

Optimality Implies Kernel Sum Classifiers are Statistically Efficient

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 - This includes low-accuracy estimators f



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- ⊙ How can considering **optimal estimators** help us understand **statistical efficiency**?



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 - θ may be convex combination, 0/1 vector, etc.



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- ⊙ But Support Vector Machines pick α in practice



How can we understand $\alpha^\top \tilde{\mathbf{K}}_\Sigma \alpha$?

If α_Σ solves the SVM problem with $\tilde{\mathbf{K}}_\Sigma$,
How does $\alpha_\Sigma^\top \tilde{\mathbf{K}}_\Sigma \alpha_\Sigma$ depend on

- ⊙ The number of kernels?
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Our Approach

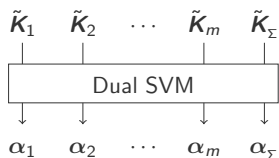
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$$\tilde{K}_1 \quad \tilde{K}_2 \quad \dots \quad \tilde{K}_m \quad \tilde{K}_\Sigma$$



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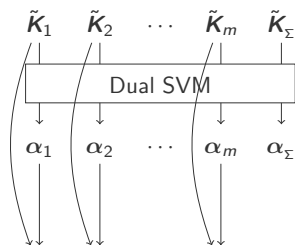
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For all $t = 1, 2, \dots, m$,
Assume $\alpha_t^\top \tilde{\mathbf{K}}_t \alpha_t \leq B^2$



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KKT Conditions

Then $\alpha_\Sigma^\top \tilde{\mathbf{K}}_\Sigma \alpha_\Sigma \leq 3m^{-0.58} B^2$



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Then $\alpha_\Sigma^\top \tilde{\mathbf{K}}_\Sigma \alpha_\Sigma \leq 3m^{-0.58} B^2$

Rademacher Complexity

Then:

Estimator $y(\mathbf{x}; \alpha_\Sigma)$ generalizes well
 $O\left(\frac{BRm^{0.208}\sqrt{\ln m}}{\sqrt{n}}\right)$



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- ⊙ Consider $\alpha^T \tilde{\mathbf{K}} \alpha$ in Multiple Kernel Learning as a specific case
- ⊙ Several possible applications of this idea beyond kernels



THANK
YOU



Corinna Cortes, Mehryar Mohri, and Afshin Rostamizadeh.
Generalization Bounds for Learning Kernels.

In *Proceedings of the 27th International Conference on International Conference on Machine Learning*, pages 247–254.
Omnipress, 2010.



Raphael Meyer and Jean Honorio.

Optimality Implies Kernel Sum Classifiers are Statistically Efficient.

In *International Conference on Machine Learning*, pages 4566–4574, 2019.