Tutorial
Characterizing the Generalization Error of Machine Learning Algorithms via Information Measures

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Slides for Part II

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- KL divergence: $\mathrm{KL}(P\|Q) \triangleq \int_{\mathcal{X}} \log\left(\frac{dP}{dQ}\right) dP$
- Symmetrized KL divergence (Jeffrey's divergence)

$$D_{\mathrm{SKL}}(P\|Q) \triangleq \mathrm{KL}(P\|Q) + \mathrm{KL}(Q\|P).$$

- Mutual information: $\mathrm{I}(X;Y) \triangleq \mathrm{KL}(P_{X,Y}\|P_X \otimes P_Y)$
- Lautum information [Palomar and Verdú, 2008]: $L(X;Y) \triangleq \mathrm{KL}(P_X \otimes P_Y\|P_{X,Y})$
- Symmetrized KL information [Aminian et al., 2015]:

$$\mathrm{I}_{\mathrm{SKL}}(X;Y) \triangleq D_{\mathrm{SKL}}(P_{X,Y}\|P_X \otimes P_Y) = \mathrm{I}(X;Y) + L(X;Y).$$

Information-theoretic Generalization Bounds

Lemma ([Xu and Raginsky, 2017])

Suppose $\ell(w, Z)$ is σ-sub-Gaussian under $Z \sim \mu$ for all $w \in \mathcal{W}$, then

$$|\mathrm{gen}(\mu, P_{W|S})| \leq \sqrt{\frac{2\sigma^2}{n}\mathrm{I}(S; W)}.$$

- Depends on every ingredient in the supervised learning problem
- Reducing dependence between W and S leads to better generalization bound
- This bound is only tight if $\mathrm{I}(S; W) = 0$ and $\mathrm{gen}(\mu, P_{W|S}) = 0$
- Multiple techniques to improve this result, including ISMI [Bu et al., 2020], CMI [Steinke and Zakynthinou, 2020], f-CMI [Harutyunyan et al., 2021], ΔL-CMI [Wang and Mao, 2023]

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Regularized ERM problem

- How can we use this result to develop a better learning algorithm?
- Regularizing mutual information $\mathrm{I}(S;W)$ during ERM

$$P^{\star}_{W|S} = \operatorname*{arg\,min}_{P_{W|S}} \left(\mathbb{E}_{P_{W,S}}[L_E(W,S)] + \frac{1}{\gamma}\mathrm{I}(S;W) \right)$$

  - inverse temperature $\gamma \geq 0$ balances between fitting and generalization
- Replacing $\mathrm{I}(S;W)$ with $\mathrm{KL}(P_{W|S}\|\pi(W)|P_S)$ for any prior $\pi(W)$
- It gives **information risk minimization** (IRM) problem

$$P^{\star}_{W|S} = \operatorname*{arg\,min}_{P_{W|S}} \left(\mathbb{E}_{P_{W,S}}[L_E(W,S)] + \frac{1}{\gamma}\mathrm{KL}(P_{W|S}\|\pi(W)|P_S) \right)$$

Information Risk Minimization

Lemma ([Zhang, 2006, Xu and Raginsky, 2017])

Solution to IRM problem is $(\gamma, \pi(w), L_E(w,s))$-**Gibbs distribution**

$$P^{\gamma}_{W|S}(w|s) \triangleq \frac{\pi(w)e^{-\gamma L_E(w,s)}}{V(s,\gamma)}, \quad \gamma \geq 0,$$

where $V(s,\gamma) \triangleq \int \pi(w)e^{-\gamma L_E(w,s)}dw$ *is partition function.*

Proof.

For any learning algorithm $P_{W|S}$ with fixed $S = s$,

$$\begin{aligned} 0 &\leq \mathrm{KL}(P_{W|S=s} \| P^{\gamma}_{W|S=s}) \\ &= \mathbb{E}_{P_{W|S=s}}\left[\log \frac{P_{W|S=s} \cdot V(s,\gamma)}{\pi(W) \cdot e^{-\gamma L_E(w,s)}}\right] \\ &= \mathrm{KL}(P_{W|S=s} \| \pi(W)) + \log V(s,\gamma) + \gamma \mathbb{E}_{P_{W|S=s}}[L_E(w,s)]. \end{aligned}$$

$$\min_{P_{W|S}} \mathbb{E}_{P_{W|S=s}}[L_E(W,s)] + \frac{1}{\gamma}\mathrm{KL}(P_{W|S=s} \| \pi) = -\frac{1}{\gamma}\log V(s,\gamma). \quad \square$$

Gibbs Algorithm

We focus on the generalization error of Gibbs algorithm (distribution)

$(\gamma, \pi(w), L_E(w, s))$-Gibbs distribution:

$$P^{\gamma}_{W|S}(w|s) \triangleq \frac{\pi(w)e^{-\gamma L_E(W,s)}}{V(s,\gamma)}, \quad \gamma \geq 0$$

where

- inverse temperature γ, reduces to standard ERM if $\gamma \to \infty$
- $\pi(w)$ arbitrary prior distribution of W
- $V(s,\gamma) \triangleq \int \pi(w)e^{-\gamma L_E(w,s)} dw$ partition function

Practical Implementation of Gibbs algorithm

- Stochastic Gradient Langevin Dynamics (SGLD)
- Metropolis adjusted Langevin algorithm (MALA)

The SGLD can be viewed as the noisy version of SGD,

$$W_{k+1} = W_k - \eta_t \nabla L_E(W_k, s) + \sqrt{\frac{2\eta_t}{\gamma}}\zeta_k, \quad k = 0, 1, \cdots,$$

where ζ_k standard Gaussian random vector; $\eta_t > 0$ step size.

