Early stopping points for gradient desccent

An application to least square regression

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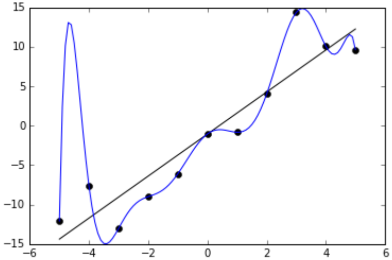
Promo : 2021

Plan

1. Introduction
   - Context
   - Settings
   - Kernels
2. Stopping rules
3. Conclusion

Context



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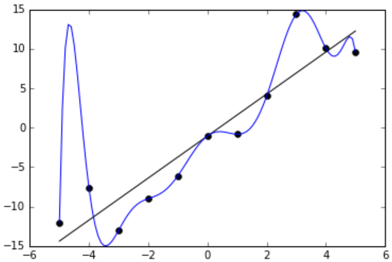

Figure: Overfitting phenomenon

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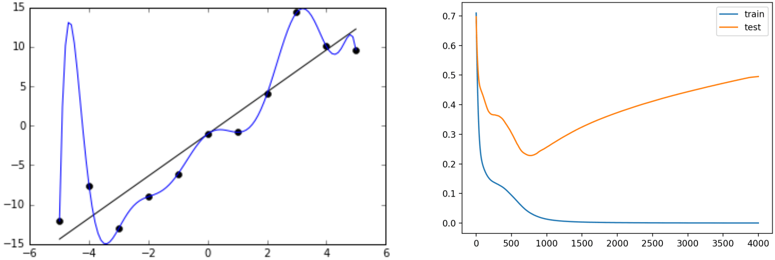

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But :

- Cost increases (Time, complexity, ...)
- Alternative : **Early stopping** : find the number of iterations $\hat{T}$, to perform before interrupting the training procedure.
- Motivated by the **Bias-Variance** balance :

Bias-Variance trade-off

Bias variance principle

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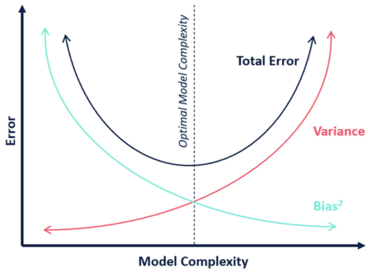
Bias variance principle



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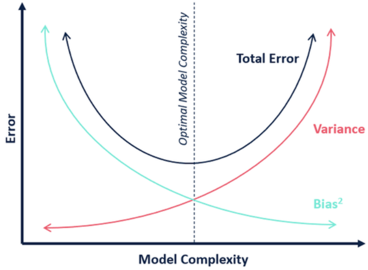

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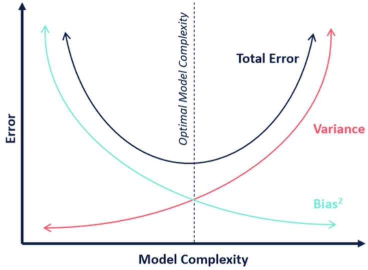

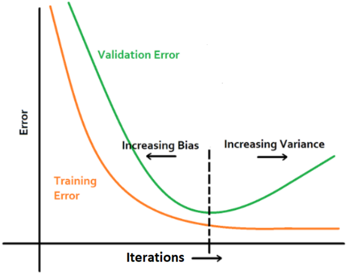

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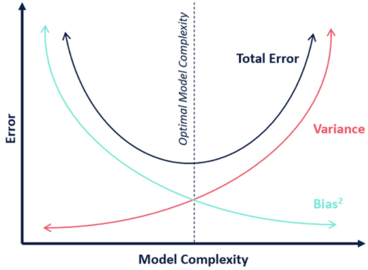

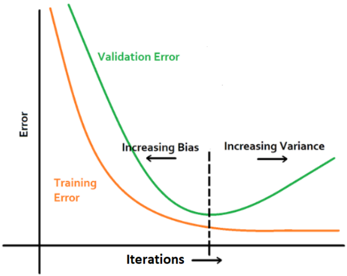

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- Bias term and variance term behave in opposite sens
- Controling their evolution may lead to consistant rules

