

Information theoretic perspectives on learning algorithms

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R Narasimhan Memorial Lecture
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Work with Adrian Tovar-Lopez (Math), Ankit Pensia (CS), Po-Ling Loh (Stats)



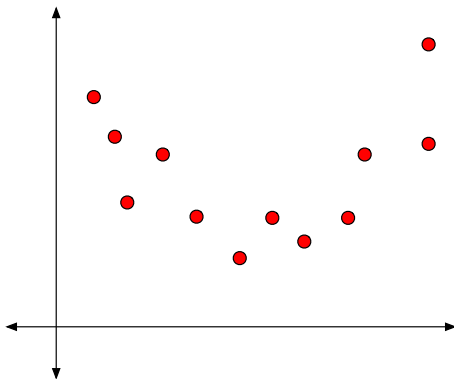
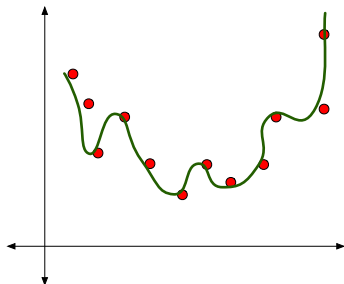
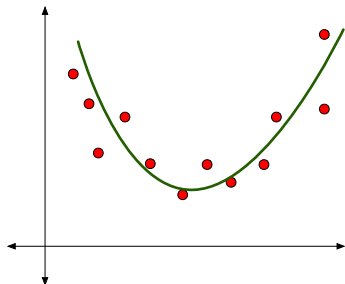


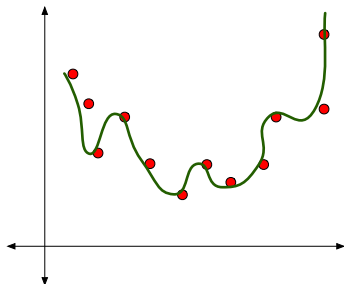
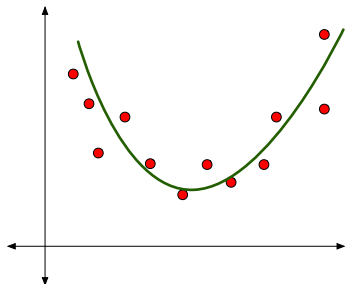
Figure: Given N points in \mathbb{R}^2 , fit a curve

- **Forward problem:** From dataset to curve

Finding the right "fit"

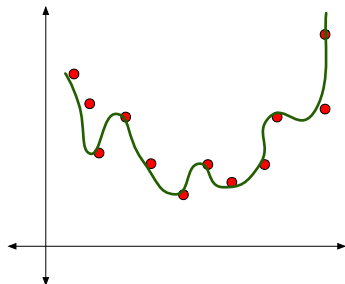
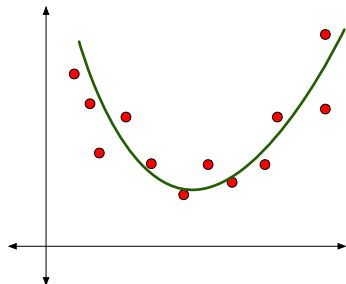


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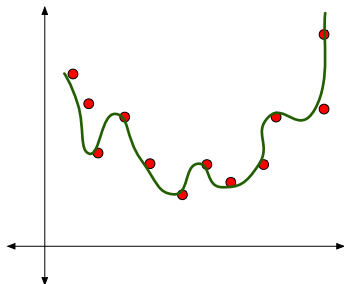
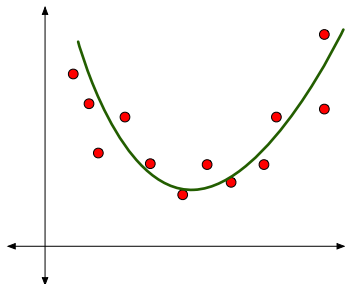
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- **Not stable**

Guessing points from curve

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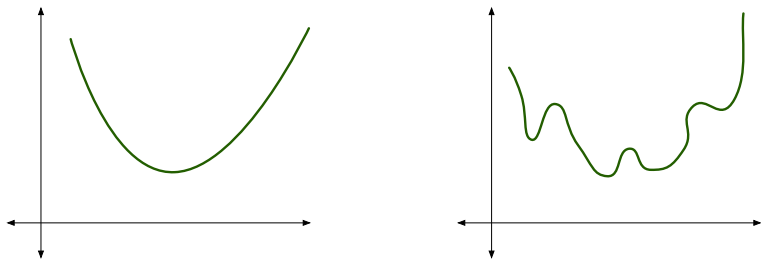