- [Raginsky et al., 2017] shows that $P_{W_k|S}$ induced by SGLD converges to $(\gamma, \pi(W_0), L_E(w_k, s))$-Gibbs distribution for sufficiently large k
- MALA is SGLD with Metropolis rejection, faster convergence

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Expected Generalization Error

An **exact** characterization of generalization error for Gibbs algorithm

Theorem

For $(\gamma, \pi(w), L_E(w,s))$*-Gibbs algorithm,*

$$P^{\gamma}_{W|S}(w|s) = \frac{\pi(w) e^{-\gamma L_E(w,s)}}{V(s,\gamma)}, \quad \gamma > 0,$$

the expected generalization error is

$$\overline{\text{gen}}(P^{\gamma}_{W|S}, P_S) = \frac{\mathrm{I}_{\mathrm{SKL}}(W;S)}{\gamma}.$$

- Highlights the fundamental role of $\mathrm{I}_{\mathrm{SKL}}(W;S)$ in learning theory
- Holds even for non-i.i.d training samples

G. Aminian*, Y. Bu*, L. Toni, M. R. Rodrigues, G. W. Wornell. "An Exact Characterization of the Generalization Error for the Gibbs Algorithm," in *Proc. Conference on Neural Information Processing Systems (***NeurIPS***)*, Dec. 2021.

Generalization Error of Gibbs Algorithm

Theorem

For Gibbs algorithm $P^{\gamma}_{W|S}(w|s) = \frac{\pi(w)e^{-\gamma L_E(w,s)}}{V(s,\gamma)}$,

$$\overline{\text{gen}}(P^{\gamma}_{W|S}, P_S) = \frac{\text{I}_{\text{SKL}}(W;S)}{\gamma}.$$

Sketch of Proof:

Symmetrized KL information can be written as

$$\begin{aligned}\text{I}_{\text{SKL}}(W;S) &= \mathbb{E}_{P_{W,S}}[\log(\frac{P^{\gamma}_{W|S}}{P_W})] + \mathbb{E}_{P_W \otimes P_S}[\log(\frac{P_W}{P^{\gamma}_{W|S}})] \\ &= \mathbb{E}_{P_{W,S}}[\log(P^{\gamma}_{W|S})] - \mathbb{E}_{P_W \otimes P_S}[\log(P^{\gamma}_{W|S})]\end{aligned}$$

Note that $P_{W,S}$ and $P_W \otimes P_S$ share the same marginal distribution,

$$\begin{aligned}\text{I}_{\text{SKL}}(W;S) &= \mathbb{E}_{P_{W,S}}[-\gamma L_E(W,S)] - \mathbb{E}_{P_W \otimes P_S}[-\gamma L_E(W,S)] \\ &= \gamma \overline{\text{gen}}(P^{\gamma}_{W|S}, P_S)\end{aligned}$$

□

Empirical risk of Gibbs algorithm

Theorem

$\log V(s,\gamma)$ is convex and differentiable infinitely many times with respect to γ. In particular,

$$\mathbb{E}_\gamma[L_E(W,s)] = -\frac{\partial \log V(s,\gamma)}{\partial \gamma},$$

$$\mathrm{Var}_\gamma[L_E(W,s)] = \frac{\partial^2 \log V(s,\gamma)}{\partial \gamma^2},$$

where $\mathbb{E}_\gamma[\,\cdot\,] \triangleq \mathbb{E}_{P^\gamma_{W|S=s}}[\,\cdot\,]$, and $\mathrm{Var}_\gamma[L_E(W,s)] \triangleq \mathbb{E}_\gamma[L_E(W,s)^2] - \mathbb{E}_\gamma[L_E(W,s)]^2$.

Expected empirical risk of the Gibbs algorithm is non-increasing w.r.t γ

- Monoticity: $L_E(W,s)$ is non-increasing with γ
- Sub-Gaussianity: $L_E(W,s)$ is sub-Gaussian under Gibbs algorithm if $\mathrm{Var}_\gamma[L_E(W,s)]$ is bounded

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Perlaza, Samir M., Gaetan Bisson, Iñaki Esnaola, Alain Jean-Marie, and Stefano Rini. "Empirical risk minimization with relative entropy regularization," *IEEE Trans. Inf. Theory*, 2024.

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Tighter Generalization Error Upper Bounds

Why do we care about upper bounds when we have exact characterization?

