Efficient Convex Algorithms for Universal Kernel Learning.

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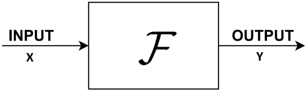
Kernel Methods are sensitive to the choice of kernel.

Function Learning Problem



Find F **minimizing** $L(F)$.

The loss function can be

$$L(F) = \sum_{i=1}^{N} \max\left\{0, \left|y_i - F(x_i)\right| - \varepsilon\right\},$$

where $\{(x_i, y_i)\}_{i=1}^{N} \subseteq \mathcal{X} \times \mathbb{R}$.

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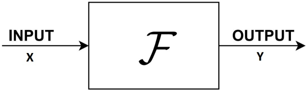

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Kernel methods

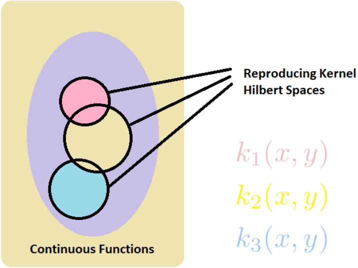
$$\min_{F \in \mathcal{H}_k} L(F)$$

$$\mathcal{H}_k = \underbrace{\left\{ \sum_i k(x, x_i)\alpha_i \;\middle|\; \alpha_i \in \mathbb{R},\ x_i \in \mathcal{X} \right\}}_{\text{Reproducing Kernel Hilbert Space}}$$

$k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is positive-definite kernel.

k is PD kernel if $K = K^T$ and $K \geq 0$

$$K = \begin{bmatrix} k(x_1, x_1) & \dots & k(x_1, x_N) \\ \vdots & & \ddots \\ k(x_N, x_1) & \dots & k(x_N, x_N) \end{bmatrix}$$



Function Space

Kernel Methods search a function for fixed k

How to **optimally** choose a kernel function?

Kernel Learning does not require the choice of Kernel.

Kernel Learning

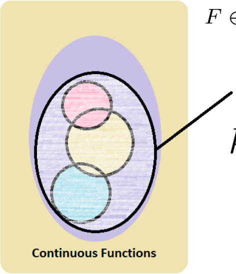
$$\min_{k \in \mathcal{K}} \min_{F \in \mathcal{H}_k} L(F)$$

$$\mathcal{H}_k = \overline{\left\{ \sum_i k(x, x_i)\alpha_i \;\middle|\; \alpha_i \in \mathbb{R},\ x_i \in \mathcal{X} \right\}}$$

where $\mathcal{K}$ **is a set of PD kernels**

$$\mathcal{K} = \left\{ k = \int_{\mathcal{Z}} N^T(x,z) P N(y,z) dz \;\middle|\; \overbrace{\substack{P \geq 0 \\ tr(P) = n_P}}^{\mathcal{P}} \right\},$$

where $N : \mathcal{X} \times \mathcal{Z} \to \mathbb{R}^{n_p}$ – chosen functions,
$\mathcal{Z} = [a, b]^{n_z}$ – integration interval.
$P \in \mathbb{R}^{n_p \times n_p}$ – Positive-Definite matrix.



Set of RKHSs

Function Space

$$F \in \mathcal{H} := \underbrace{\cup_{k \in \mathcal{K}} \mathcal{H}_k}_{\text{Set of RKHSs}}$$

$$k \in \mathcal{K}$$

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Kernel Learning

$$\min_{k\in\mathcal{K}} \min_{F\in\mathcal{H}_k} L(F)$$

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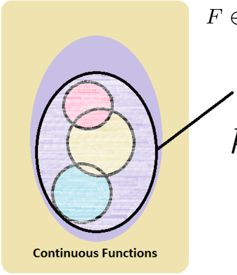

Function Space

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Finite-Dimensional Optimization

$$\min_{P\in\mathcal{P}} \min_{\alpha\in\mathbb{R}^N} L(F_{\alpha,P})$$
$$F_{\alpha,P}(x) = \sum_{i=1}^N k_P(x,x_i)\alpha_i$$
$$k_P(x_1,x_2) = \int_{\mathcal{Z}} N^T(x,z)PN(y,z)dz$$

BUT, the objective is not convex in both variables!

$$L(F_{\alpha,P}) \sim \underbrace{\max\left\{0, \left|y_i - \sum_{j=1}^N k_P(x_i,x_j)\alpha_j\right| - \varepsilon\right\}}_{\text{linear in } k \text{ and linear in } \alpha}$$

Direct method to solve[*] $\Longrightarrow$ Time complexity $O(N^4)$

Q: How to efficiently solve **Kernel Learning** Problem?

[*] G. Lanckriet and et. al. "Learning the kernel matrix with semidefinite programming." *JMLR*, 2004.

How to solve Kernel Learning Problem?

