

# Stability of Tikhonov Regularization

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9.520 Class 7

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**Goal** To show that Tikhonov regularization in RKHS satisfies a strong notion of stability, namely  $\beta$ -stability, so that we can derive generalization bounds using the results in the last class.

- Review of Generalization Bounds via Stability
- Stability of Tikhonov Regularization Algorithms

A **learning algorithm**  $\mathcal{A}$  is a map

$$S \mapsto f_S^\lambda$$

where  $S = (x_1, y_1) \dots (x_n, y_n)$ .

A **generalization bound** is a (probabilistic) bound on the defect (generalization error)

$$D[f_S^\lambda] = I[f_S^\lambda] - I_S[f_S^\lambda]$$

Let  $S = \{z_1, \dots, z_n\}$ ;  $S^{i,z} = \{z_1, \dots, z_{i-1}, z, z_{i+1}, \dots, z_n\}$

An algorithm  $\mathcal{A}$  is  $\beta$ -stable if

$$\forall (S, z) \in \mathcal{Z}^{n+1}, \forall i, \sup_{z' \in \mathcal{Z}} |V(f_S^\lambda, z') - V(f_{S^{i,z}}^\lambda, z')| \leq \beta.$$

# Generalization Bounds Via Uniform Stability

From the last class we have that,

- If  $\beta = \frac{k}{n}$  for some  $k$ ,
- the loss is bounded by  $M$ ,

then:

$$P \left( |I[f_S^\lambda] - I_S[f_S^\lambda]| \geq \frac{k}{n} + \epsilon \right) \leq 2 \exp \left( -\frac{n\epsilon^2}{2(k+M)^2} \right).$$

Equivalently, with probability  $1 - \delta$ ,

$$I[f_S^\lambda] \leq I_S[f_S^\lambda] + \frac{k}{n} + (2k + M) \sqrt{\frac{2 \ln(2/\delta)}{n}}.$$

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Today we prove that Tikhonov regularization

$$f_S^\lambda = \arg \min_{f \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^n V(f(x_i), y_i) + \lambda \|f\|_K^2 \right\}$$

satisfies

$$\forall (S, z) \in Z^{n+1}, \forall i, \sup_{z' \in Z} |V(f_S^\lambda, z') - V(f_{S_i, z}^\lambda, z')| \leq \beta.$$

We assume the loss to be Lipschitz

$$|V(f_1(x), y') - V(f_2(x), y')| \leq L \|f_1 - f_2\|_\infty = L \sup_{x \in X} |f_1(x) - f_2(x)|$$

- The hinge loss and the  $\epsilon$ -insensitive loss are both  $L$ -Lipschitz with  $L = 1$  (exercise!).
- The square loss function is  $L$  Lipschitz if we can bound the values of  $y$  and  $f(x)$ .
- The 0 – 1 loss function is not  $L$ -Lipschitz (why?)

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If  $f \in \mathcal{H}$  is in a RKHS with

$$\sup_{x \in X} K(x, x) \leq \kappa^2 < \infty$$

then

$$\|f\|_{\infty} \leq \kappa \|f\|_K.$$

In particular this implies

$$\|f - f'\|_{\infty} \leq \kappa \|f - f'\|_K.$$

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## A key lemma

We will prove the following lemma about **Tikhonov regularization**:

$$\|f_S^\lambda - f_{S^{i,z}}^\lambda\|_K^2 \leq \frac{L \|f_S^\lambda - f_{S^{i,z}}^\lambda\|_\infty}{\lambda n}$$

This result is not straightforward and will be the most difficult part of the proof.

# Proving Stability

- 1 assumption:  $|V(f_1(x), y') - V(f_2(x), y')| \leq L\|f_1 - f_2\|_\infty$
- 2 property of RKHS:  $\|f - f'\|_\infty \leq \kappa\|f - f'\|_K$ , for any  $f, f' \in \mathcal{H}$ .
- 3 lemma:  $\|f_S^\lambda - f_{S^i, z}^\lambda\|_K^2 \leq \frac{L\|f_S^\lambda - f_{S^i, z}^\lambda\|_\infty}{\lambda n}$

putting all together:

$$\begin{aligned} |V(f_S^\lambda, z) - V(f_{S^i, z}^\lambda, z)| &\leq L\|f_S^\lambda - f_{S^i, z}^\lambda\|_\infty \\ &\leq L\kappa\|f_S^\lambda - f_{S^i, z}^\lambda\|_K \\ &\leq \frac{L^2\kappa^2}{\lambda n} \\ &=: \beta \end{aligned}$$

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# Proving the Lemma

We now prove

$$\|f_S^\lambda - f_{S^{i,z}}^\lambda\|_K^2 \leq \frac{L \|f_S^\lambda - f_{S^{i,z}}^\lambda\|_\infty}{\lambda n}$$

Note that it holds only when we consider the minimizers of Tikhonov regularization.

