Solving Non-Linear SVM in Linear Time? A Nyström Approximated SVM with Applications to Image Classification

Ming-Hen Tsai, Academia Sinica, Taiwan (now at Google Inc.)
Joint work with
Yi-Ren Yeh, Intel-NTU Connected Context Computing Center
Yuh-Jye Lee, Dept. CSIE, National Taiwan University Science & Technology
Yu-Chiang Frank Wang, Research Center for IT Innovation, Academia Sinica

May 21, 2013

Outline

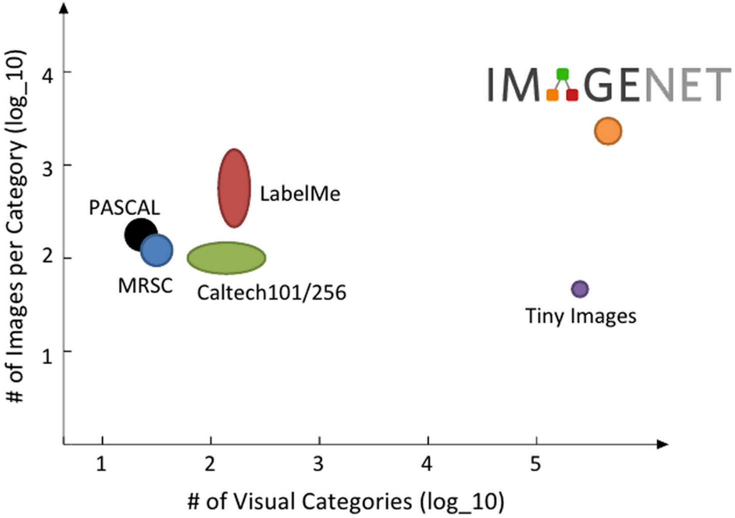
- Introduction
- The Nyström Method for Kernel Approximation
- The Nyström Method for Linear SVM Classification
- Experiments and Conclusions

Outline

- Introduction
- The Nyström Method for Kernel Approximation
- The Nyström Method for Linear SVM Classification
- Experiments and Conclusions

Visual Classification: Faces, Objects, and Beyond

Example: Some Image Classification Data Sets



We Have Known...

- Non-linear SVM: powerful but slow
- Linear SVM: simple but fast

  Paper: "Training Linear SVMs in Linear Time" by Joachims KDD'06

  Software: LIBLINEAR, VW, etc.

We Had Always Wondered...

- But we want something **powerful** and **fast**: train faster than non-linear SVM and generate a more accurate model than linear SVM.

We Had Always Wondered...

- But we want something **powerful** and **fast**: train faster than non-linear SVM and generate a more accurate model than linear SVM.

  Is this even possible?

We Had Always Wondered...

- But we want something **powerful** and **fast**: train faster than non-linear SVM and generate a more accurate model than linear SVM.

  Is this even possible?

  Yes. Do approximation!

Outline

- Introduction
- The Nyström Method for Kernel Approximation
- The Nyström Method for Linear SVM Classification
- Experiments and Conclusions

Definitions and a Brief Review (1/2)

- Input Data: $\{(\mathbf{y}, X)\} = \{(y_i, \mathbf{x}_i)\}_{i=1}^{\ell}$. y_i: label, $\mathbf{x}_i$: feature vector.
- Dimension of $\mathbf{x}_i$: d
- Non-linear mapping $\phi(\mathbf{x})$ (e.g. bi-gram features)
- Kernel function: $K(\mathbf{u}, \mathbf{v}) = \phi(\mathbf{u})^T \phi(\mathbf{v})$, usually computed in linear time.
- For ease of representation, for $U = [\mathbf{u}_1, \ldots, \mathbf{u}_\ell]$ and $V = [\mathbf{v}_1, \ldots, \mathbf{v}_{\tilde{\ell}}]$, we define $Q = K(U, V)$, where $Q_{ij} = K(\mathbf{u}_i, \mathbf{v}_j)$