1. **Reformulate** as a saddle-point optimization problem. $\mathbf{1} = \begin{bmatrix}1 & \dots & 1\end{bmatrix}^T$

Primal Subproblem

$$\min_{P \in \mathcal{P}} \overbrace{\min_{\alpha \in \mathbb{R}^d} \quad L(F_{\alpha,k})}^{\text{Primal Subproblem}}$$

$$F_{\alpha,k}(x) = \sum_{i=1}^{N} k_P(x, x_i)\alpha_i$$

Dual Subproblem

$$\min_{P \in \mathcal{P}} \overbrace{\max_{\alpha \in \mathcal{A}} \quad L_D(F_{\alpha,P})}^{\text{Dual Subproblem}}$$

$$\mathcal{A} = \{\alpha \mid \mathbf{1}^T\alpha = 0, \ \alpha_i \in [-1, 1]\}$$

$$L_D(F_{\alpha,P}) = \underbrace{\sum_{i=1}^{N} y_i\alpha_i - \varepsilon \sum_{i=1}^{N} |\alpha_i| - \frac{1}{C} \sum_{i,j=1}^{N} k_P(x_i, x_j)\alpha_i\alpha_j}_{\text{concave in } \alpha \text{ and linear in } k \text{ (convex)}}$$

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concave in α and linear in k (convex)

3. Propose an algorithm.

```
Initialize P_0 = I
For i = 1 to m do
    • α_i = arg max_{α∈A} L_D(α, P_i)
    • S_i = arg min_{P∈P} L_D(α_i, P)
    • γ_i = arg min_{γ∈[0,1]} L_D(α_i, P_i + γ(S_i − P_i))
    • P_{i+1} = P_i + γ_k(S_i − P_i)
enddo
Return α_m, P_m.
```

← SV regression $O(N^{2.3})$

← SDP (using analytic solution)

← line-search for P updates

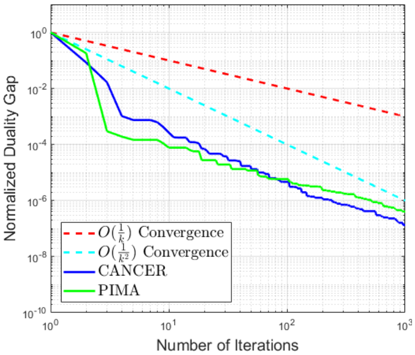
vs SDP $O(N^4)$

Time complexity is $\sim O(mN^{2.3})$

m is number of iterations

N is size of data set.

Convergence of Algorithm



Min-Max Formulation

$$\min_{P \in \mathcal{P}} \max_{\alpha \in \mathcal{A}} L_D(\alpha, P),$$

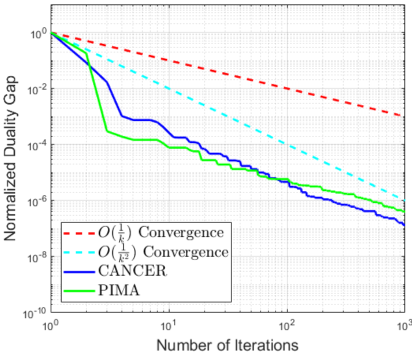
where $L_D(\alpha, P)$ is convex in α and concave in P.

$$\text{Duality Gap} = \left| \min_{P \in \mathcal{P}} L_D(\alpha, P) - \max_{\alpha \in \mathcal{A}} L_D(\alpha, P) \right|$$

- Just few iterations enough for convergence

Numerical Examples

Convergence of Algorithm



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Kernel Learning for Regression

Data set	Method	Error	Time (s)
Gas	Kernel Learning	**0.23 ± 0.01**	**13580 ± 2060**
$d = 11$	NNet	0.27 ± 0.03	1172 ± 100
$N = 30000$	RF	0.38 ± 0.02	16.44 ± 0.57
	XGBoost	0.33 ± 0.005	49.46 ± 1.93

N – number of data points
d – dimension of the data set

$$\text{Error} = \sum_{i=1} \|y_i - F(x_i)\|^2$$

Using mutliple data sets => KL outperforms other algorithms by 23.6%

Conclusion Remarks

Conclusion

- **Parameterize kernels** using positive-definite matrices.
- Formulate KL problem as **the saddle point problem**
- Propose the **algorithm for solving Kernel Learning**

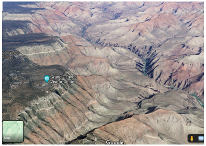
More details in the paper.

- **The convergence proof**.
- The time and memory **complexity** of the algorithm
- More numerical experiments
- **Alternative algorithm** for solving Kernel Learning

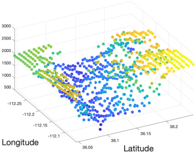
Future Plans

- **Scalability** of Kernel Learning
- New class of kernel function
- Improved algorithm for Kernel Learning

Learning for the Grand Canyon



Data



Fitting