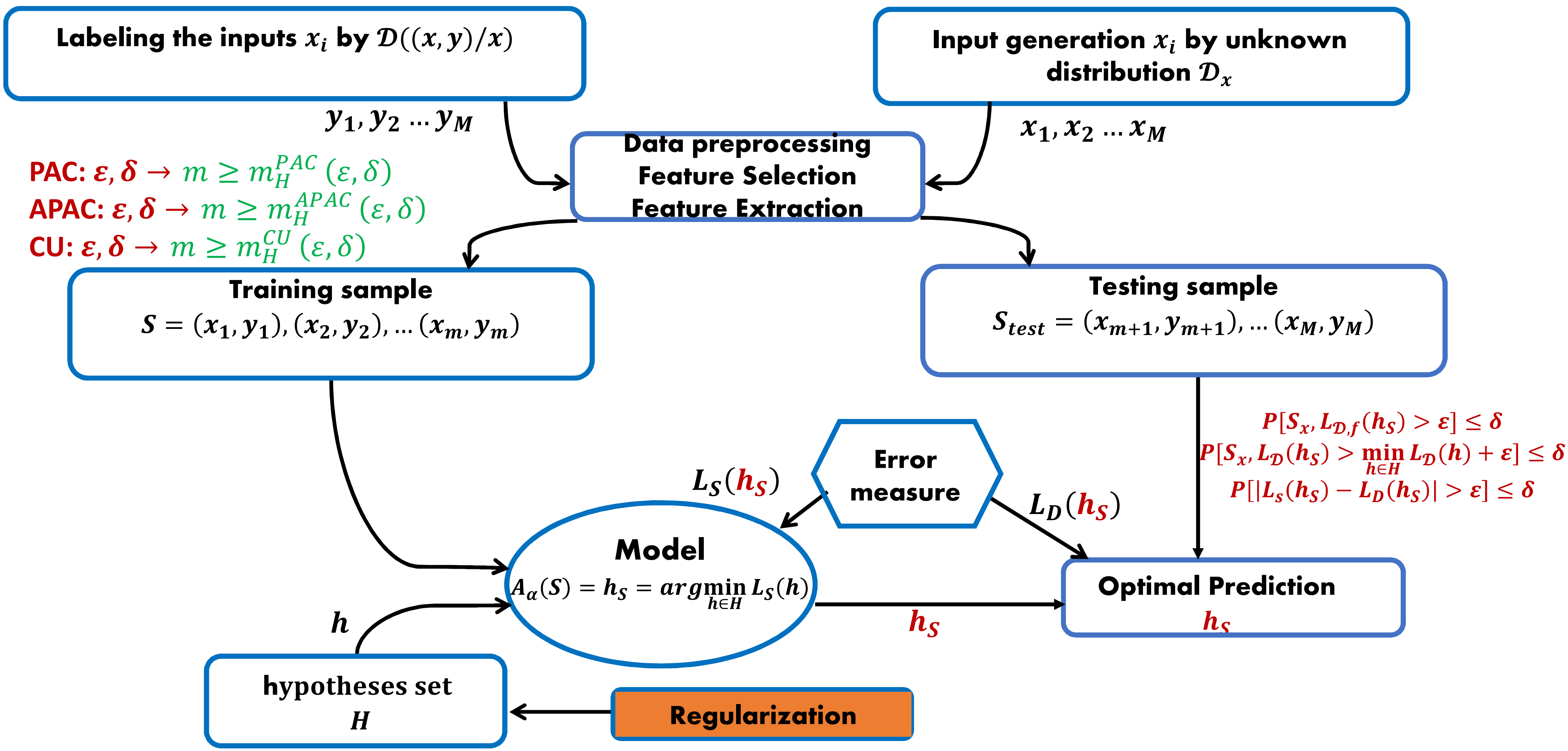
Part 3: Overfitting Underfitting

1. Validation/Cross-Validation
2. Regularization:
   1. Minimisation of regularized cost
   2. Algorithm stability
   3. Tikhonov Regularizer
   4. Stability-Adaption tradeoff

Supervised Learning Passive Offline Algorithm (SLPOA)



Recall

Definition: APAC learning model

H follows agnostic PAC learning, if there exist $m_{\mathcal{H}}:\ (0,1)^2\ \rightarrow \mathbb{N}$ and A_α.

