Generalization Error of Generalized Linear Models in High Dimensions

    

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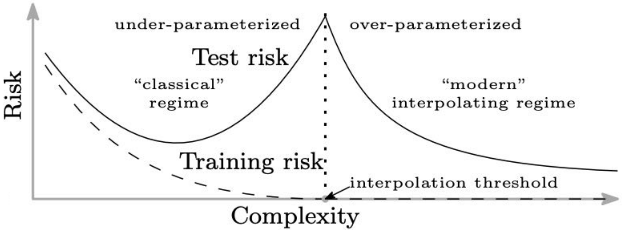
ICML 2020

Overview

- Generalization Error: Performance on new data
- Fundamental question in modern systems:
  - Low generalization error despite over-parameterization

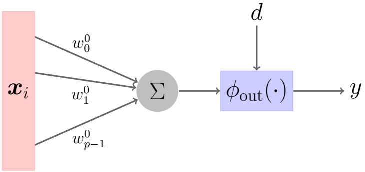


[BHMM19]

- **This work**: Exact calculation of generalization error for GLMs
  - High dimensional regime
  - *Double descent* phenomenon

Overview

- Generalized linear models (GLMs): $y = \phi_{\text{out}}(\langle \boldsymbol{x}, \boldsymbol{w}^0 \rangle, d)$



- Regularized ERM:

$$\widehat{\boldsymbol{w}} = \underset{\boldsymbol{w}}{\text{argmin}} \quad F_{\text{out}}(\boldsymbol{y}, \mathbf{X}\boldsymbol{w}) + F_{\text{in}}(\boldsymbol{w})$$

- Generalization error:

$$\mathbb{E}\, f_{\text{ts}}(y_{\text{ts}}, \widehat{y}_{\text{ts}}) \tag{1}$$

  - Test sample: $(\boldsymbol{x}_{\text{ts}}, y_{\text{ts}})$
  - $y_{\text{ts}} = \phi_{\text{out}}(\left\langle \boldsymbol{x}_{\text{ts}}, \boldsymbol{w}^0 \right\rangle, d_{\text{ts}}), \quad \widehat{y}_{\text{ts}} = \phi(\langle \boldsymbol{x}_{\text{ts}}, \widehat{\boldsymbol{w}} \rangle)$

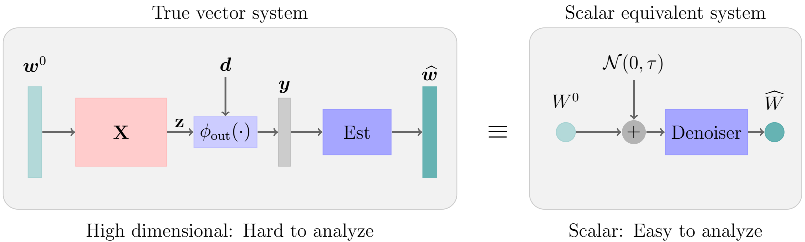
Overview

- Prior work
  - Understanding generalization in deep neural nets [BMM18, BHX19, BLLT19, NLB+18, ZBH+16, AS17]
  - Linear models [MRSY19, DKT19, MM19, HMRT19, GAK20]
  - GLMs with uncorrelated features [BKM+19]
- **Our contribution**:
  - A procedure for characterizing generalization error (1)
  - General test metrics, training losses, regularizers, link function
  - Correlated covariates
  - Train-test distributional mismatch
  - Over-parameterized and under-parameterized regime

Outline

- Main Result
  - Scalar Equivalent System
  - Main Theorem
- Examples
  - Linear Regression
  - Logistic Regression
  - Non-linear Regression
- Proof Technique
  - Multi-layer VAMP
- Future Directions

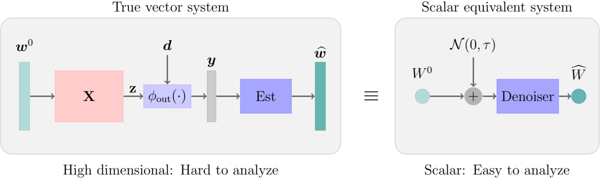
Scalar Equivalent System



$$\hat{\boldsymbol{w}} = \underset{\boldsymbol{w}}{\text{argmin}} \quad F_{\text{out}}(\boldsymbol{y}, \mathbf{X}\boldsymbol{w}) + F_{\text{in}}(\boldsymbol{w}) \tag{2}$$

- **Key tool**: Approximate Message Passing (AMP) framework [DMM09, BM11, RSF19, FRS18, PSAR+20]
  - As a constructive proof technique
  - Performance of the estimates:
    $\rightarrow$ deterministic recursive equations: *state evolution* (SE)

Main Result



Theorem (Generalization error of GLMs)