Figure: Given curve, find N points

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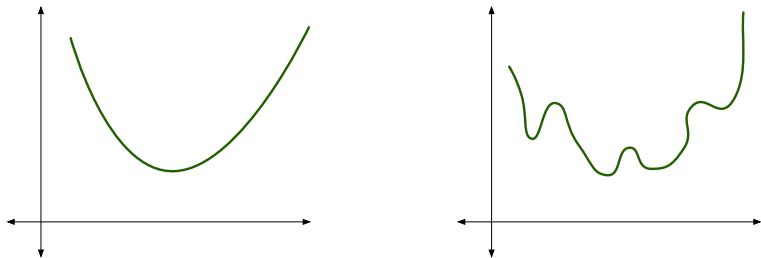


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- Backward problem easier for overfitted curve!

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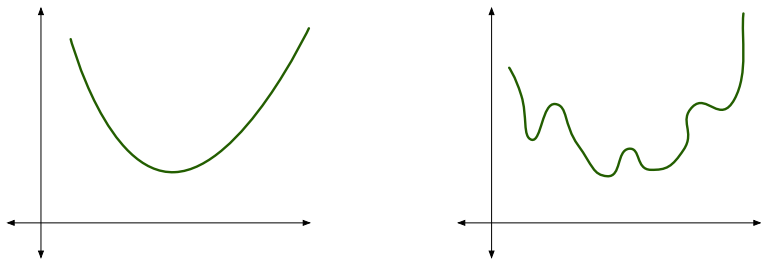


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- **Backward problem:** From curve to dataset
- Backward problem easier for overfitted curve!
- Curve contains **more information** about dataset

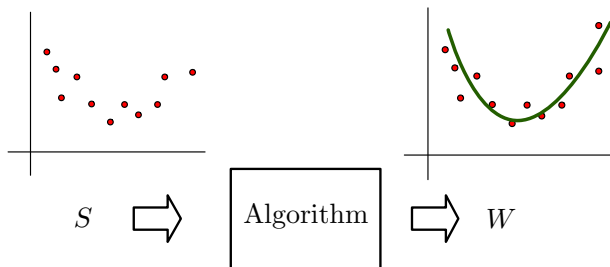
This talk

- Explore [information and overfitting](#) connection (Xu & Raginsky, 2017)

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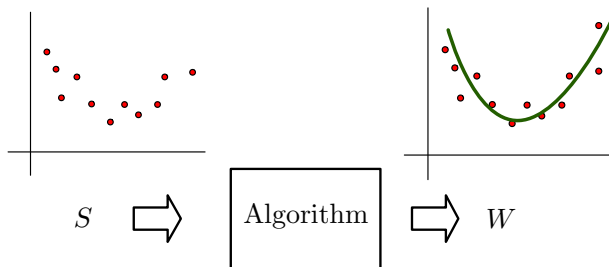
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- Speculations and open problems

Learning algorithm as a channel



- **Input:** Dataset S with N i.i.d. samples $(X_1, X_2, \dots, X_n) \sim \mu^{\otimes n}$
- **Output:** W

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- **Output:** W
- **Algorithm equivalent to designing $\mathbb{P}_{W|S}$. Very different from channel coding!**

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- Can't always get what we want...
- Minimize empirical loss instead

$$\ell_N(w, S) = \frac{1}{N} \sum_{i=1}^N \ell(w, X_i)$$

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- Generalization error = test error - train error

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- Ideally, we want both small. Often, both are analyzed separately.