- Quantify how $\overline{\text{gen}}(P^{\gamma}_{W|S}, P_S)$ depends on number of i.i.d. samples n
- Useful when directly evaluating $\mathrm{I}_{\mathrm{SKL}}(W;S)$ is hard

Theorem

Suppose that

- $S = \{Z_i\}_{i=1}^{n}$ *are i.i.d generated from the distribution* P_Z
- $\ell(w, Z)$ *is* σ*-sub-Gaussian*
- $C_E \leq \frac{\mathrm{L}(W;S)}{\mathrm{I}(W;S)}$ *for some* $C_E \geq 0$*,*

$$\overline{\text{gen}}(P^{\gamma}_{W|S}, P_S) \leq \frac{2\sigma^2\gamma}{(1 + C_E)n}.$$

G. Aminian*, Y. Bu*, L. Toni, M. R. Rodrigues, G. W. Wornell. “An Exact Characterization of the Generalization Error for the Gibbs Algorithm,” in *Proc. Conference on Neural Information Processing Systems (* **NeurIPS** *)*, Dec. 2021.

Tighter Generalization Error Upper Bounds

Sketch of Proof:

Recall the mutual information-based bound,

$$\sqrt{\frac{2\sigma^2}{n}\mathrm{I}(S;W)} \geq \overline{\mathrm{gen}}(P^{\gamma}_{W|S}, P_S) = \frac{\mathrm{I}(W;S) + L(W;S)}{\gamma}$$

$$\geq \frac{(1+C_E)}{\gamma}\mathrm{I}(W;S)$$

$$\overline{\mathrm{gen}}(P^{\gamma}_{W|S}, P_S) \leq \sqrt{\frac{2\sigma^2}{n}\mathrm{I}(S;W)} \leq \frac{2\sigma^2\gamma}{(1+C_E)n} \qquad \square$$

[Choice of C_E]

- $C_E = 0$ is always valid, which gives $\overline{\mathrm{gen}}(P^{\gamma}_{W|S}, P_S) \leq \frac{2\sigma^2\gamma}{n}$
- $C_E = 1$, $L(S;W) \geq \mathrm{I}(S;W)$ holds for any Gaussian channel $P_{W|S}$

Example: Mean Estimation

- Learning mean $\boldsymbol{\mu} \in \mathbb{R}^d$ of Z using n i.i.d training samples $S = \{\boldsymbol{z}_i\}_{i=1}^n$
- Not necessary Gaussian, but covariance matrix $\Sigma_Z = \sigma_Z^2 \boldsymbol{I}_d$
- Mean-squared loss $\ell(\boldsymbol{w}, \boldsymbol{z}) = \|\boldsymbol{z} - \boldsymbol{w}\|_2^2$
- Gaussian prior $\pi(\boldsymbol{w}) = \mathcal{N}(\boldsymbol{\mu}_0, \sigma_0^2 \boldsymbol{I}_d)$
- Then, $(\gamma, \mathcal{N}(\boldsymbol{\mu}_0, \sigma_0^2 \boldsymbol{I}_d), L_E(\boldsymbol{w}, s))$-Gibbs algorithm is given by the following Gaussian posterior

$$P_{W|S}^{\gamma}(\boldsymbol{w}|\boldsymbol{z}^n) \sim \mathcal{N}\Big(\alpha \boldsymbol{\mu}_0 + (1-\alpha)\bar{\boldsymbol{z}}, \alpha \sigma_0^2 \boldsymbol{I}_d\Big),$$

with

$$\alpha \triangleq \frac{1}{2\sigma_0^2 \gamma + 1}, \quad \bar{\boldsymbol{z}} \triangleq \frac{1}{n}\sum_{i=1}^{n} \boldsymbol{z}_i.$$

Example: Mean Estimation

Since $P^{\gamma}_{W|S}$ is Gaussian,

$$\mathrm{I}(S;W) = \frac{d\sigma_0^2\sigma_Z^2\gamma}{(n\sigma_0^2 + \frac{1}{2\gamma})} - \mathrm{KL}\big(P_W \| \mathcal{N}(\boldsymbol{\mu}_W, \sigma_1^2 I_d)\big),$$
$$L(S;W) = \frac{d\sigma_0^2\sigma_Z^2\gamma}{(n\sigma_0^2 + \frac{1}{2\gamma})} + \mathrm{KL}\big(P_W \| \mathcal{N}(\boldsymbol{\mu}_W, \sigma_1^2 I_d)\big),$$

with $\boldsymbol{\mu}_W = \alpha\boldsymbol{\mu}_0 + (1-\alpha)\boldsymbol{\mu}$.

The generalization error can be computed exactly as:

$$\overline{\mathrm{gen}}(P^{\gamma}_{W|S}, P_S) = \frac{\mathrm{I}_{\mathrm{SKL}}(W;S)}{\gamma} = \frac{2d\sigma_0^2\sigma_Z^2}{n(\sigma_0^2 + \frac{1}{2\gamma})}.$$

As a comparison, the ISMI-based bound gives a sub-optimal bound $\mathcal{O}\left(1/\sqrt{n}\right)$, as $n \to \infty$.

Check Point

Generalization error or empirical risk is one part of the story

Our goal is to **design** (or guide the design) algorithms that minimize population risk.

