Large Scale Learning with String Kernels

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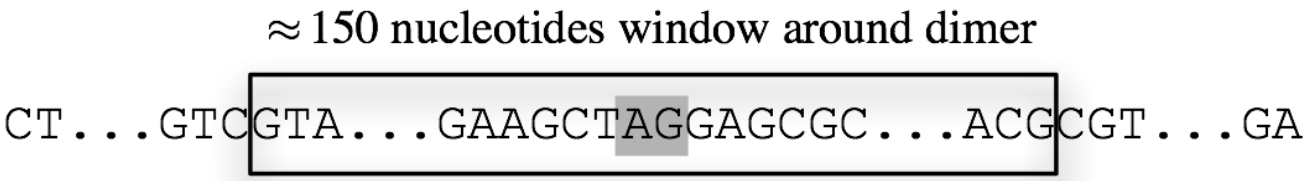
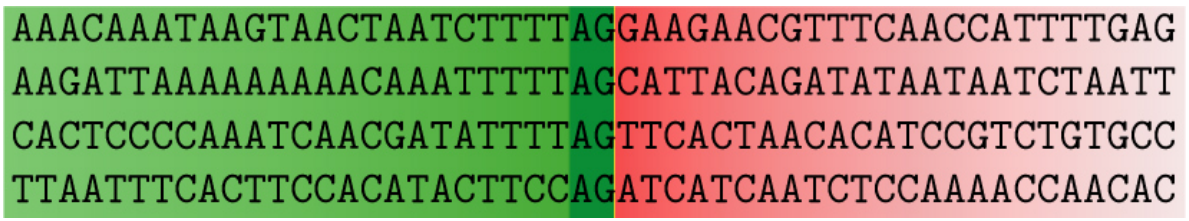
The Motivating Application - Splice Site recognition

Discriminate true signal positions against all other positions



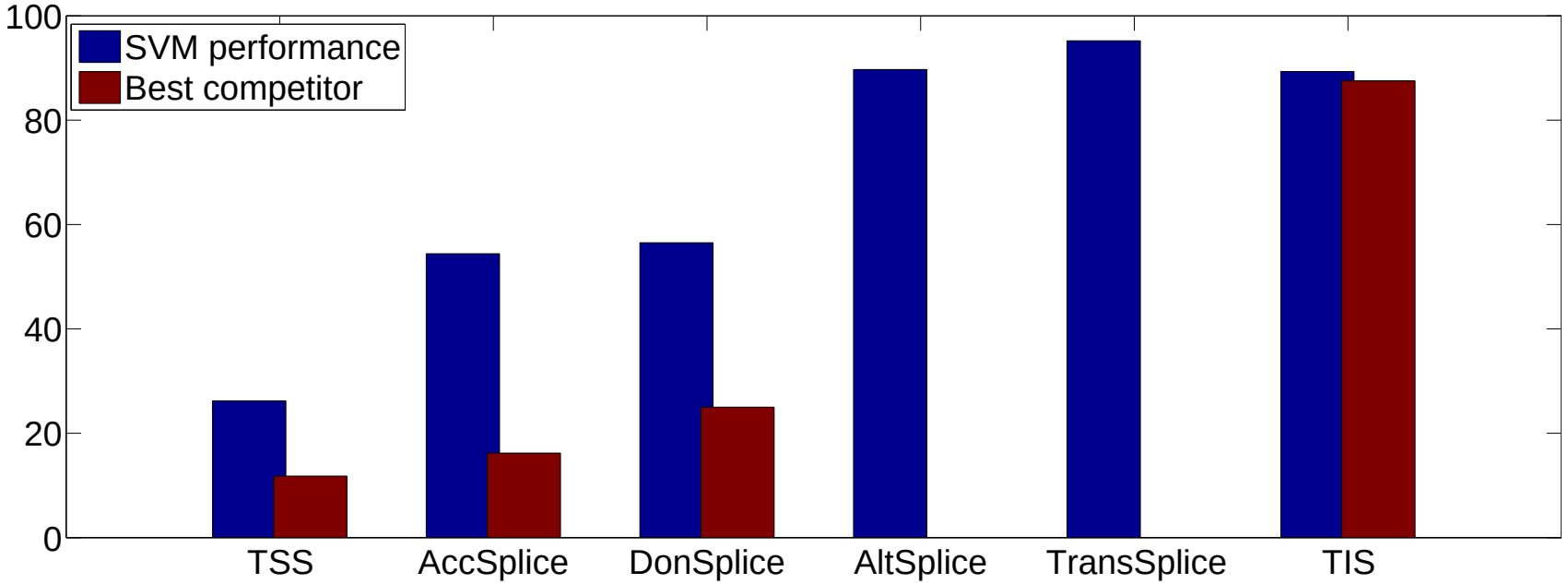
- True sites: fixed window around a true splice site
- Decoy sites: all other consensus sites