Definitions and a Brief Review (1/2)

- Input Data: $\{(\mathbf{y}, X)\} = \{(y_i, \mathbf{x}_i)\}_{i=1}^{\ell}$. y_i: label, $\mathbf{x}_i$: feature vector.
- Dimension of $\mathbf{x}_i$: d
- Non-linear mapping $\phi(\mathbf{x})$ (e.g. bi-gram features)
- Kernel function: $K(\mathbf{u}, \mathbf{v}) = \phi(\mathbf{u})^T \phi(\mathbf{v})$, usually computed in linear time.
- For ease of representation, for $U = [\mathbf{u}_1, \ldots, \mathbf{u}_\ell]$ and $V = [\mathbf{v}_1, \ldots, \mathbf{v}_{\tilde{\ell}}]$, we define $Q = K(U, V)$, where $Q_{ij} = K(\mathbf{u}_i, \mathbf{v}_j)$
- Lower bound for data storage and training: $\Omega(\ell d)$.

Definitions and a Brief Review (2/2)

- Primal SVM:

$$\min_{\mathbf{w},b} \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{i=1}^{\ell} \max(1 - y_i\mathbf{w}^T\phi(\mathbf{x}_i), 0)$$

- Dual SVM:

$$\begin{aligned} \min_{\boldsymbol{\alpha}} \ & \frac{1}{2}\boldsymbol{\alpha}^T Q\boldsymbol{\alpha} - \mathbf{e}^T\boldsymbol{\alpha} \\ \text{s.t. } & 0 \le \alpha_i \le C \quad \forall i. \end{aligned}$$

- Primal-Dual Correspondence: $\mathbf{w} = \sum_{i=1}^{\ell} y_i\alpha_i\phi(\mathbf{x}_i)$

Kernel in Non-linear SVM

- Dual form:

$$\min_{\boldsymbol{\alpha}} \frac{1}{2}\boldsymbol{\alpha}^T Q \boldsymbol{\alpha} - \mathbf{e}^T \boldsymbol{\alpha}$$
$$\text{s.t. } 0 \leq \alpha_i \leq C \quad \forall i.$$

- Kernel matrix Q with $Q_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$.

Kernel in Non-linear SVM

- Dual form:

$$\begin{aligned}\min_{\boldsymbol{\alpha}} \ & \frac{1}{2}\boldsymbol{\alpha}^T Q\boldsymbol{\alpha} - \mathbf{e}^T\boldsymbol{\alpha} \\ \text{s.t. } & 0 \leq \alpha_i \leq C \quad \forall i.\end{aligned}$$

- Kernel matrix Q with $Q_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$.
  Computational time: $O(\ell^2 d) \sim \ell$ times data size.
  Space: $O(\ell^2)$.

Kernel in Non-linear SVM

- Dual form:

$$\begin{aligned} \min_{\boldsymbol{\alpha}} \ & \frac{1}{2}\boldsymbol{\alpha}^T Q \boldsymbol{\alpha} - \mathbf{e}^T \boldsymbol{\alpha} \\ \text{s.t. } & 0 \le \alpha_i \le C \quad \forall i. \end{aligned}$$

- Kernel matrix Q with $Q_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$.

  Computational time: $O(\ell^2 d) \sim \ell$ times data size.

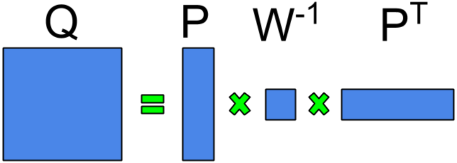
  Space: $O(\ell^2)$.
- $1M$ images: $1M$ times more computational time than the linear counterpart.

Nyström Method

- A low-rank kernel approximation method. (Why?)