Having the following property: $\forall \varepsilon, \delta \in (0,1), \forall\, \mathcal{D}$ on $X \times Y$.

Then, if we run A_α on $m \geq m_{\mathcal{H}}(\varepsilon, \delta)$ generated $(i.i.d.)$ such that S is selected with a probability at least $(1-\delta)$, A_α will generate the hypothesis h_S such that:

$$L_{\mathcal{D}}(h_S) \leq \min_{h \in H} L_{\mathcal{D}}(h) + \varepsilon.$$

In other words:

$$P_{S \sim \mathcal{D}^m}\left[L_{\mathcal{D}}(h_S) > \min_{h \in H} L_{\mathcal{D}}(h) + \varepsilon\right] \leq \delta\ \ for\ all\ m \geq m_H(\varepsilon, \delta)$$

Recall

Definition: Uniform Convergence

We say that H has the uniform convergence property with respect to (Z, l), if there exist:

- a function $m_H^{CU}(\varepsilon, \delta)$: $[0,1]^2 \longrightarrow \mathbb{N}$, such that: $\forall(\varepsilon, \delta) \in [0,1]^2 and\ \forall\ \mathcal{D}$ over Z.
- S is a sample of size $m \geq m_H^{CU}(\varepsilon, \delta)$, whose points are drawn $(i.i.d.)$ by $\mathcal{D}$, such that with probability of at least $(1-\delta)$, S is ε-representative:

$$P[|L_s(h) - L_D(h)| \leq \varepsilon] \geq 1 - \delta \Leftrightarrow P[|L_s(h) - L_D(h)| > \varepsilon] \leq \delta$$

Recall

- If $|H| \approx \infty \boldsymbol{|L_s(h_S) - L_D(h_S)| \leq g}(d_{CV}) \boldsymbol{= \varepsilon \in V(0)}$
$$d_{CV} < \infty \; or \; N_C < \infty \Leftrightarrow CU \;\Leftrightarrow APAC \Leftrightarrow PAC$$
- If $|H| < \infty$
  - $If\ \ target\ function\ exist\ then\ PAC$
  - $If\ Target\ function\ is\ stochastic\ then\ CU\ \Longrightarrow APAC$

Example: Regression

$$x_i = \left(x_i^1, x_i^2\right)$$

$$f(x_i) = w_0 x_i^1 + w_1 x_i^2 + w_2 x_i^1 x_i^2 + w_3 \left(x_i^1\right)^2 + w_4 \left(x_i^2\right)^2 = y_i$$

If $L_D(h) \gg L_S(h)$ then we reduce the degree of polynomial that is to reduce the size of $w = (w_0, w_1, w_2, w_3, w_4)$

Motivation

If $L_D(h) \gg L_S(h)$ we have the Overfitting Problem .

To remedy this problem, we should penalize the model parameters.

Objective:

- How to penalize the learning.

Tool:

- Regularization.

1. Minimization of regularized cost

$$A_\alpha(S) = h_S \in \underset{w \in \mathbb{R}^d}{\operatorname{argmin}} \{L_S(w)\}$$

If we have the Overfitting Problem , we penalize the model parameters as following .

$$\begin{cases} \boldsymbol{Min} & \boldsymbol{L_S(w)} \\ \boldsymbol{s.t} & \boldsymbol{\|w\| < C} \\ & \boldsymbol{w \in \mathbb{R}^d} \end{cases}$$

- $\Longrightarrow L(w, \lambda) = L_S(w) + \lambda(\|w\| - C) = L_S(w) + \mathrm{R(w)}$

$$\Rightarrow A_\alpha(S) = h_S \in \underset{w \in \mathbb{R}^d}{\operatorname{argmin}} \{L_S(w) + R(w)\}$$

- $d(w, 0) = \|w\|$
- $\|w\| = \|w\|_1 = \sum_{i=1}^{d} |w_i|$ with $w \in l_1$
- $\|w\| = \|w\|_2^2 = \sum_{i=1}^{d} {w_i}^2$ with $\mathrm{w} \in l_2$
- $L_S \in L_2$

1. Minimization of regularized cost

Definition : RLM algorithm

RLM is a learning algorithm used to minimize the sum of the empirical error and the regularization function $R: \mathbb{R}^d \longrightarrow \mathbb{R}$.