We need again some preliminary facts and definitions...

# Preliminaries: Derivative of a Functional

Let  $F : \mathcal{H} \rightarrow \mathbb{R}$ ,  $f$  is differentiable at  $f_0$  if

$$\lim_{t \rightarrow 0} \frac{F(f_0 + th) - F(f_0)}{t} = \langle \nabla F(f_0), h \rangle, \quad \forall h \in \mathcal{H}$$

and  $\nabla F(f_0)$  is the derivative.

Example:  $F(f) = \|f\|^2 = \langle f, f \rangle$

$$\frac{\langle f_0 + th, f_0 + th \rangle - \langle f_0, f_0 \rangle}{t} = \frac{2t\langle f_0, h \rangle - t^2\langle h, h \rangle}{t}$$

and taking  $t \rightarrow 0$

$$\nabla F(f_0) = 2f_0.$$

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# Preliminaries: Bregman Divergence

Let  $F : \mathcal{H} \rightarrow \mathbb{R}$  be a convex and differentiable function.

The Bregman divergence

$$d_F(f_2, f_1) = F(f_2) - F(f_1) - \langle f_2 - f_1, \nabla F(f_1) \rangle.$$

It can be seen as the error we make when we know  $F(f_1)$  for some  $f_1$  and “guess”  $F(f_2)$  by considering a linear approximation to  $F$  at  $f_1$ :

$$F(f_2) = F(f_1) + \langle f_2 - f_1, \nabla F(f_1) \rangle.$$

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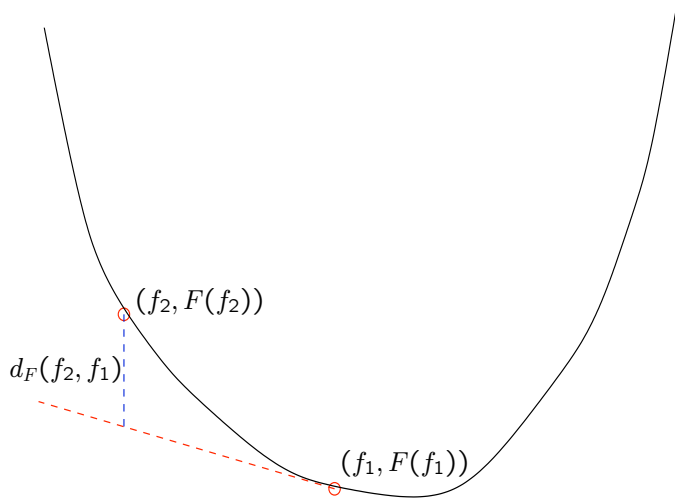
## The Bregman divergence

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# Divergences Illustrated





# Properties of Bregman Divergence

$$d_F(f_2, f_1) = F(f_2) - F(f_1) - \langle f_2 - f_1, \nabla F(f_1) \rangle.$$

We will need the following key facts about divergences:

- $d_F(f_2, f_1) \geq 0$
- If  $f_1$  minimizes  $F$ , then the gradient is zero, and  $d_F(f_2, f_1) = F(f_2) - F(f_1)$ .
- If  $F = A + B$ , where  $A$  and  $B$  are also convex and differentiable, then  $d_F(f_2, f_1) = d_A(f_2, f_1) + d_B(f_2, f_1)$  (derivative is additive).

# The Tikhonov Functionals

We use the following short notation:

$$T_S(f) = \frac{1}{n} \sum_{i=1}^n V(f(x_i), y_i) + \lambda \|f\|_K^2,$$

$$I_S(f) = \frac{1}{n} \sum_{i=1}^n V(f(x_i), y_i)$$

$$N(f) = \|f\|_K^2.$$

Hence,  $T_S(f) = I_S(f) + \lambda N(f)$ . If the loss function is convex (in the first variable), then all three functionals are convex.