- Sequences are compared via String-Kernels
  - For each position a Weighted Degree Kernel compares all k-mers up to maximal length K

SVM ≈ 3 times more accurate than IMCs
(54.4% vs. 16.2% auPRC)

Beauty in Generality

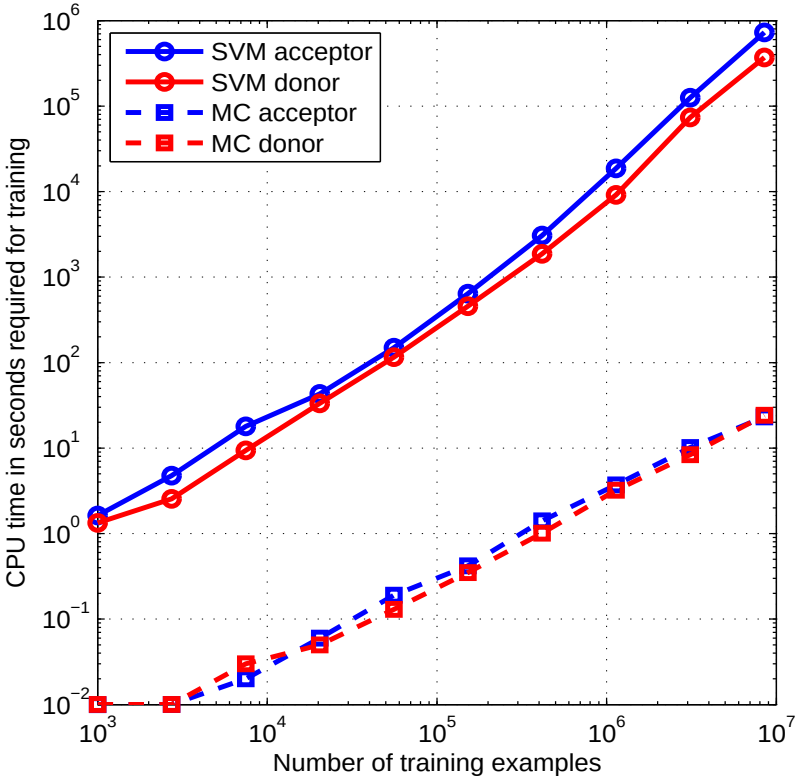


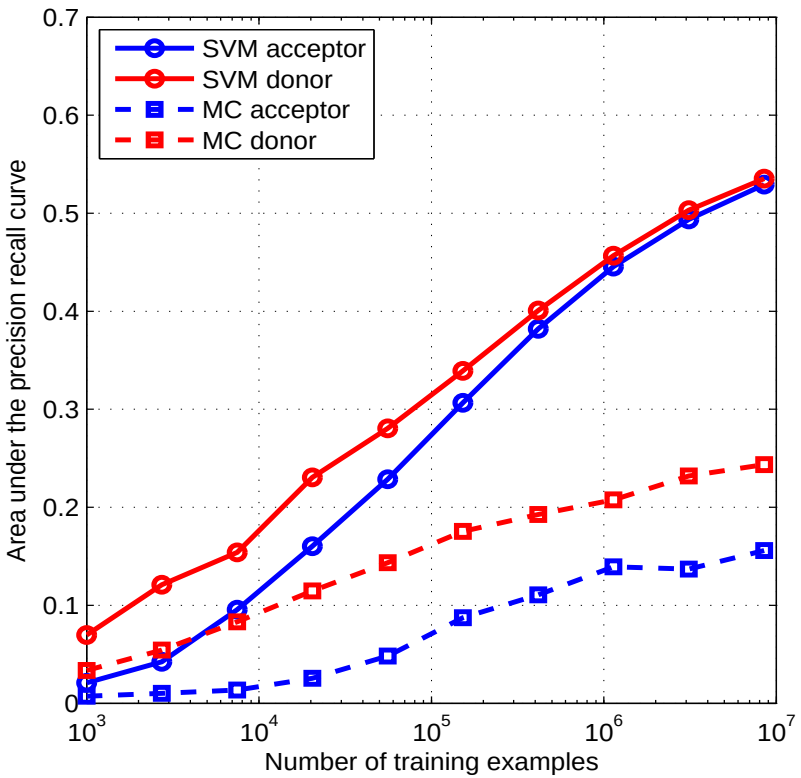
- Transcription Start (Sonnenburg et al., Eponine Down et al.)
- Acceptor Splice Site (Philips et al.)
- Donor Splice Site (Philips et al.)
- Alternative Splicing (Rätsch et al., -)
- Transsplicing (Schweikert et al., -)
- Translation Initiation (Sonnenburg et al., Saeys et al.)