It generates the following hypothesis:

$$A_\alpha(S) = h_S \in \underset{w}{\operatorname{argmin}}\{L_S(w) + R(w)\}$$

Notice :

- The RLM algorithm shares the same similarities with SRM and MDL, such that the complexity of the hypotheses is measured by a regularization function $R(w)$.
- Similarly to MDL, there exist many types of regularization functions that depend on the type of problem to deal with.

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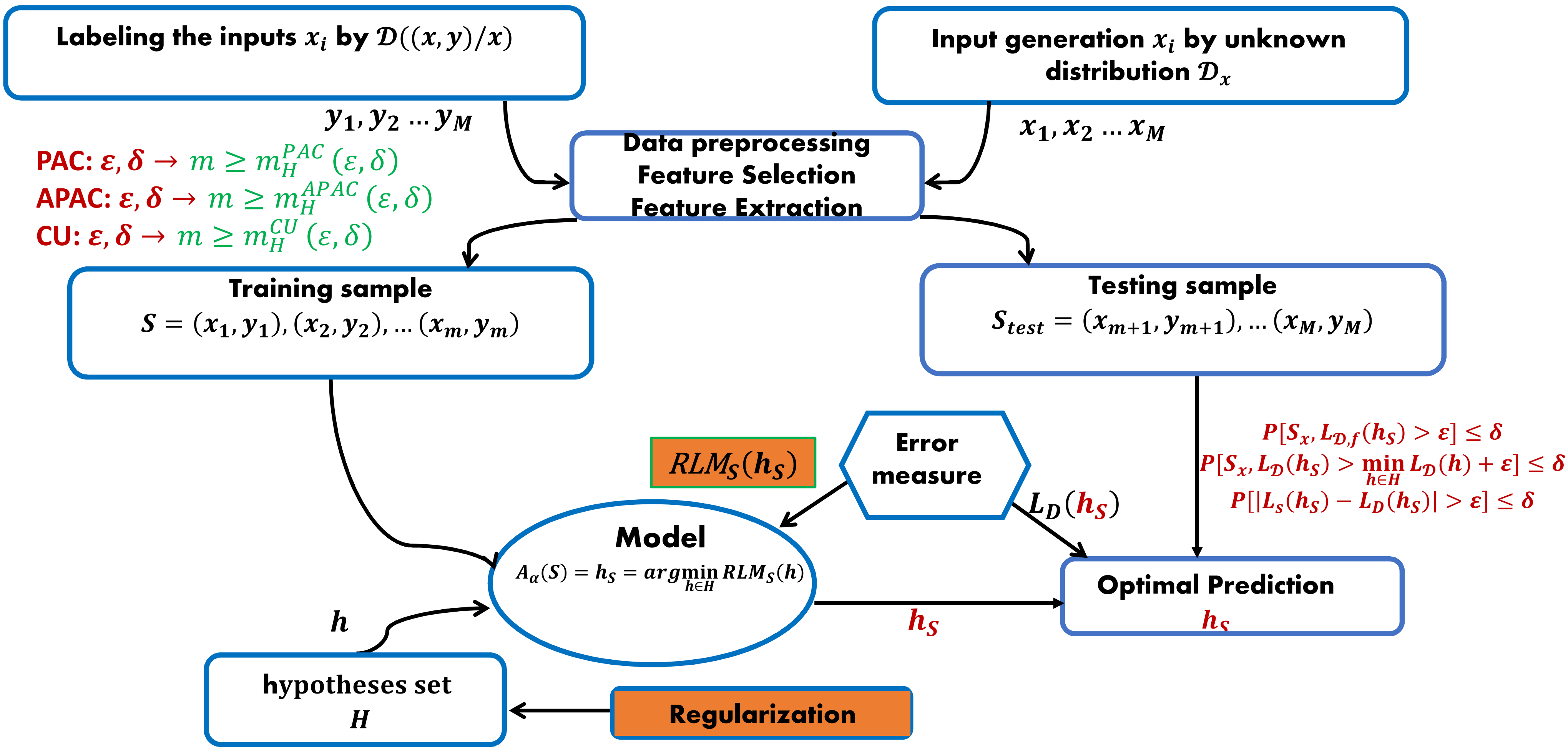