There are three elements in $(\gamma, \pi(w), L_E(w, s))$-Gibbs algorithm

- inverse temperature $\gamma \longrightarrow$ Optimal hyper-parameter
- empirical risk $L_E(w, s)$, or model family $\longrightarrow$ Information criteria for model selection
- prior distribution $\pi(w) \longrightarrow$ Transfer learning

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Expected Test Loss

For fixed training data s and testing data s', consider expected test loss

$$L_P(\gamma, s, s') \triangleq \mathbb{E}_\gamma[L_E(W, s')],$$

and expected generalization error

$$\overline{\mathrm{gen}}(\gamma, s, s') \triangleq \mathbb{E}_\gamma[L_E(W, s') - L_E(W, s)].$$

Theorem

For $\gamma \geq 0$ such that $\log V(s, \gamma) < \infty$, the first order derivative of the expected test loss is given by

$$\frac{\partial}{\partial \gamma} L_P(\gamma, s, s') = -\mathrm{Cov}_\gamma[L_E(W, s'), L_E(W, s)],$$

with

$$\mathrm{Cov}_\gamma[L_E(W, s'), L_E(W, s)] \triangleq \mathbb{E}_\gamma[L_E(W, s) L_E(W, s')] - \mathbb{E}_\gamma[L_E(W, s)]\mathbb{E}_\gamma[L_E(W, s')].$$

$\mathrm{Cov}_\gamma[L_E(W, s'), L_E(W, s)]$ can be positive/negative, no monotonicity

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Y. Bu, "Towards Optimal Inverse Temperature in the Gibbs Algorithm," in IEEE ISIT 2024

Expected Generalization Error

Corollary

For $\gamma \geq 0$ such that $\log V(s,\gamma) < \infty$, the first order derivative of the expected generalization error is given by

$$\frac{\partial}{\partial\gamma}\overline{\mathrm{gen}}(\gamma, s, s') = \mathrm{Var}_\gamma(L_E(W,s)) - \mathrm{Cov}_\gamma[L_E(W,s'), L_E(W,s)].$$

- Cannot show that the $\overline{\mathrm{gen}}$ is non-decreasing, Cauchy-Schwarz Inequality only guarantees that

$$\left|\mathrm{Cov}_\gamma[L_E(W,s'), L_E(W,s)]\right| \leq \sqrt{\mathrm{Var}_\gamma(L_E(W,s))\mathrm{Var}_\gamma(L_E(W,s'))}.$$

- [Aminian et al., 2021] provides a bound of order $\mathcal{O}\left(\frac{\gamma}{n}\right)$ by simply combining the I_{SKL} characterization with the MI bound, which may hint that $\overline{\mathrm{gen}}$ is always increasing with γ.
- However, we will illustrate how $\overline{\mathrm{gen}}$ rises from zero and then decreases as γ increases.

Example: Mean Estimation

$(\gamma, \mathcal{N}(\boldsymbol{\mu}_0, \sigma_0^2 \boldsymbol{I}_d), L_E(\boldsymbol{w}, s))$-Gibbs algorithm is given by the following Gaussian posterior

$$P^{\gamma}_{W|S}(\boldsymbol{w}|\boldsymbol{z}^n) \sim \mathcal{N}\Big(\alpha \boldsymbol{\mu}_0 + (1-\alpha)\bar{\boldsymbol{z}}, \alpha\sigma_0^2 \boldsymbol{I}_d\Big)$$

Population risk has the following exact characterization

$$L_P(P^{\gamma}_{W|S}, P_S) = \underbrace{\frac{4d\sigma_0^2\sigma_Z^2\gamma}{n(1+2\sigma_0^2\gamma)}}_{\text{generalization error}} + \underbrace{\frac{\|\boldsymbol{\mu}_0 - \boldsymbol{\mu}\|_2^2 + d\sigma_z^2/n}{(1+2\sigma_0^2\gamma)^2} + \frac{d\sigma_0^2}{1+2\sigma_0^2\gamma} + \frac{n-1}{n} d\sigma_Z^2.}_{\text{empirical risk}}$$

To find optimal γ minimizes L_P

- Optimize over γ using the above equation directly
- Evaluate the derivative of $L_P(\gamma, s, s')$ by computing covariance

Example: Mean Estimation

γ^* depends on other parameters of the problem in a non-trivial manner

$$\gamma^* = \begin{cases} +\infty, & \text{if } \frac{\sigma_Z^2}{n} \in [0, \frac{\sigma_0^2}{2}), \text{ (high-SNR)} \\ \frac{\|\boldsymbol{\mu}-\boldsymbol{\mu}_0\|^2 + d\sigma_0^2/2}{d(2\sigma_Z^2/n - \sigma_0^2)\sigma_0^2}, & \text{if } \frac{\sigma_Z^2}{n} \in [\frac{\sigma_0^2}{2}, \infty). \text{ (low-SNR)} \end{cases}$$

- $\frac{\sigma_Z^2}{n}$ only depends on S, can be interpreted as normalized noise
- σ_0^2 and $\|\boldsymbol{\mu} - \boldsymbol{\mu}_0\|^2$ captures the confidence and bias of prior knowledge
- high-SNR regime, high-quality training samples, discarding prior distribution and employing standard ERM
- low-SNR regime, where we should incorporate knowledge from both training samples and prior, optimal γ depends on everything
- If $\boldsymbol{\mu}_0 = \boldsymbol{\mu}$ and $\sigma_0^2 = 0$, $\gamma^* = 0$

Example: Linear Regression

- Training data $S = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$, with $\mathcal{X} = \mathbb{R}^d$ and $\mathcal{Y} = \mathbb{R}$
- Data is generated using true weights $W^* \in \mathbb{R}^d$ with additive noise,

$$Y_i = X_i \cdot W^* + \varepsilon_i, \quad \varepsilon \sim \mathcal{N}(0, \sigma_\varepsilon^2).$$