Basics of mutual information

- Mutual information $I(X; Y)$ precisely quantifies information between $(X, Y) \sim \mathbb{P}_{XY}$:

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- Chain rule:

$$I(X_1, X_2; Y) = I(X_1; Y) + I(X_2; Y|X_1)$$

Theorem (Xu & Raginsky (2017))

Assume that $\ell(w, X)$ is R -subgaussian for every $w \in \mathcal{W}$. Then the following bound holds:

$$|\text{gen}(\mu, \mathbb{P}_{W|S})| \leq \sqrt{\frac{2R^2}{n} I(S; W)}.$$

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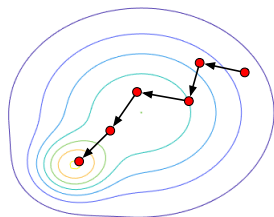


Figure: Update W_t using some update rule to generate W_{t+1}

- Many learning algorithms are **iterative**
- Generate $W_0, W_1, W_2, \dots, W_T$, and output $W = f(W_0, \dots, W_T)$.
For example, $W = W_T$ or $W = \frac{1}{T} \sum_i W_i$

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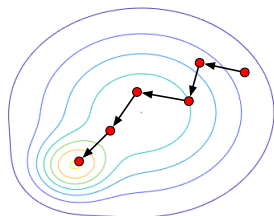


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- **Bound $I(W; S)$ by controlling information at each iteration**

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- Run for T steps, output $W = f(W_0, \dots, W_T)$

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- **Assumption 3:** Sampling is done without looking at W_t 's; i.e.,

$$\mathbb{P}(Z_{t+1} \mid Z^{(t)}, W^{(t)}, S) = \mathbb{P}(Z_{t+1} \mid Z^{(t)}, S)$$

Main result

Theorem (Pensia, J., Loh (2018))

The mutual information satisfies the bound

$$I(S; W) \leq \sum_{t=1}^T \frac{d}{2} \log \left(1 + \frac{\eta_t^2 L^2}{d\sigma_t^2} \right).$$

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- Depends on T — longer you optimize, higher the risk of overfitting

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Corollary (Bound on expectation)

The generalization error of our class of iterative algorithms is bounded by

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Corollary (High-probability bound)

Let $\epsilon = \sum_{t=1}^T \frac{d}{2} \log \left(1 + \frac{\eta_t^2 L^2}{d\sigma_t^2} \right)$. For any $\alpha > 0$ and $0 < \beta \leq 1$, if $n > \frac{8R^2}{\alpha^2} \left(\frac{\epsilon}{\beta} + \log\left(\frac{2}{\beta}\right) \right)$, we have

$$\mathbb{P}_{S,W} (|L_\mu(W) - L_S(W)| > \alpha) \leq \beta, \quad (1)$$

where the probability is with respect to $S \sim \mu^{\otimes n}$ and W .

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- Common experimental practices for SGLD [Welling & Teh, 2011]:
 - 1 the noise variance $\sigma_t^2 = \eta_t$,
 - 2 the algorithm is run for K epochs; i.e., $T = nK$,
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- **Expectation bounds:** Using $\sum_{t=1}^T \frac{1}{t} \leq \log(T) + 1$

$$|\text{gen}(\mu, \mathbb{P}_{W|S})| \leq \frac{RL}{\sqrt{n}} \sqrt{\sum_{t=1}^T \eta_t} \leq \frac{RL}{\sqrt{n}} \sqrt{c \log T + c}$$

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- Best known bounds by Mou et al. (2017) are $O(1/n)$ —but our bounds more general

- Perturbed SGD (Ge et al. 2015): Similar to SGLD, but different noise distribution:

$$W_t = W_{t-1} - \eta (\nabla_w \ell(W_{t-1}, Z_t) + \xi_t),$$

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- A modified version of stochastic gradient Hamiltonian Monte-Carlo, Chen et al. (2014):

$$\begin{aligned} V_t &= \gamma_t V_{t-1} + \eta_t \nabla_w \ell(W_{t-1}, Z_t) + \xi'_t, \\ W_t &= W_{t-1} - \gamma_t V_{t-1} - \eta_t \nabla_w \ell(W_{t-1}, Z_t) + \xi''_t, \end{aligned}$$

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- Same bound also holds for “noisy” Nesterov’s accelerated gradient descent method (1983)

Proof sketch

Lots of Markov chains!