1. Minimization of regularized cost

Definition : Tikhonov regularizer

Tikhonov regularization function has the following from :

$$R(w) = \lambda\|w\|^2$$

With :

$\lambda > 0$ is a scalar. And $\|.\|$ is the l_2 norm:

$$\|w\| = \sqrt{\sum_{i=1}^{d} {w_i}^2}$$

The learning rule becomes :

$$A_\alpha(S) = h_S = \underset{w}{\operatorname{argmin}}(L_S(w) + \lambda\|w\|^2)$$

1. Minimization of regularized cost – Ridge Regression

Consider a problem of linear regression and the training data $(x_1, y_1), \ldots, (x_m, y_m)$.

We want to minimize: L_2 norm

$$L_S(w) = \frac{1}{m}\sum_{i=1}^{m}(w^T x_i - y_i)^2 = \frac{1}{m}(Xw - y)^T(Xw - y)$$

In that case the solution is: $w_{lin} = (X^T X)^{-1} X^T y$

Hard constraint:

$$w_i = 0 \text{ pour } i > 0.$$

Soft constraint:

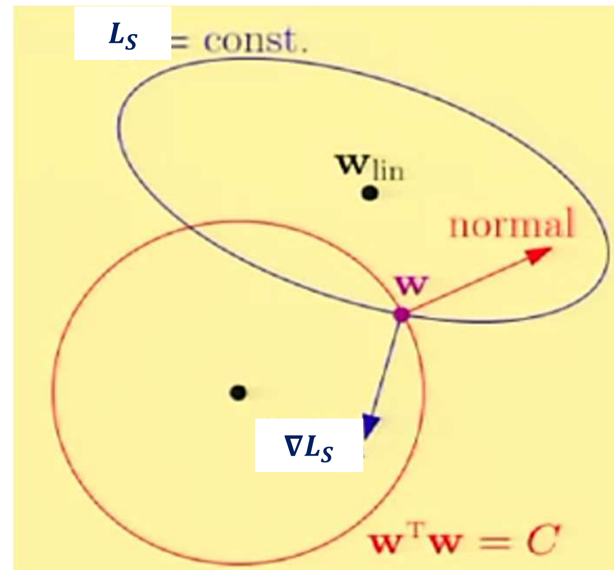
$$\sum_{i=0}^{d} w_i^2 \leq C$$

Instead of eliminating weights, we are going to minimize their values.

1. Minimization of regularized cost – Ridge Regression

We can use the multiples of Lagrange to solve that problem:

$$\begin{cases} Min \quad L_S(w) = \dfrac{1}{m}(Xw - y)^T(Xw - y) \\ w^T w \leq C \end{cases}$$



the solution is w_{reg} instead of w_{lin}.