(a) Under some regularity conditions on $f_{\text{ts}}, \phi, \phi_{\text{out}}$, the above convergence is rigorous:

$$\lim_{N\to\infty} \frac{1}{N}\sum_{i=1}^{N} f(w_i^0, \widehat{w}_i) = \mathbb{E} f(W^0, \widehat{W}) \quad a.s.$$

$$\widehat{W} = \text{prox}_{f_{\text{in}}/\gamma}(W^0 + Q), \quad Q = \mathcal{N}(0,\tau) \quad (\textit{independent of } W^0)$$

(b) Generalization error:

$$\mathcal{E}_{\text{ts}} = \mathbb{E}\, f_{\text{ts}}\left(\phi_{\text{out}}(Z_{\text{ts}}, D), \phi(\widehat{Z}_{\text{ts}})\right), \quad (Z_{\text{ts}}, \widehat{Z}_{\text{ts}}) \sim \mathcal{N}(\mathbf{0}_2, \mathbf{M})$$

τ, γ, *and* $\mathbf{M}$ *are computed by SE equations, and* $D \perp\!\!\!\perp (Z_{\text{ts}}, \widehat{Z}_{\text{ts}})$

Example Setting

- Train-test distributional mismatch
  - $\boldsymbol{x}_{\text{train}} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}_{\text{tr}})$, $\boldsymbol{x}_{\text{test}} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}_{\text{ts}})$, $\boldsymbol{\Sigma}_{\text{tr}}$ and $\boldsymbol{\Sigma}_{\text{ts}}$ commute
  - i.i.d. log-normal eigenvalues

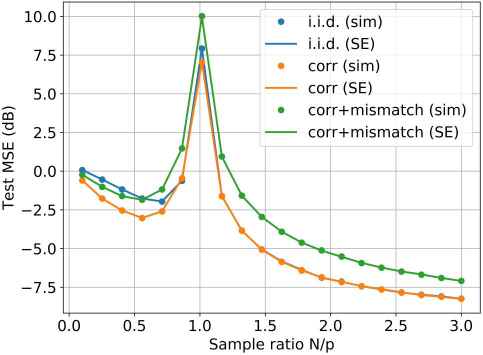
$$\begin{bmatrix} \log(S_{\text{tr}}^2) \\ \log(S_{\text{ts}}^2) \end{bmatrix} \overset{\text{i.i.d.}}{\sim} \mathcal{N}\left(\mathbf{0}, \sigma \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix}\right) \quad \forall\ i$$

- 3 different cases :

(i) Uncorrelated features ($\sigma = 0$) $\quad \boldsymbol{\Sigma}_{\text{tr}} = \boldsymbol{\Sigma}_{\text{ts}} = \boldsymbol{I}$
(ii) Correlated features ($\sigma > 0,\ \rho = 1$) $\quad \boldsymbol{\Sigma}_{\text{tr}} = \boldsymbol{\Sigma}_{\text{ts}} \neq \boldsymbol{I}$
(iii) Mismatched features ($\sigma > 0,\ \rho < 1$) $\quad \boldsymbol{\Sigma}_{\text{tr}} \neq \boldsymbol{\Sigma}_{\text{ts}}$

Example: Linear Regression

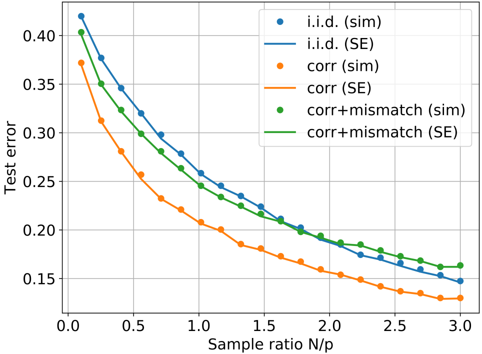
- Under-regularized linear regression:
  - $\phi_{\text{out}}(p, d) = p + d$, and $d \sim \mathcal{N}(0, \sigma_d^2)$
  - MSE output loss
  - *double descent* phenomenon



(Recovered result of [HMRT19])

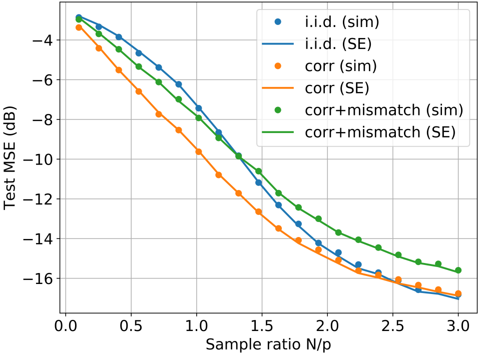
Example: Logistic Regression

- Logistic regression
  - Logistic output $P(y=1) = 1/(1+e^{-p})$
  - Binary cross-entropy loss with ℓ_2 regularization