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- $I(W; S) \leq I(W_0^T; Z_1^T)$ because

$$S \rightarrow Z_1^T \rightarrow W_0^T \rightarrow W$$

Figure: Data processing inequality

- Iterative structure means

$$W_0 \rightarrow Z_1 W_1 \rightarrow Z_2 W_2 \rightarrow Z_3 W_3 \cdots \rightarrow W_T$$

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- [Bottomline](#): Bound “one step” information between W_t and Z_t

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$$I(W_t; Z_t | W_{t-1}) = \underbrace{h(W_t | W_{t-1})}_{\text{Variance}(W_t | W_{t-1}) \leq \eta_t^2 L^2 + \sigma_t^2} - \underbrace{h(W_t | W_{t-1}, Z_t)}_{=h(\xi_t)}$$

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- Gaussian distribution maximizes entropy for fixed variance, giving

$$I(W_t; Z_t | W_{t-1}) \leq \frac{d}{2} \log \left(1 + \frac{\eta_t^2 L^2}{d\sigma_t^2} \right)$$

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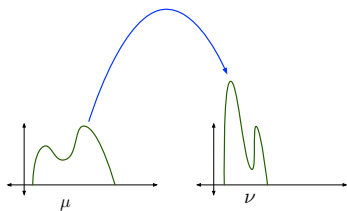
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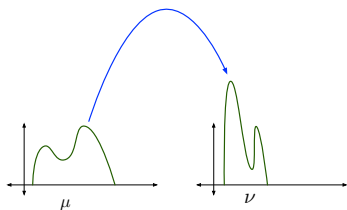
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- ...many cases when mutual information $I(W; S)$ shoots to infinity
- Cannot use bounds for stochastic gradient descent (SGD) :(
- “Noisy” algorithms are *essential* for using mutual information based bounds

Wasserstein metric





- Wasserstein distance given by

$$W_p(\mu, \nu) = \left(\inf_{\mathbb{P}_{XY} \in \Pi(\mu, \nu)} \mathbb{E} \|X - Y\|^p \right)^{1/p}$$

where $\Pi(\mu, \nu)$ is the set of coupling such that marginals are μ and ν

- Lots of fascinating theory¹ for W_p

¹Topics in Optimal Transportation by Cedric Villani

Main result: Wasserstein bounds on $\text{gen}(\mu, \mathbb{P}_{W|S})$

- **Assumption:** $\ell(w, x)$ is Lipschitz in x for each fixed w ; i.e.

$$|\ell(w, x_1) - \ell(w, x_2)| \leq L \|x_1 - x_2\|_p$$

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If $\ell(w, \cdot)$ is L -Lipschitz in $\|\cdot\|_p$, generalization error satisfies the following bound:

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- Measure **average separation** of $\mathbb{P}_{S|W}$ from \mathbb{P}_S (looks like a p -th moment in the space of distributions)

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- In particular, for Gaussian data, Wasserstein bound strictly stronger

- Recall generalization error expression:

$$\text{gen}(\mu, \mathbb{P}_{W|S}) = |\mathbb{E}l_N(\bar{S}, \bar{W}) - \mathbb{E}l_N(S, W)|,$$

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- **Key insight:** Any **coupling** of (\bar{S}, \bar{W}, S, W) that has the “correct” **marginals** on (S, W) and (\bar{S}, \bar{W}) leads to the same expected value above
- Just pick a nice coupling!

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Speculations and open problems

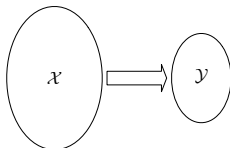
- **Stability:** How much does W change with S changes a little?
- Property of the **forward channel** $\mathbb{P}_{W|S}$
- **Generalization upper bound:** How much does S change when W changes a little?
- Property of the **backward channel** $\mathbb{P}_{S|W}$
- Pre-process data to deliberately make backward channel noisy (data augmentation, smoothing, etc.)

Relation to rate distortion theory?

Speculations and open problems

Relation to rate distortion theory?

- Branch of information theory dealing with **lossy data compression**

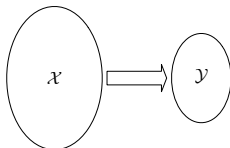


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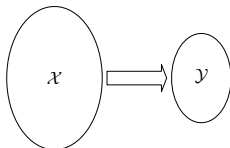
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- **Minimize distortion given by $\ell_N(W, S)$** subject to mutual information constraint $I(W; S) \leq \epsilon$
- Essentially same problem, but more connections need to be developed

References

- *Generalization error for noisy, iterative algorithms*. Ankit Pensia, Varun Jog, Po-Ling Loh. ISIT 2018.
- *Wasserstein distance based bounds on generalization error*. Adrian Tovar Lopez, Varun Jog. ITW 2018.

Thank you!