# Proving the Lemma

We want to prove that

$$\|f_{S^{i,z}}^\lambda - f_S^\lambda\|_K^2 \leq \frac{2L\|f_S^\lambda - f_{S^{i,z}}^\lambda\|_\infty}{\lambda n}$$

The proof consists of two steps:

Step 1: prove that

$$2\|f_{S^{i,z}}^\lambda - f_S^\lambda\|_K^2 = d_N(f_{S^{i,z}}^\lambda, f_S^\lambda) + d_N(f_S^\lambda, f_{S^{i,z}}^\lambda)$$

Step 2: prove that

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Recalling that  $\nabla N(f) = 2f$ , we have

$$\begin{aligned} d_N(f_{S^{i,z}}^\lambda, f_S^\lambda) &= \|f_{S^{i,z}}^\lambda\|_K^2 - \|f_S^\lambda\|_K^2 - \langle f_{S^{i,z}}^\lambda - f_S^\lambda, \nabla \|f_S^\lambda\|_K^2 \rangle \\ &= \|f_{S^{i,z}}^\lambda - f_S^\lambda\|_K^2 \end{aligned}$$

$$d_N(f_{S^{i,z}}^\lambda, f_S^\lambda) + d_N(f_S^\lambda, f_{S^{i,z}}^\lambda) \leq \frac{2L \|f_S^\lambda - f_{S^{i,z}}^\lambda\|_\infty}{\lambda n}$$

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# The Lemma

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# Stability of Tikhonov

- 1 assumption:  $|V(f_1(x), y') - V(f_2(x), y')| \leq L\|f_1 - f_2\|_\infty$
- 2 property of RKHS:  $\|f - f'\|_\infty \kappa \leq \|f - f'\|_K$ , for any  $f, f' \in \mathcal{H}$ .
- 3 lemma:  $\|f_S^\lambda - f_{S^{j,z}}^\lambda\|_K^2 \leq \frac{L\|f_S^\lambda - f_{S^{j,z}}^\lambda\|_\infty}{\lambda n}$

putting all together:

$$\begin{aligned} |V(f_S^\lambda, z) - V(f_{S^{j,z}}^\lambda, z)| &\leq L\|f_S^\lambda - f_{S^{j,z}}^\lambda\|_\infty \\ &\leq L\kappa\|f_S^\lambda - f_{S^{j,z}}^\lambda\|_K \\ &\leq \frac{L^2\kappa^2}{\lambda n} \\ &=: \beta \end{aligned}$$

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# Bounding the Loss

We have shown that Tikhonov regularization with an  $L$ -Lipschitz loss is  $\beta$ -stable with  $\beta = \frac{L^2 \kappa^2}{\lambda n}$ .  
To apply the theorems and get the generalization bound, we need to bound the loss

$$V(f_S^\lambda, z) \leq M < \infty, \quad \forall z = (x, y)$$

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# Bounding the Loss (cont.)

$$V(f_S^\lambda, z) \leq M < \infty, \quad \forall z = (x, y)$$

- Assume that  $V(0, z) \leq C_0 < \infty$ , then

$$\begin{aligned} \lambda \|f_S^\lambda\|_K^2 &\leq T_S(f_S^\lambda) \leq T_S(0) \\ &= \frac{1}{n} \sum_{i=1}^n V(0, y_i) \leq C_0. \end{aligned}$$

- Then  $\|f_S^\lambda\|_K^2 \leq \frac{C_0}{\lambda} \implies \|f_S^\lambda\|_\infty \leq \kappa \|f_S^\lambda\|_K \leq \kappa \sqrt{\frac{C_0}{\lambda}}$
- Finally  $|V(f_S^\lambda(x), y)| \leq |V(f_S^\lambda(x), y) - V(0, y)| + |V(0, y)|$

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$$\beta = \frac{L^2 \kappa^2}{\lambda n}, \quad M = \kappa L \sqrt{\frac{C_0}{\lambda}} + C_0$$

so that, with probability  $1 - \delta$ ,

$$I[f_S^\lambda] \leq I_S[f_S^\lambda] + \frac{L^2 \kappa^2}{\lambda n} + \left( \frac{2L^2 \kappa^2}{\lambda} + C_0 + \kappa L \sqrt{\frac{C_0}{\lambda}} \right) \sqrt{\frac{2 \ln(2/\delta)}{n}}.$$

Keeping  $\lambda$  fixed as  $n$  increase  $n$ , the generalization bound will tighten as  $O\left(\frac{1}{\sqrt{n}}\right)$ .

However, fixing  $\lambda$  fixed we keep our hypothesis space fixed. As we get more data, we want  $\lambda$  to get smaller. If  $\lambda$  gets smaller too fast, the bounds become trivial...

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