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- **Goal :** fit function space $\mathcal{H}$ to the model via gradient descent

Using RKHS setting gives broad class of functions and algebraic properties

$$f_{t+1} = f_t + \alpha \nabla \mathcal{L}(f_t), \quad f^* \in \arg\min_{f \in \mathcal{H}} \mathcal{L}(f), \ \ \mathcal{L}(f) = \mathbb{E}_y \frac{1}{n} \sum_{i=1}^{n} \phi(y_i, f(x_i))$$

Oracle

Denote by : $R_{OR}(f_t) = \|f^* - f_t\|_n^2$. We might attempt for the **Oracle** rule :

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- **data independent** rule : with $\mathcal{D}_{train} \neq \mathcal{D}'_{train}$ we have the same performance.
- **Not computable in practice** !!!

Hold out

- Let's suppose that the size of the full data $\{x_i\}_{i=1}^n$ is even. S_{te}, and S_{tr} the train/test sets .
- at each iteration, the training data is used to estimate the risk $R_{HO}(f_t) = \frac{1}{n}\sum_{i\in S_{te}}(y_i - f_{tr,t}(x_i))^2$.

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- at each iteration, the training data is used to estimate the risk $R_{HO}(f_t) = \frac{1}{n}\sum_{i \in S_{te}}(y_i - f_{tr,t}(x_i))^2$.
- Possible rule
  $\hat{T}_{HO} = \arg\min \left\{ t \in \mathbb{N}, R_{HO}(f_{tr,t+1}) > R_{HO}(f_{tr,t}) \right\} - 1$

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- **RKHS** mathematical setting

RKHS setting : consequences

Representation theorem

Consider a $\mathcal{H}$ to be a **RKHS** defined with a kernel $\mathbb{K}$ over a domain $\mathcal{X}$. let $(x_1, x_2, ..., x_n) \in \mathcal{X}^n$. Let a functional $\Psi : \mathbb{R}^{n+1} \to \mathbb{R}$ increasing wrt (with respect to) its last variable. Then

$$\min_{f \in \mathcal{F}} \Psi(f(x_1), ..., f(x_n), \|f\|^2_{\mathcal{F}})$$

is reached at some $f = \sum_{i=1}^n \alpha_i \mathbb{K}(x_i, .)$

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- we have the inner products $\langle f, g \rangle_{L^2(\mathcal{X})} = \sum_{j=1}^{\infty} \mu_j a_j b_j$ and $\langle f, g \rangle_{\mathcal{H}} = \sum_{j=1}^{\infty} a_j b_j$
- recall the fact that :$\langle f, g \rangle_{L^2(\mathcal{X})} = \int_{\mathcal{X}} f(x) g(x) d\mathbb{P}(x)$

RKHS consequences

- Define the **Local Rademacher upper bound** :
  $\mathcal{R}_K(\epsilon) = \left[\frac{1}{n}\sum_{i=1}^{n} \min(\hat{\lambda}_i, \epsilon^2)\right]^{\frac{1}{2}}$ where $K = UAU^T$ the empirical kernel matrix, $r = \mathrm{rank}(K)$ its rank, and finally :
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- Define the empirical radius :$\hat{\epsilon_n} = \inf\left\{\epsilon > 0 \; |\mathcal{R}_K(\epsilon) \leq \frac{\epsilon^2}{2e\sigma}\right\}$
- Define the stopping time :

$$\hat{T} := \arg\min\left\{t \in \mathbb{N} \mid \mathcal{R}_k\left(\frac{1}{\sqrt{\eta_t}}\right) > \frac{1}{2e\sigma\eta_t}\right\} - 1$$

where η_t is the the sum of step sizes (*learning rates*) untill time $t - 1$

Theorem : regression case (fixed design)

For regression problems, [2] have proved that :

Theorem : Raskutti, Wainwright [2]

Suppose wa have a **valid step-size**. Then define $\hat{T}$ as previous. There are universal positive constants (c_1, c_2), such that, the following events hold with probability at least $1 - c_1 \exp\left(-c_2 n \hat{\epsilon}_n^2\right)$:

(a) : for all iterations t = 1, 2, ..., $\hat{T}$:

$$\|f_t - f^*\|_n^2 \leq \frac{4}{e \eta_t}$$

(b) : At the iteration $\hat{T}$ we have :

$$\|f_t - f^*\|_n^2 \leq 12 \hat{\epsilon}_n^2$$

(c) : Moreover, for all $t > \hat{T}$:

$$\mathbb{E}\left[\|f_t - f^*\|_n^2\right] \geq \frac{\sigma^2}{4} \eta_t \hat{R}_k^2 \left(\frac{1}{\eta_k}\right)$$

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- Claiming results in high probability is true only if the decay of the empirical radius is of a minimum $n^{\frac{\alpha-1}{2}}$ for $\alpha > 0$
- Norms control : the paper uses the property : $\|f\|_{\mathcal{H}} \leq B$ for some $B > 0$ for all $f \in \mathbb{B}_{\mathcal{H}}(f^*, 1)$ and as consequence $\|f\|_\infty \leq B$ for all $f \in \mathbb{B}_{\mathcal{H}}(f^*, 1)$.

Numerical illustration

$f^*(x) = |x - \frac{1}{2}| - \frac{1}{2}$ and $(x, y) \in [0, 1] \times [0, 1]$ and $x_i = \frac{i}{n}$ $i = 0, ..., n - 1$

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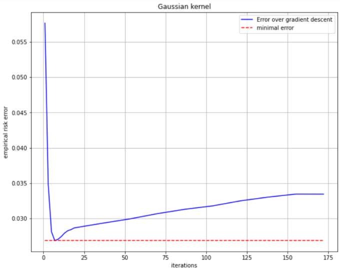

Figure: Gaussian kernel

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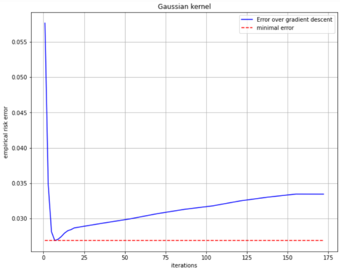

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- Gaussian kernel $T = 9$ iterations (infinitely differentiable functions)

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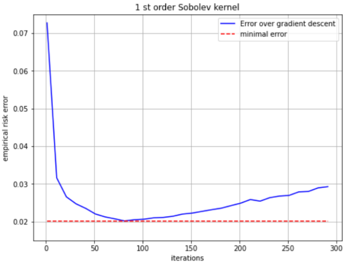
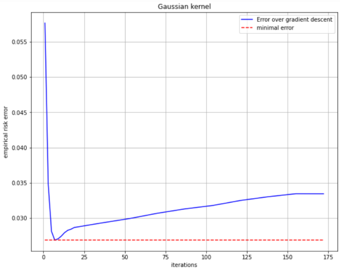


Figure: First order Sobolev kernels



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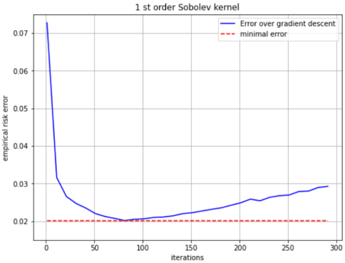

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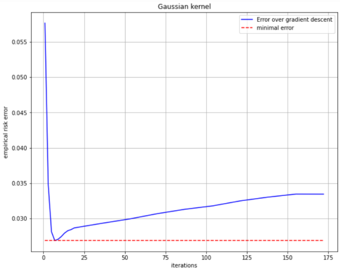

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- Gaussian kernel $T = 9$ iterations (infinitely differentiable functions)
- Sobolev kernel $T = 70$ iterations (Lipchitz functions)

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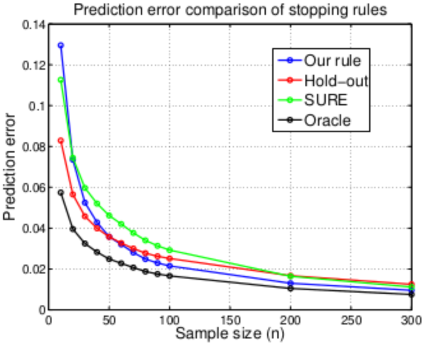

Figure: Different rules

Conclusion

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