So:

$$\nabla L_S(w_{reg}) \propto -w_{reg}$$
$$= -2\lambda w_{reg}$$
$$\nabla L_S(w_{reg}) + 2\lambda w_{reg} = 0$$

The minimisation problem becomes:

$$Min \quad L_S(w) + \lambda w^T w$$

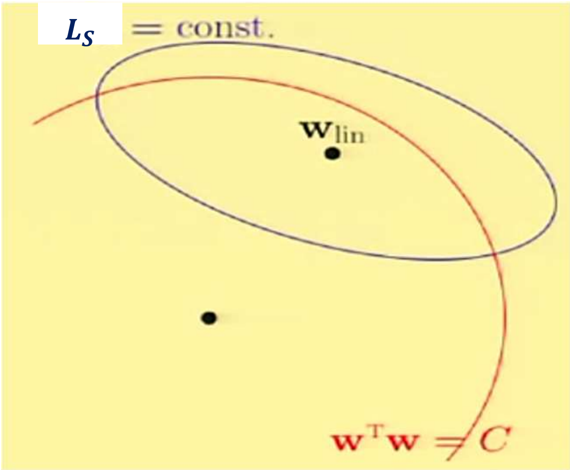
$$Min\, L_S(w) + \lambda w^T w = \frac{1}{m}(Xw - y)^T(Xw - y) + \lambda w^T w$$

1. Minimization of regularized cost – Ridge Regression

$$\nabla\left(\frac{1}{m}(Xw-y)^T(Xw-y)+\lambda w^T w\right)=0$$

$$X^T(Xw-y)+\lambda w=0$$

$$w_{reg}=(X^TX+\lambda I)^{-1}X^Ty$$



Hence, the unconditional minimization problem.

If C ↑ so λ ↓ : non-severe regularization.

If C ↓ so λ ↑ : severe regularization.

Definition : Ridge regression

Ridge regression is a combination between linear regression (having the squared cost) and Tikhonov regularization. The learning rule becomes:

$$A_\alpha(S)=\underset{w\in\mathbb{R}^d}{\operatorname{argmin}}\left\{\lambda\|w\|_2^2+\frac{1}{m}\sum_{i=1}^{m}\frac{1}{2}(\langle w,x_i\rangle-y_i)^2\right\}$$

2. Model's Stability

Definition :

A Model is said to be stable if a small changing in its inputs implies a small changing in its outputs.

Notice:

Let A_α be a Learning Model, let $S = \{z_1, \dots, z_m\}$ be a training set of size m, let $A_\alpha(S)$ be the output of the Model A_α.

Consider another example z'. Let $S^{(i)}$ be the training set obtained by replacing the example z_i in S by z' :

$$S^{(i)} = \{z_1, \dots, z_{i-1}, z', z_{i+1}, \dots, z_m\}$$

Replacing z_i by z' defines the small changing in its inputs, this means we train $A_\alpha(S^{(i)})$ instead of $A_\alpha(S)$.

2. Model's Stability

Theorem :

Soit la distribution D, soit $S = \{z_1, \dots, z_m\}$ une séquence $i.i.d$ d'exemples, soit z' un autre exemple $i.i.d$. Soit $U(m)$ une distribution uniforme sur $[m]$. Donc $\forall A_\alpha$:

$$E_{S \sim D^m}\left[L_D\left(A_\alpha(S)\right) - L_S\left(A_\alpha(S)\right)\right] = E_{(S,z') \sim D^{m+1}, i \sim U(m)}\left[\, l\left(A_\alpha\left(S^{(i)}\right), z_i\right) - l(A_\alpha(S), z_i)\right]$$

Notice :

- If the différence $l\left(A_\alpha\left(S^{(i)}\right), z_i\right) - l(A_\alpha(S), z_i)$ is large, we say the Model overfits the data.
- If the différence $l\left(A_\alpha\left(S^{(i)}\right), z_i\right) - l(A_\alpha(S), z_i)$ is small, we say the Model is stable.

2. Model's Stability

Definition : Model's stability

Let $\varepsilon: \mathbb{N} \longrightarrow \mathbb{R}$ be a monotonic decreasing function, we say that the Model A_α is stable (On-Average-Replace-One-Stable) with two rates $\varepsilon(m)$, if $\forall D$:

$$E_{(S,z')\sim D^{m+1}, i\sim U(m)}\left[\, l\left(A_\alpha\left(S^{(i)}\right), z_i\right) - l(A_\alpha(S), z_i)\right] \leq \varepsilon(m)$$

Notice :