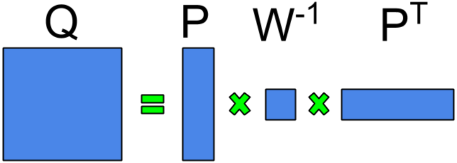
Nyström Method

- A low-rank kernel approximation method. (Why?)
- Sample $\tilde{\ell}(\ll \ell)$ feature vectors from X with a basis set $B = \{\mathbf{b}_i\}_{i=1}^{\tilde{\ell}}$.
  The low-rank apprxoimated kernel: $Q \sim \tilde{Q} = PW^{-1}P^T$, where $P_{ij} = K(\mathbf{x}_i, \mathbf{b}_j)$ and $W_{ij} = K(\mathbf{b}_i, \mathbf{b}_j)$.



Nyström Method

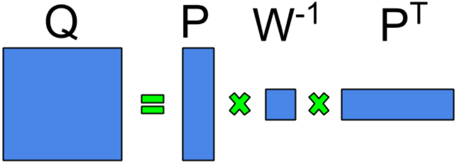
- A low-rank kernel approximation method. (Why?)
- Sample $\tilde{\ell}(\ll \ell)$ feature vectors from X with a basis set $B = \{\mathbf{b}_i\}_{i=1}^{\tilde{\ell}}$.
  The low-rank apprxoimated kernel: $Q \sim \tilde{Q} = PW^{-1}P^T$, where $P_{ij} = K(\mathbf{x}_i, \mathbf{b}_j)$ and $W_{ij} = K(\mathbf{b}_i, \mathbf{b}_j)$.



- Time: Basis Selection + $O(\ell^2 \max(\tilde{\ell}, d))$ overall. (Alright...)
  Space: $O(\ell \max(\tilde{\ell}, d))$. (Good! Don't know how large is $\tilde{\ell}$..)

Nyström Method

- A low-rank kernel approximation method. (Why?)
- Sample $\tilde{\ell}(\ll \ell)$ feature vectors from X with a basis set $B = \{\mathbf{b}_i\}_{i=1}^{\tilde{\ell}}$.
  The low-rank apprxoimated kernel: $Q \sim \tilde{Q} = PW^{-1}P^T$, where $P_{ij} = K(\mathbf{x}_i, \mathbf{b}_j)$ and $W_{ij} = K(\mathbf{b}_i, \mathbf{b}_j)$.



- Time: Basis Selection + $O(\ell^2 \max(\tilde{\ell}, d))$ overall. (Alright...)
  Space: $O(\ell \max(\tilde{\ell}, d))$. (Good! Don't know how large is $\tilde{\ell}$..)
- Set our basis size, $\tilde{\ell}$ to d. The space consumption is optimal.

Outline

- Introduction
- The Nyström Method for Kernel Approximation
- The Nyström Method for Linear SVM Classification
- Experiments and Conclusions

An Equivalent Representation (1/2)

- Bottleneck: kernel matrix Q of size $O(\ell^2)$.

  But observe the following...

An Equivalent Representation (1/2)

- Bottleneck: kernel matrix Q of size $O(\ell^2)$.

  But observe the following...
- $Q = \tilde{X}^T \tilde{X}$ by Cholesky decomposition. (This is valid because Q is PSD by definition.)
- Investigate the columns of $\tilde{X} = [\tilde{\mathbf{x}}_1 \ldots \tilde{\mathbf{x}}_\ell]$. We have $\tilde{\mathbf{x}_i}^T \tilde{\mathbf{x}_j} = Q_{ij} = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j) = K(\mathbf{x}_i, \mathbf{x}_j)$.

An Equivalent Representation (1/2)

- Bottleneck: kernel matrix Q of size $O(\ell^2)$.