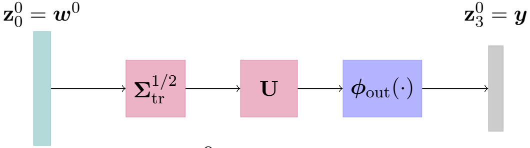


Example: Non-linear Regression

- Non-linear Regression
  - $\phi_{\text{out}}(p, d) = \tanh(p) + d, \quad d \sim \mathcal{N}(0, \sigma_d^2)$
  - $f_{\text{out}}(y, p) = \frac{1}{2\sigma_d^2}(y - \tanh(p))^2$



Proof Technique: Multi-Layer Representation



- Represent the mapping $\boldsymbol{w}^0 \mapsto \boldsymbol{y}$ as a multi-layer network

$$\boldsymbol{y} = \phi_{\mathrm{out}}(\mathbf{X}\boldsymbol{w}, \mathbf{d})$$

- Decompose Gaussian training data $\mathbf{X}$ with covariance $\boldsymbol{\Sigma}_{\mathrm{tr}}$

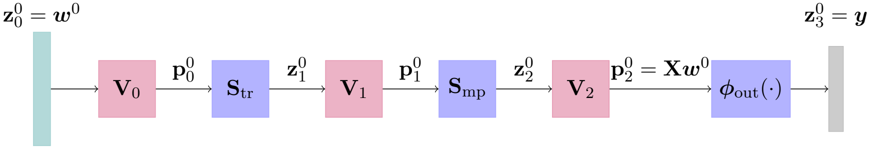
$$\mathbf{X} = \mathbf{U}\boldsymbol{\Sigma}_{\mathrm{tr}}^{\frac{1}{2}}, \quad \mathbf{U} \text{ i.i.d. Gaussian}$$

- Use SVD of $\mathbf{U}$ and eigendecomposition of $\boldsymbol{\Sigma}_{\mathrm{tr}}^{\frac{1}{2}}$:

$$\boldsymbol{\Sigma}_{\mathrm{tr}} = \frac{1}{p}\mathbf{V}_0^{\mathsf{T}}\mathrm{diag}(\mathbf{s}_{\mathrm{tr}}^2)\mathbf{V}_0, \quad \mathbf{U} = \mathbf{V}_2\mathbf{S}_{\mathrm{mp}}\mathbf{V}_1$$

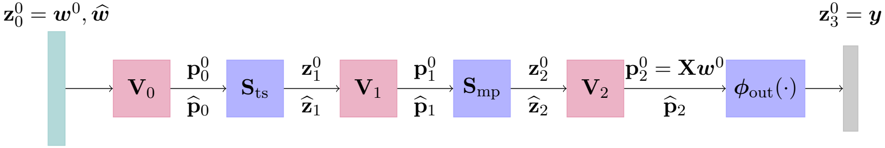
- $\mathbf{V}_0$, $\mathbf{V}_1$, $\mathbf{V}_2$: Haar-distributed
- $\mathbf{S}_{\mathrm{mp}}$: Singular values of $\mathbf{U}$
  - converges in distribution to Marchenko-Pastur law

Proof Technique: Multi-Layer VAMP



- Algorithm to solve inference problem in deep neural networks
- Similar to ADMM algorithm for optimization
- Statistical guarantees:
  - Joint distribution of $(W^0, \widehat{W})$ and other hidden signals

Proof Technique: Generalization Error



- ML-VAMP $\Rightarrow$ Joint distribution of $(W^0, \widehat{W})$ (part (a) of Thm)
- Given test data:

$$\boldsymbol{x}_{\text{ts}}^{\mathsf{T}} = \mathbf{u}^{\mathsf{T}}\text{diag}(\mathbf{s}_{\text{ts}})\mathbf{V}_0$$

- Find joint distribution of $(P_2^0, \widehat{P}_2)$ for test data (part (b) of Thm)

$$(P_2^0, \widehat{P}_2) \sim \mathcal{N}(\mathbf{0}_2, \mathbf{M})$$

- Obtain generalization error

$$\mathcal{E}_{\text{ts}} = \mathbb{E}\, f_{\text{ts}}\Big(\phi_{\text{out}}(P_2^0, D), \phi(\widehat{P}_2)\Big)$$

Future Directions

- Generalize results to:
  - Non-Gaussian covariates
  - Multitask GLMs using multi-layer matrix-valued VAMP
  - Deeper models like two-layer neural networks
  - Non-asymptotic regimes
- Use results to get:
  - Generalization errors in reproducing kernel Hilbert spaces, such as NTK space

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