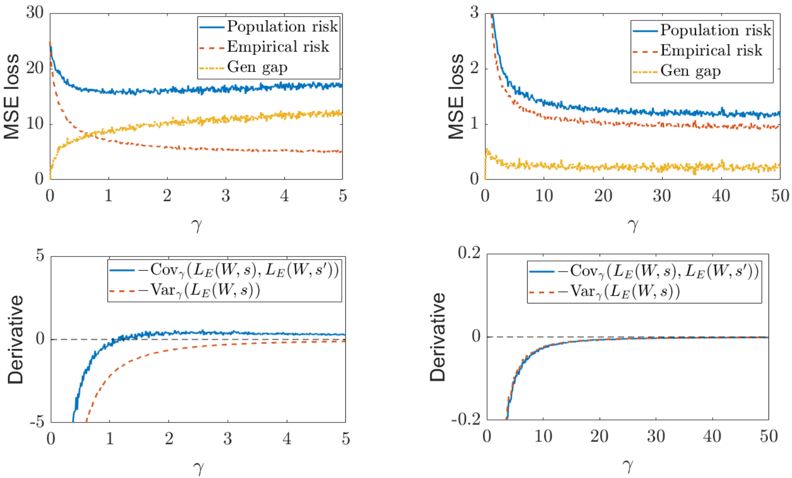
- Mean-squared loss $\ell(\boldsymbol{w}, \boldsymbol{z}) = (y - \boldsymbol{x} \cdot \boldsymbol{w})^2$
- Gaussian prior $\pi(\boldsymbol{w}) = \mathcal{N}(0, \sigma_0^2 \boldsymbol{I}_d)$
- $(\gamma, \mathcal{N}(0, \sigma_0^2 \boldsymbol{I}_d), L_E(\boldsymbol{w}, s))$-Gibbs algorithm is Gaussian

$$P_{W|S}^{\gamma}(\boldsymbol{w}|S) \sim \mathcal{N}\left(\boldsymbol{\Sigma}^{-1} \boldsymbol{X}^\top \boldsymbol{Y}, \frac{n}{2\gamma} \boldsymbol{\Sigma}^{-1}\right),$$

with $\boldsymbol{\Sigma} \triangleq \boldsymbol{X}^\top \boldsymbol{X} + \frac{n}{2\sigma_0^2 \gamma} \boldsymbol{I}_d$, and $\boldsymbol{X} \in \mathbb{R}^{n \times d}$, $\boldsymbol{Y} \in \mathbb{R}^n$ are the matrix form of the training data.

Simulation of Linear Regression

Low SNR regime, $n = 10$ and $\sigma_\varepsilon^2 = 3$; high SNR regime, $n = 100$ and $\sigma_\varepsilon^2 = 1$.



Low-SNR High-SNR

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Asymptotic Behavior of Generalization Error

- Can we show something for ERM by letting $\gamma \to \infty$?
  - Previous upper bound has order $\mathcal{O}(\frac{\gamma}{n})$
- Asymptotic normality of Gibbs algorithm
  - **Single-well** case: there exists a unique $W^*(S)$

$$W^*(S) = \arg\min_{w \in \mathcal{W}} L_E(w, S).$$

  - If $H^*(S) \triangleq \nabla_w^2 L_E(w, S)\big|_{w=W^*(S)}$ is invertible [Hwang, 1980],

$$P_{W|S}^{\gamma} \to \mathcal{N}(W^*(S), \frac{1}{\gamma} H^*(S)^{-1})$$

G. Aminian*, Y. Bu*, L. Toni, M. R. Rodrigues, G. W. Wornell. "An Exact Characterization of the Generalization Error for the Gibbs Algorithm," in *Proc. Conference on Neural Information Processing Systems (*__NeurIPS__*)*, Dec. 2021.

Asymptotic Behavior of MLE

Maximum likelihood estimates (MLE) in the asymptotic regime $n \to \infty$.

- n i.i.d. training samples generated from distribution P_Z
- Fit training data with distribution family $f(z_i|\boldsymbol{\theta})$, $\boldsymbol{\theta} \in \mathbb{R}^p$
- $P_Z = f(\cdot|\boldsymbol{\theta}^*)$ for $\boldsymbol{\theta}^* \in \mathcal{W}$
- log-loss $\ell(\boldsymbol{w}, z) = -\log f(z|\boldsymbol{w})$

As $\gamma \to \infty$, Gibbs algorithm converges to ERM algorithm (MLE),

$$\hat{W}_{\mathrm{ML}} \triangleq \arg\max_{\boldsymbol{\theta} \in \mathcal{W}} \sum_{i=1}^{n} \log f(Z_i|\boldsymbol{\theta}).$$

Compute $\mathrm{I}_{\mathrm{SKL}}(W; S)$ using Gaussian approximation

$$\overline{\mathrm{gen}}(P_{W|S}^{\infty}, P_S) = \frac{d}{n}.$$

Connection to Model Selection

- K candidate models $M_1, M_2, \ldots, M_K$
- Each model M_k is characterized by parametric probabilistic model $P_k(\boldsymbol{z}|\boldsymbol{\theta}_k)$ and prior $\pi_k(\boldsymbol{\theta}_k)$
- log likelihood as the loss function $\ell_{\log}(w, \boldsymbol{z}) \triangleq -\log P(\boldsymbol{z}|w)$

How to select the *optimal* model?