  But observe the following...
- $Q = \tilde{X}^T \tilde{X}$ by Cholesky decomposition. (This is valid because Q is PSD by definition.)
- Investigate the columns of $\tilde{X} = [\tilde{\mathbf{x}}_1 \ldots \tilde{\mathbf{x}}_\ell]$. We have $\tilde{\mathbf{x}_i}^T \tilde{\mathbf{x}_j} = Q_{ij} = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j) = K(\mathbf{x}_i, \mathbf{x}_j)$.
- We represent the kernelized linear products as regular linear products. Let's call $\tilde{X}$ a compact representation.

An Equivalent Representation (2/2)

- SVM Dual:

$$\begin{aligned} &\min_{\boldsymbol{\alpha}} \frac{1}{2}\boldsymbol{\alpha}^T Q\boldsymbol{\alpha} - \mathbf{e}^T\boldsymbol{\alpha} \\ &\text{s.t. } 0 \leq \alpha_i \leq C \quad \forall i. \end{aligned}$$

An Equivalent Representation (2/2)

- SVM Dual:

$$\min_{\boldsymbol{\alpha}} \frac{1}{2}\boldsymbol{\alpha}^T Q \boldsymbol{\alpha} - \mathbf{e}^T \boldsymbol{\alpha}$$
$$\text{s.t. } 0 \le \alpha_i \le C \quad \forall i.$$

- SVM Primal:

$$\min_{\mathbf{w},b} \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{i=1}^{\ell} \max(1 - y_i\mathbf{w}^T\tilde{\mathbf{x}}_i, 0)$$

An Equivalent Representation (2/2)

- SVM Dual:

$$\min_{\boldsymbol{\alpha}} \frac{1}{2}\boldsymbol{\alpha}^T Q\boldsymbol{\alpha} - \mathbf{e}^T\boldsymbol{\alpha}$$
$$\text{s.t. } 0 \le \alpha_i \le C \quad \forall i.$$

- SVM Primal:

$$\min_{\mathbf{w},b} \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{i=1}^{\ell} \max(1 - y_i\mathbf{w}^T\tilde{\mathbf{x}}_i, 0)$$

- Issue: computing $\tilde{\mathbf{x}}_i$ requires the computation of the ℓ^2-sized kernel.

Nyströms' Equivalent Representation

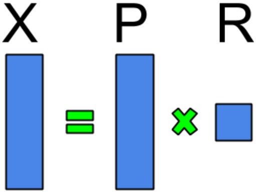
- Let's go back to kernel approximation!

Nystöms' Equivalent Representation

- Let's go back to kernel approximation!
- As $\tilde{Q} = PW^{-1}P^T$, we can find a matrix R such that $W^{-1} = RR^T$, and $(PR)^T$ is our a compact representation.

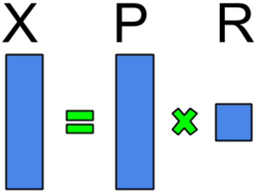
Nystöms' Equivalent Representation

- Let's go back to kernel approximation!
- As $\tilde{Q} = PW^{-1}P^T$, we can find a matrix R such that $W^{-1} = RR^T$, and $(PR)^T$ is our a compact representation.



Nystroms' Equivalent Representation

- Let's go back to kernel approximation!
- As $\tilde{Q} = PW^{-1}P^T$, we can find a matrix R such that $W^{-1} = RR^T$, and $(PR)^T$ is our a compact representation.

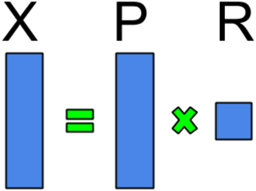


Time: Basis selection time $+ \, O(\ell\tilde{\ell}d)$ overall.

Space: $O(\ell \max(\tilde{\ell}, d))$.

Nystöms' Equivalent Representation

- Let's go back to kernel approximation!
- As $\tilde{Q} = PW^{-1}P^T$, we can find a matrix R such that $W^{-1} = RR^T$, and $(PR)^T$ is our a compact representation.



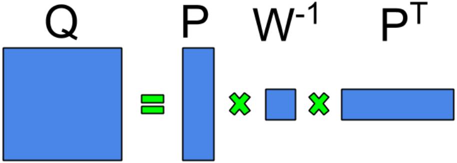
Time: Basis selection time $+\ O(\ell\tilde{\ell}d)$ overall.

