GaKCo: a Fast GApped k-mer string Kernel using COunting

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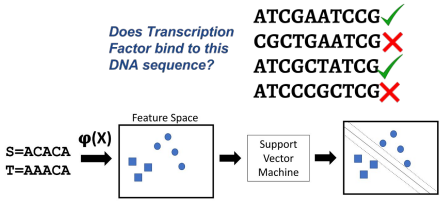
1. Overview

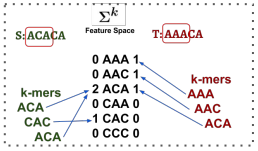
String Kernel techniques, especially those using gapped k-mers as features, have obtained great success in classifying sequences like DNA, protein, and text. However, the state-of-the-art gk-SVM runs extremely slow when we increase the dictionary size (Σ) or allow more mismatches (M). We propose a fast algorithm for calculating Gapped k-mer Kernel using Counting (GaKCo)-

1. *Faster* than state-of-the-art gk-SVM
2. Independent of dictionary size Σ and can *scale up* to large values of M and Σ.
3. *Parallelizable*

2. String Kernel + SVM framework

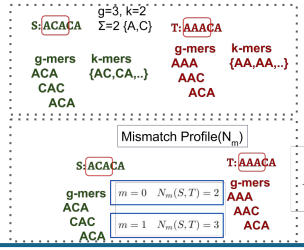


3. Spectrum Kernel

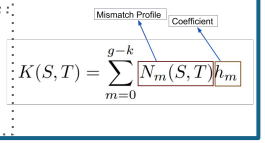


$$K(S,T) = \sum_{\gamma \in \Gamma_k} c_S(\gamma) \cdot c_T(\gamma)$$

4. Gapped k-mer Kernel



$$K(S,T) = \sum_{\gamma \in \Theta_g} c_S(\gamma) \cdot c_T(\gamma)$$



5. GaKCo

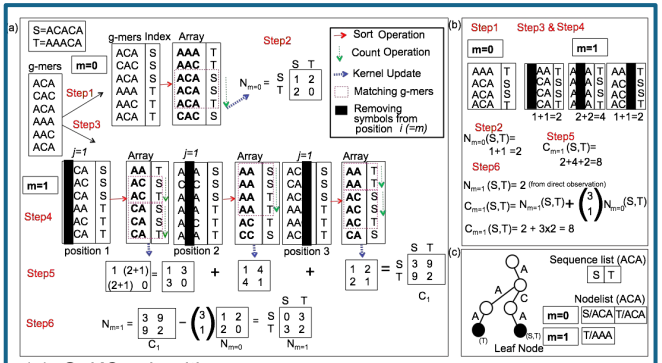
-*Algorithm*: GaKCo performs g-mer based cumulative counting of cooccurence to calculate N_m (independent of dictionary size(Σ)).

-*Parallelization*: GaKCo groups computations for each value of m into an independent function, making it naturally parallelizable.

Algorithm 1 GaKCo

Require: L, g, k ▨ L=Array list of g-mers

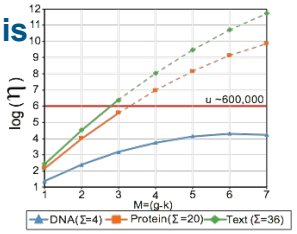
```
procedure CalculateKernel (L, g, k)
    M = g − k
    N = MismatchProfile (L, g, M)
    K = 0
    for m : 0 ..... M do
        h_m = C(g−k, m)
        K = K + N_m · h_m
procedure MismatchProfile (L, g, M)
    for m = 0 ...M do                ▨ Parallel threads
        C_m = 0                      ▨ Cumulative Profile
        n_pos = C(g, m)              ▨ Number of positions
        for i : 0..... n_pos do
            C^i_m = 0
            L^i = removePosition (L, i)
            L^i = sort (L^i)
            C^i_m = countAnd Update (L^i)
            C_m = C_m + C^i_m
    for m : 0 = M do
        N_m = C_m
        for j : 0 = m − 1 do
            N_m = N_m − C(g−j, m−j) N_j
    return N                         ▨ N = [N_0, ..., N_M]
Ensure: K                            ▨ Kernel Matrix
```



(a). GaKCo algorithm
(b). Overcounting when calculating cumulative mismatch profile for m=1.
(c). *gkm-SVM* uses a trie based data structure and a separate nodelist at each leafnode for calculating N_m.

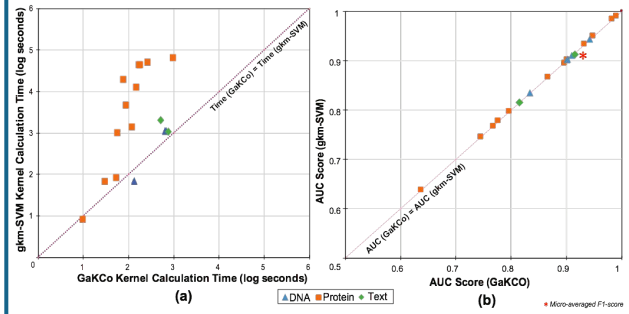
6. Theoretical Analysis

	GaKCo	gkm-SVM
Pre-processing	c_{gk} gNI	gNI + ηug
Kernel updates	c_{gk} zN ^{2}	ηuN ^{2}



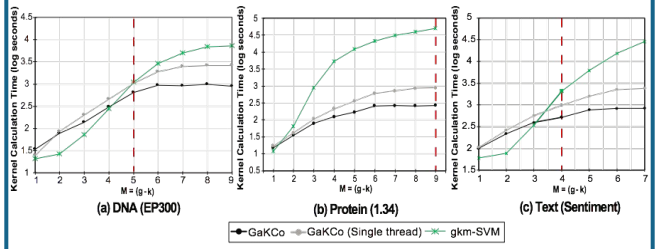
7. Experiments and Results

Data: We perform 19 different classification tasks to evaluate the performance of GaKCo. These tasks belong to three categories: (1) Transcription Factor (TF) binding site prediction (DNA dataset), (2) Remote Protein Homology prediction (protein dataset), and (3) Character based English text classification (text dataset).



Comparisons:

- (a). Kernel Calculation times (log(seconds)) of GaKCo(X-axis) vs gkm-SVM(Y-axis).*GaKCo is faster for 16/19 datasets.*
- (b). Empirical performance for the same 19 datasets of GaKCo (X-axis) versus gkm-SVM (Y-axis). *GaKCo achieves the same AUC-scores as gkm-SVM.*



Kernel calculation times with varying mismatches (M): scales well with increasing Σ and M.

References

1. Mahmoud Ghandi, Dongwon Lee, Morteza Mohammad-Noori, and Michael A Beer. Enhanced regulatory sequence prediction using gapped k-mer features. PLoS Comput Biol, 10(7):e1003711, 2014.
2. Mahmoud Ghandi, Morteza Mohammad-Noori, and Michael A Beer. Robust k-mer frequency estimation using gapped k-mers. Journal of mathematical biology, 69(2):469–500, 2014