- Information Criteria for Model Selection
  - Akaike Information Criterion (AIC)
  - Bayesian Information Criterion (BIC)

Akaike Information Criterion (AIC)

AIC selects the model that minimizes population risk:

$$\arg\min_k \ \mathrm{KL}(P_Z \| P_k(\boldsymbol{z}|\hat{\boldsymbol{\theta}}^{(k)}_{\mathrm{ML}})) = \arg\min_k \mathbb{E}_{P_Z}\big[-\log P_k(Z|\hat{\boldsymbol{\theta}}^{(k)}_{\mathrm{ML}})\big].$$

AIC approximates it using empirical risk and generalization error

$$\mathrm{AIC} = \arg\min_k L_E(\hat{\boldsymbol{\theta}}^{(k)}_{\mathrm{ML}}, S) + \overline{gen}(\hat{\boldsymbol{\theta}}^{(k)}_{\mathrm{ML}}, P_Z).$$

In classic regime where $n \to \infty$, and certain regularization conditions

$$\mathrm{AIC} = \arg\min_k L_E(\hat{\boldsymbol{\theta}}^{(k)}_{\mathrm{ML}}, S) + \frac{p}{n}.$$

Bayesian Information Criterion (BIC)

BIC selects the model that maximizes marginal likelihood:

$$m_k(\boldsymbol{z}^n) \triangleq \int P_k(\boldsymbol{z}^n|\boldsymbol{\theta}_k)\,\pi_k(\boldsymbol{\theta}_k)\,d\boldsymbol{\theta}_k,$$

which is equivalent to maximizing posterior probability $P(M_k|\boldsymbol{z}^n)$.

$$\begin{aligned}\mathrm{BIC} &= \arg\min_k \; -\frac{1}{n}\log m_k(\boldsymbol{z}^n) \\ &= \arg\min_k \; L_E(\hat{\boldsymbol{\theta}}^{(k)}_{\mathrm{ML}}, S) + \frac{p_k \log n}{2n},\end{aligned}$$

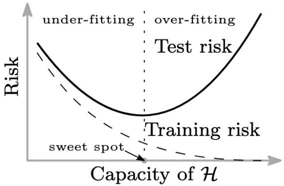
where Laplace approximation is applied as $n \to \infty$.

Comparison between AIC and BIC

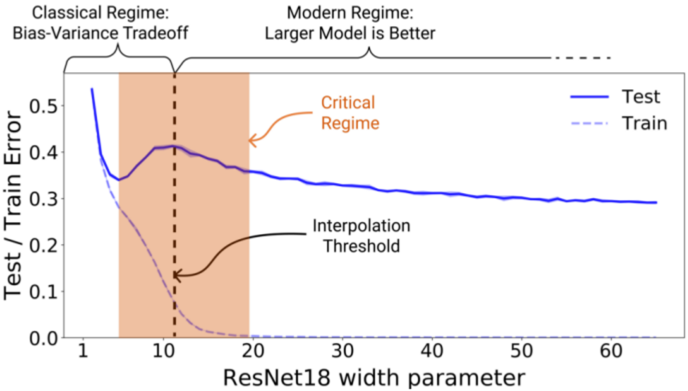
$$\mathrm{AIC} = \arg\min \; L_E(\hat{\theta}_{\mathrm{ML}}, S) + \frac{p}{n}$$

$$\mathrm{BIC} = \arg\min \; L_E(\hat{\theta}_{\mathrm{ML}}, S) + \frac{p \log n}{2n}.$$

- AIC minimizes population risk (optimal prediction performance)
- BIC maximizes the marginal likelihood (identifying the true model)
- BIC imposing a **larger** penalty for more complex models.



Double-descent in Over-parameterized Regime



- When $p \leq n$, the classical $\cup$-shaped curve is valid.
- When $p \geq n$, test loss can decrease again.

Challenges in Over-parameterized regime

Asymptotic normality (AIC) and Laplace Approximation (BIC) do not hold in this new regime!

There are some efforts to extend these information criteria:

- Akaike's Information Corrected Criterion (AICC), fixed p, small n
- Widely applicable BIC (WBIC), singular Hessian matrix

More recent work trying to demystify double-descent

- Neural Tangent Kernel (NTK), lazy training
- Random feature model
- Mean-field approach

Marginal likelihood of Gibbs algorithm

Recall the **information risk minimization** for motivating the Gibbs algorithm.

$$\min_{P_{W|S}} \mathbb{E}_{P_{W|S=s}}\left[L_E(W,s)\right] + \frac{1}{\gamma}\mathrm{KL}(P_{W|S=s}\|\pi) = -\frac{1}{\gamma}\log V(s,\gamma).$$