Space: $O(\ell \max(\tilde{\ell}, d))$.

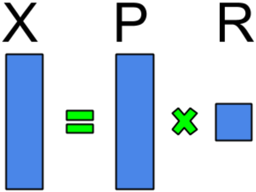
- Needs a linear feature selection method!

Brief Recap

- Nyström approximation



- Nyström approximation for linear representation



Another View of Basis Selection (1/2)

- Recall that: $P_{i:} = [K(\mathbf{x}_i, \mathbf{b}_1), \ldots, K(\mathbf{x}_i, \mathbf{b}_{\tilde{\ell}})]$
- Can we view PR as input data and do feature selection?

Another View of Basis Selection (1/2)

- Recall that: $P_{i:} = [K(\mathbf{x}_i, \mathbf{b}_1), \ldots, K(\mathbf{x}_i, \mathbf{b}_{\tilde{\ell}})]$
- Can we view PR as input data and do feature selection?
- No! R introduces dependency between dimensions.

Another View of Basis Selection (1/2)

- Recall that: $P_{i:} = [K(\mathbf{x}_i, \mathbf{b}_1), \ldots, K(\mathbf{x}_i, \mathbf{b}_{\tilde{\ell}})]$
- Can we view PR as input data and do feature selection?
- No! R introduces dependency between dimensions.
- We remove R! Each dimension is then independent of other basis vector.
- L1-regularized linear SVM which runs linear time in data size is used in the work.

Another View of Basis Selection (2/2)

- Does it hurt by removing R?

Another View of Basis Selection (2/2)

- Does it hurt by removing R?
- Say $\mathbf{x}_+$ and $\mathbf{x}_-$ are two samples with different labels.

Another View of Basis Selection (2/2)

- Does it hurt by removing R?
- Say $\mathbf{x}_+$ and $\mathbf{x}_-$ are two samples with different labels.
- If for a $\mathbf{w}$, $\mathbf{w}^T\mathbf{x}_+ > \mathbf{w}^T\mathbf{x}_-$ (separable), then $\mathbf{w}^T R^{T^{-1}} R^T \mathbf{x}_+ > \mathbf{w}^T R^{T^{-1}} R^T \mathbf{x}_-$.

Another View of Basis Selection (2/2)

- Does it hurt by removing R?
- Say $\mathbf{x}_+$ and $\mathbf{x}_-$ are two samples with different labels.
- If for a $\mathbf{w}$, $\mathbf{w}^T\mathbf{x}_+ > \mathbf{w}^T\mathbf{x}_-$ (separable), then $\mathbf{w}^T R^{T^{-1}} R^T \mathbf{x}_+ > \mathbf{w}^T R^{T^{-1}} R^T \mathbf{x}_-$.
- $R^{T^{-1}}\mathbf{w}$ separates $R^T\mathbf{p}_+$ and $R^T\mathbf{p}_-$.

Another View of Basis Selection (2/2)

- Does it hurt by removing R?
- Say $\mathbf{x}_+$ and $\mathbf{x}_-$ are two samples with different labels.
- If for a $\mathbf{w}$, $\mathbf{w}^T\mathbf{x}_+ > \mathbf{w}^T\mathbf{x}_-$ (separable), then $\mathbf{w}^T {R^T}^{-1} R^T \mathbf{x}_+ > \mathbf{w}^T {R^T}^{-1} R^T \mathbf{x}_-$.
- ${R^T}^{-1}\mathbf{w}$ separates $R^T\mathbf{p}_+$ and $R^T\mathbf{p}_-$.
- When doing the linear tranformation by R, we preserve separability.