Drawback: SVM Training Time too large

Task

- Human splice sites: $5 \cdot 10^7$ strings of length ≈ 200
- Note: Raw data is already 9GB in size

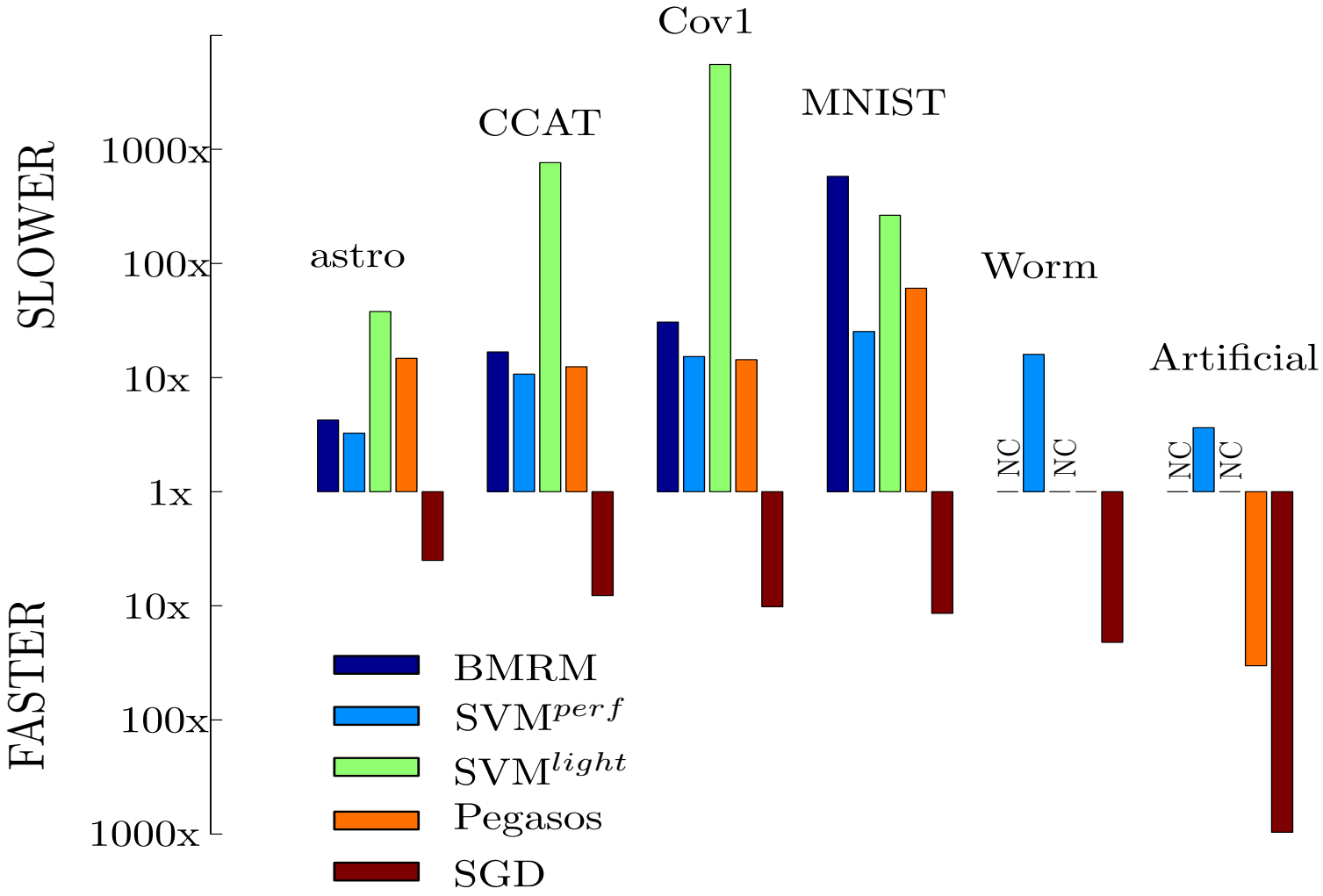




Train string-kernel SVM on all available data

Idea - Use recent advances in learning *linear* SVMs

Optimized Cutting Plane SVM (OCAS, Franc et al.)



Effort $\mathcal{O}(N)$ instead of $\mathcal{O}(N^2)$ to $\mathcal{O}(N^3)$

String Kernel SVM Scoring Function

$$s(\mathbf{x}) := \mathbf{w} \cdot \Phi(\mathbf{x}) + b = \sum_{k=1}^{K} \sum_{i=1}^{L-k+1} w\left(\mathbf{x}[i]^k, i\right) + b$$

k-mer	pos. 1	pos. 2	pos. 3	pos. 4	$\cdots$
A	+0.1	-0.3	-0.2	+0.2	$\cdots$
C	0.0	-0.1	+2.4	-0.2	$\cdots$
G	+0.1	-0.7	0.0	-0.5	$\cdots$
T	-0.2	-0.2	0.1	+0.5	$\cdots$
AA	+0.1	-0.3	+0.1	0.0	$\cdots$
AC	+0.2	0.0	-0.2	+0.2	$\cdots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$
TT	0.0	-0.1	+1.7	-0.2	$\cdots$
AAA	+0.1	0.0	0.0	+0.1	$\cdots$
AAC	0.0	-0.1	+1.2	-0.2	$\cdots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$
TTT	+0.2	-0.7	0.0	0.0	$\cdots$

Training Linear SVMs in String Kernel Feature Space

Mapping

- A-priory compute $\Phi(\mathbf{x}_i)$ for all $i = 1, \ldots, N$