If we adopt log-loss function $\ell(w,\boldsymbol{z}) = -\log P(\boldsymbol{z}|w)$, and set $\gamma = n$

$$\begin{aligned}
-\frac{1}{\gamma}\log V(s,\gamma) &= -\frac{1}{n}\log\int \pi(w)e^{-nL_E(w,s)}dw \\
&= -\frac{1}{n}\log\int \pi(w)P(\boldsymbol{z}^n|w)dw \\
&= -\frac{1}{n}\log m(\boldsymbol{z}^n)
\end{aligned}$$

Gibbs based Information Criteria

Gibbs-based AIC:

$$\mathrm{AIC}^{+} \triangleq L_E(\hat{W}_{\mathrm{Gibbs}}, \boldsymbol{z}^n) + \frac{1}{n}\mathrm{I}_{\mathrm{SKL}}(P^*_{\hat{W}|S}, P_S).$$

Gibbs-based BIC:

$$\mathrm{BIC}^{+} \triangleq L_E(\hat{W}_{\mathrm{Gibbs}}, \boldsymbol{z}^n) + \frac{1}{n}\mathrm{KL}(P^*_{W|S=\boldsymbol{z}^n} \| \pi),$$

$$\mathrm{BIC}^{-} \triangleq \mathbb{E}_{\pi}\left[L_E(W, \boldsymbol{z}^n)\right] - \frac{1}{n}\mathrm{KL}(\pi \| P^*_{W|S=\boldsymbol{z}^n}).$$

We can show that in the classic regime where p is fixed and $n \to \infty$, they all reduce back to their classical forms.

H. Chen, Y. Bu, G. W. Wornell, "Gibbs-Based Information Criteria and the Over-Parameterized Regime," in *Proc. International Conference on Artificial Intelligence and Statistics (**AISTATS**)*, 2024.

Random Feature Model

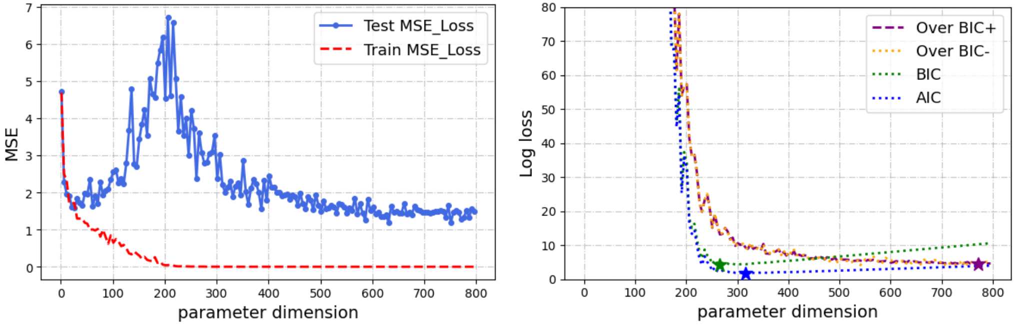
The output of **Random Feature (RF) model** with input data $\boldsymbol{x} \in \mathbb{R}^d$ is

$$g(\boldsymbol{x}) \triangleq \sum_{j=1}^{p} f\left(\frac{\langle \boldsymbol{x}, \boldsymbol{F}_j \rangle}{\sqrt{d}}\right) \boldsymbol{w}_j = f\left(\frac{\boldsymbol{x}^\top \boldsymbol{F}}{\sqrt{d}}\right) \boldsymbol{w},$$

- Two-layer neural network with i.i.d Gaussian weights $\boldsymbol{F} \in \mathbb{R}^{d \times p}$ in the first layer, only the second layer is trainable
- $f()$ is the non-linear activation function
- The dimensionality of input data d is not entangled with number of parameters p

Experiment

Evaluating the BIC^{+} and BIC^{-} using $n = 200$ samples in RF models



- We observe **Double-descent** in population risk for RF model
- Our Gibbs-based BICs prefer **over-parameterized models**

Check point

- Provide information criteria for the Gibbs algorithm, with different **information measures** as the penalty terms.

- Generalize our information-theoretic analysis to **over-parameterized** random feature.

- The **mismatch** between **marginal likelihood (BIC)** and **generalization error (AIC)** in the over-parameterized setting, which highly depends on the prior distributions.

Table of Contents (Part II)

Generalization of Transfer Learning

- Source data set $D^s = \{Z_i^s\}_{i=1}^m$, generated from P_{D^s}
- Target data set $D^t = \{Z_j^t\}_{j=1}^n$, generated from P_{D^t}
- The empirical risk of source and target task

$$L_E(w, d^s) \triangleq \frac{1}{m}\sum_{j=1}^{m} \ell(w, z_j^s), \qquad L_E(w, d^t) \triangleq \frac{1}{n}\sum_{j=1}^{n} \ell(w, z_j^t).$$

- The population risk of the target task

$$L_P(w, P_{D^t}) \triangleq \mathbb{E}_{P_{D^t}}[L_E(w, D^t)].$$

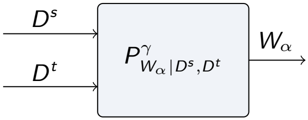
- Expected Transfer Generalization Error

$$\overline{\mathrm{gen}}(P_{W|D^s,D^t}, P_{D^s}, P_{D^t}) \triangleq \mathbb{E}_{P_{W,D^s,D^t}}[L_P(W, P_{D^t}) - L_E(W, D^t)].$$