The Algorithm Workflow

1. Input data: $(\mathbf{y}, X)$, a kernel K.
2. Run basis selection on $K(X, B)$.
3. Compute the new data $\tilde{X} = RK(X, B)$, where $R^T R = K(B, B)^{-1}$.
4. Train on $(\mathbf{y}, \tilde{X})$

The Algorithm Workflow

1. Input data: $(\mathbf{y}, X)$, a kernel K.
2. Run basis selection on $K(X, B)$.
3. Compute the new data $\tilde{X} = RK(X, B)$, where $R^T R = K(B, B)^{-1}$.
4. Train on $(\mathbf{y}, \tilde{X})$

   If we use $\tilde{\ell}$ samples to do Step 2.

The Algorithm Workflow

1. Input data: $(\mathbf{y}, X)$, a kernel K.
2. Run basis selection on $K(X, B)$.
3. Compute the new data $\tilde{X} = RK(X, B)$, where $R^T R = K(B, B)^{-1}$.
4. Train on $(\mathbf{y}, \tilde{X})$

   If we use $\tilde{\ell}$ samples to do Step 2.

   Time: $O(\ell\tilde{\ell}d)$ overall.

   Space: $O(\ell \max(\tilde{\ell}, d))$.

Outline

- Introduction
- The Nyström Method for Kernel Approximation
- The Nyström Method for Linear SVM Classification
- Experiments and Conclusions

Experimental Settings

- We conduct experiments on two benchmark datasets: USPS and MNIST.
- We randomly split 70% of the data for training and the remaining 30% for testing. (Repeat 5 times)
- We perform a five-fold cross validation to select the parameters γ and C.

Table: Dataset descriptions (with the number ℓ of instances and the dimension d of the data). The sizes for storing the data ℓd and the associated kernel matrices ℓ^2 are also listed.

	ℓ	d	kernel size ℓ^2	data size ℓd
USPS	7291	256	53M	2M
MNIST	60000	780	3.6G	47M

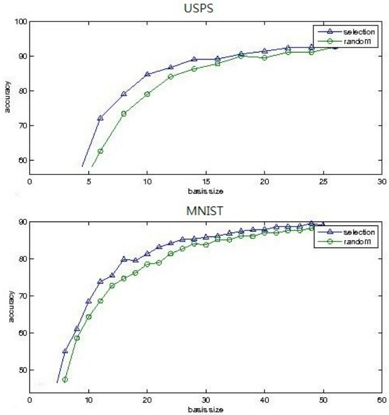
Compare Accuracy between Different Types of Methods

- Our method achieved improved accuracy than linear SVMs
- The time for training and testing using our proposed model is comparable to that of linear SVMs
- The standard nonlinear SVM utilizes the full kernel matrix whose time complexity is quadratically scaled-up with ℓ.

USPS	Accuracy	Training Time	Testing Time
Nyström primal SVM	97.057 ± 0.402	3.764	0.320
nonlinear SVM	98.007 ± 0.198	14.507	4.129
linear SVM	95.009 ± 0.275	2.274	0.079
MNIST	Accuracy	Training Time	Testing Time
Nyström primal SVM	93.833 ± 0.115	24.6092	2.006
nonlinear SVM	98.547 ± 0.066	3650.334	524.487
linear SVM	91.917 ± 0.077	14.510	0.381

Comparisons to Random Basis Selection

- Compare basis matrix determined by our method to
- the random sampling basis selection strategy



Conclusion

- Primal low-rank representation of Nytröm-approximated dual SVM.

  Training: linearly in time and space.

  Accuracy: almost as good as non-linear SVM.

  Prediction: nearly as fast as linear SVM. (e.g. Realtime robot vision applications.)
- Connect feature selection with basis selection in Nyström method.

  A basis selection method that preserves separability.
- Applications: Large-Scale Image Retrieval, Realtime Machine Vision (training/test should be nearly as fast as feature extraction,) etc.

Thank You

The most update-to-date code and slides are at `https://github.com/scan33scan33`.
Feel free to drop me questions and discussions.