- Train linear SVM classifier using, e.g., OCAS

Limitations

1. Only small order possible
   ($K = 8 \Rightarrow$ 87,380 dimensions, per position)
2. Explicit (sparse) representation too costly

Simple Trick

- Only $\mathbf{w} \leftarrow \mathbf{w} + \alpha\Phi(\mathbf{x})$ and $\mathbf{w} \cdot \Phi(\mathbf{x})$ required

$\Rightarrow$ Compute $\Phi(\mathbf{x})$ on-the-fly and parallelize!

Preliminary Results

Human splice dataset

1. Linear SVM in primal (OCAS, 4 CPUs) (**proposed method**)
   - $5 \cdot 10^7$ strings of length 140
   - WD kernel of order 6 (and 8)
   - Dimensionality of $\mathbf{w}$ is $12 \cdot 10^6$ (requires 80M)

N	Time	auPRC
10^6	90 sec	34.35%
10^7	70 min	47.47%
$5 \cdot 10^7$	8 hrs	53.92%

2. WD Kernel order > 20 (SVM^{light} + `linadd`, ≥ 4 CPUs)

N	Time	auPRC
10^6	≈ 3 hrs	≈ 45.00
$8 \cdot 10^6$	> 8 days	54.12

Discussion

Conclusions

- Simple speedup trick for string kernels
- Shared memory parallelization, able to train on **50 million** human splice sites with **12 million** dimensions within a day

Discussion

- Limited to low $K-$mer length
- Is large K really necessary biology-wise?
- How to improve feature space?

Implemented in SHOGUN `http://www.shogun-toolbox.org`