- With this definition, the Model A_α doesn't suffer from overfitting if and only if it is sable.
- To have a good Model, it should not overfit the data, moreover its empirical error should be small :

$$L_D(A_\alpha(\mathrm{S})) \approx L_S(A_\alpha(\mathrm{S})) \text{ and } L_S(A_\alpha(\mathrm{S})) \approx 0$$

3. Tikhonov Regularizer – Lipschitz Cost Function

Definition : ρ-Lipschitz function

Let $C \subset \mathbb{R}^d$, we say that the function $f : \mathbb{R}^d \rightarrow \mathbb{R}^k$ is ρ-Lipschitz on C, if $\forall w_1, w_2 \in C$, we have :

$$\|f(w_1) - f(w_2)\| \leq \rho \|w_1 - w_2\|$$

Corollary :

Let's suppose that the cost function is convex and ρ-Lipschitz. So, RLM algorithm, having the Tikhonov regularizer $\lambda\|w\|^2$, is stable with the rate $\varepsilon(m) = \frac{2\rho^2}{\lambda m}$. So :

$$\boldsymbol{E_{S \sim D^m}\left[L_D\left(A_\alpha(S)\right) - L_S\left(A_\alpha(S)\right)\right] \leq \frac{2\rho^2}{\lambda m}}$$

3. Tikhonov Regularizer – Smooth Cost Function

Definition : β-Smooth function

We say that the function $f : \mathbb{R}^d \to \mathbb{R}$ is β- Smooth if its gradient is β-Lipschitz.

That means $\forall v, w$:

$$\|\nabla f(v) - \nabla f(w)\| \leq \beta \|v - w\|$$

- This implies that, $\forall v, w$ we have :

$$f(v) \leq f(w) + \langle \nabla f(w), v - w \rangle + \frac{\beta}{2} \|v - w\|^2$$

- If f is β-Smooth and convex, we have $\forall v, w$:

$$f(w) + \langle \nabla f(w), v - w \rangle \leq f(v) \leq f(w) + \langle \nabla f(w), v - w \rangle + \frac{\beta}{2} \|v - w\|^2$$

- If $\forall v$ we have $f(v) \geq 0$, and if f is β-Smooth, we say that f is a self-bounded function :

$$\|\nabla f(w)\|^2 \leq 2\beta f(w)$$

3. Tikhonov Regularizer – Smooth Cost Function

Corollary :

Let's suppose that the cost function is convex, β-Smooth and non-negative. So, RLM algorithm, having the Tikhonov regularizer $\lambda\|w\|^2$ such that $\lambda \geq \frac{2\beta}{m}$, is stable with rate :

$$\varepsilon(m) = \frac{48\beta}{\lambda m} E\left[L_S\left(A_\alpha(S)\right)\right]$$

So :

$$E_{S\sim D^m}\left[L_D\left(A_\alpha(S)\right) - L_S\left(A_\alpha(S)\right)\right] \leq \frac{48\beta}{\lambda m} E\left[L_S\left(A_\alpha(S)\right)\right]$$

Notice :

- For the two types of the cost function,

when $\lambda \longrightarrow \infty$, $E_{S\sim D^m}\left[L_D\left(A_\alpha(S)\right) - L_S\left(A_\alpha(S)\right)\right] \longrightarrow 0$

