vs. not learning



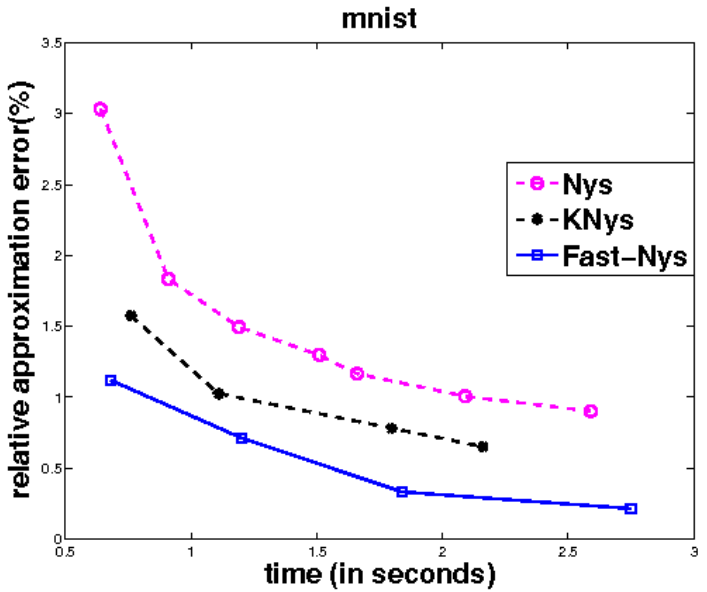
Results on Kernel Approximation

Relative kernel approximation error $\|G - \tilde{G}\|_F / \|G\|_F$.

- Time vs. kernel approximation error:



(c) a9a, polynomial.



(d) mnist,Gaussian.