Transfer Learning: α-Weighted ERM

- Output hypothesis w_α is trained by minimizing a convex combination of the source and target task empirical risks [Ben-David et al., 2010], for $\alpha \in [0,1]$

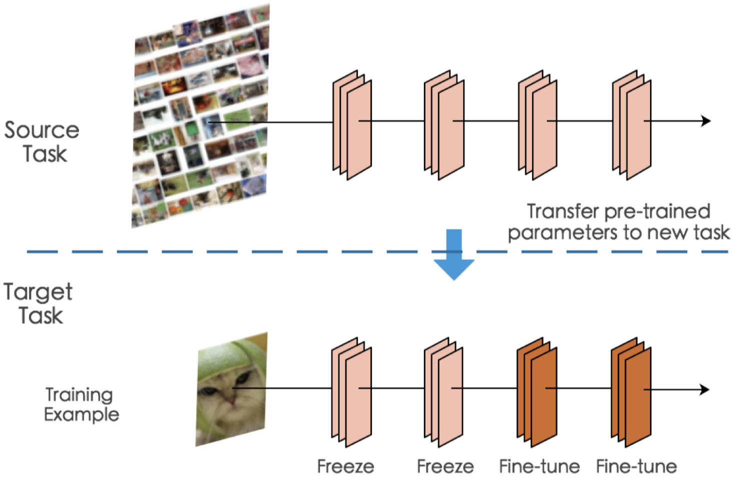
$$L_E(w_\alpha, d^s, d^t) = (1-\alpha)L_E(w_\alpha, d^s) + \alpha L_E(w_\alpha, d^t)$$



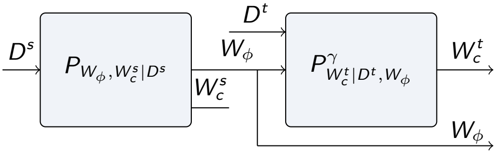
- **α-weighted Gibbs algorithm** generalizes the α-weighted-ERM by considering the $(\gamma, \pi(w_\alpha), L_E(w_\alpha, d^s, d^t))$-Gibbs algorithm

$$P^{\gamma}_{W_\alpha|D^s,D^t}(w_\alpha|d^s, d^t) = \frac{\pi(w_\alpha)e^{-\gamma L_E(w_\alpha, d^s, d^t)}}{V_\alpha(d^s, d^t, \gamma)}.$$

Transfer Learning: Two-stage ERM



Two-stage-ERM Transfer Learning



- **First Stage:** Learn shared feature extractor $w_\phi \in \mathcal{W}_\phi$

$$[W_\phi, W_c^s] = \arg\min_{w} L_E^{S1}(w, d^s).$$

- **Second Stage:** Freeze W_ϕ, and learn target-specific hypothesis w_c^t

$$W_c^t = \arg\min_{w_c} L_E^{S2}([W_\phi, w_c], d^t)$$

Expected Transfer Generalization Error

Theorem

The expected transfer generalization error of the α-weighted Gibbs algorithm is given by

$$\overline{\text{gen}}_\alpha(P_{D^s}, P_{D^t}) = \frac{\mathrm{I}_{\mathrm{SKL}}(W_\alpha; D^t|D^s)}{\alpha\gamma}.$$

Theorem

The expected transfer generalization error of the two-stage Gibbs algorithm is given by

$$\overline{\text{gen}}_\beta(P_{D^s}, P_{D^t}) = \frac{\mathrm{I}_{\mathrm{SKL}}(W_c^t; D^t|W_\phi)}{\gamma}.$$

Y. Bu*, G. Aminian*, L. Toni, M. R. Rodrigues, G. W. Wornell. "Characterizing and Understanding the Generalization Error of Transfer Learning with Gibbs Algorithm," in *Proc. International Conference on Artificial Intelligence and Statistics (***AISTATS***)* 2022.

Asymptotic Behavior of MLE

Maximum likelihood estimates

- n i.i.d. target samples, m i.i.d. source samples
- Fit training data with distribution family $f(z|\boldsymbol{w})$, $\boldsymbol{w} = (\boldsymbol{w}_\phi, \boldsymbol{w}_c) \in \mathbb{R}^d$, $\boldsymbol{w}_c \in \mathbb{R}^{d_c}$
- $P_{Z^t} = f(\cdot|\boldsymbol{w}^*)$ for $\boldsymbol{w}^* \in \mathcal{W}$
- log-loss $\ell(\boldsymbol{w}, z) = -\log f(z|\boldsymbol{w})$

	Standard target ERM	α-weighted ERM	Two-stage ERM
$\overline{\mathrm{gen}}$	$\mathcal{O}(\frac{d}{n})$	$\mathcal{O}(\frac{d}{m+n})$	$\mathcal{O}(\frac{d_c}{n})$

Table of Contents (Part II)

Conclusion

- Connect **operational quantity** in learning theory (generalization error, marginal likelihood) with different **information measures** for Gibbs algorithm
- Demonstrate the **versatility** of our approach in multiple applications
  - Optimal Inverse temperature
  - Gibbs-based BIC for over-parameterized model selection
  - Gibbs based-**transfer** learning
- Our Gibbs-based analysis provides an information-theoretic **framework** for understanding generalization behavior in modern machine learning, still a lot to be explored!

Q & A

Thank you for your attention!

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