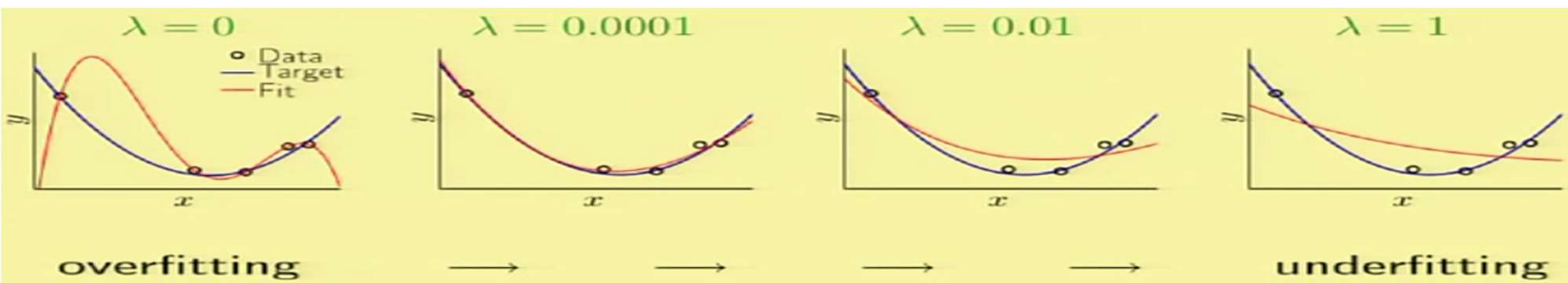
4. Stability-Adaption tradeoff

We can write the estimation of the generalization error as:

$$E_S[L_D(A_\alpha(S))] = E_S\left(L_S(A_\alpha(S))\right) + E_S[L_D(A_\alpha(S)) - L_S(A_\alpha(S))]$$

- The first term is the empirical error, it implies **the adaption** of the Model $A_\alpha$to training data $\boldsymbol{S}$.
- The second term is the difference between the general error and the empirical error, it implies the **stability** of the Model $A_\alpha$to small changings of inputs.

- If λ increases $\longrightarrow$ $L_S(A_\alpha(S))$ increases $\longrightarrow$ adaption decreases $\longrightarrow$ underfitting.
- If λ decreases $\longrightarrow L_D(A_\alpha(S)) - L_S(A_\alpha(S))$ increases $\longrightarrow$ stability decreases $\longrightarrow$ overfitting.



4. Stability-Adaption tradeoff - Lipschitz Cost Function

Corollary :

Let's suppose that the cost function is convex and ρ-Lipschitz. So, RLM algorithm, having the Tikhonov regularizer $\lambda\|w\|^2$, such that $\forall w^*$:

$$E_S\left[L_D\left(A_\alpha(S)\right)\right] \leq L_D(w^*) + \lambda\|w^*\|^2 + \frac{2\rho^2}{\lambda m}$$

Corollary : APAC learning for convex-Lipschitz bounded problems.

Let (H, Z, l) be a learning problem convex, Lipschitz and bounded having the parameters ρ and B.

For any training set of size m, let $\lambda = \sqrt{\frac{2\rho^2}{B^2 m}}$.

So, RLM algorithm having the Tikhonov regularizer $\lambda\|w\|^2$ meets :

$$E_S\left[L_D\left(A_\alpha(S)\right)\right] \leq \min_{w \in H} L_D(w) + \rho B\sqrt{\frac{8}{m}}$$

In particular, $\forall \varepsilon > 0$, if $m \geq \frac{8\rho^2 B^2}{\varepsilon^2}$, so for any distribution D :

$$E_S\left[L_D\left(A_\alpha(S)\right)\right] \leq \min_{w \in H} L_D(w) + \varepsilon$$

4. Stability-Adaption tradeoff - Smooth Cost Function

Corollary :

Let's suppose that the cost function is convex and β-Lipschitz and non-negative. So, RLM algorithm, having the Tikhonov regularizer $\lambda\|w\|^2$ and for any $\lambda \geq \frac{2\beta}{m}$, such that $\forall w^*$:

$$E_S\left[L_D\left(A_\alpha(S)\right)\right] \leq (1 + \frac{48\beta}{\lambda m})(L_D(w^*) + \lambda\|w^*\|^2)$$

Corollary : APAC learning for convex-smooth bounded problems.

Let (H, Z, l) be a learning problem convex-Smooth and bounded having the parameters β and B. Suppose that $l(0, z) \leq 1$ for any $z \in Z$.

$\forall \varepsilon \in [0,1]$, let $m \geq \frac{150\beta B^2}{\varepsilon^2}$ and $\lambda = \varepsilon/3B^2$, so for any distribution D :

$$E_S\left[L_D\left(A_\alpha(S)\right)\right] \leq \min_{w \in H} L_D(w) + \varepsilon$$