Information theoretic perspectives on learning algorithms

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Shannon Channel Hangout!

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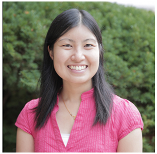
Jointly with Adrian Tovar-Lopez (Math), Ankit Pensia (CS), Po-Ling Loh (Stats)





Curve fitting

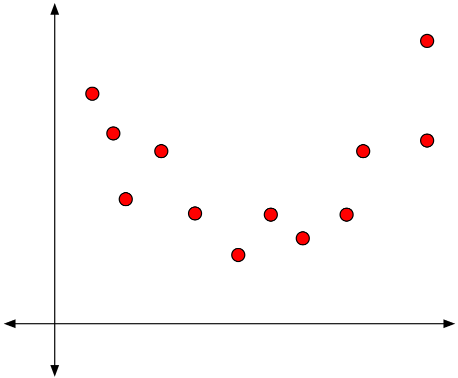


Figure: Given N points in $\mathbb{R}^2$, fit a curve

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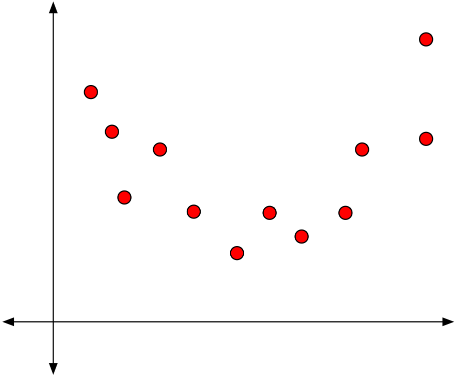

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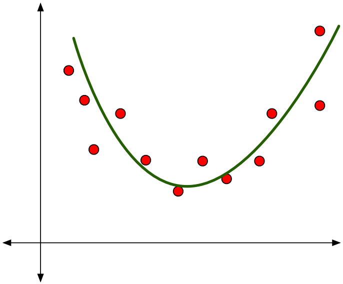
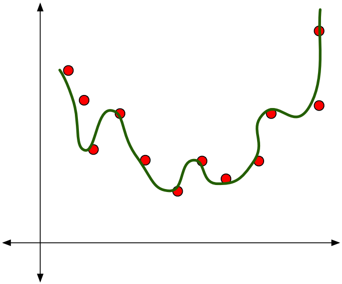
- Forward problem: From dataset to curve

Finding the right "fit"





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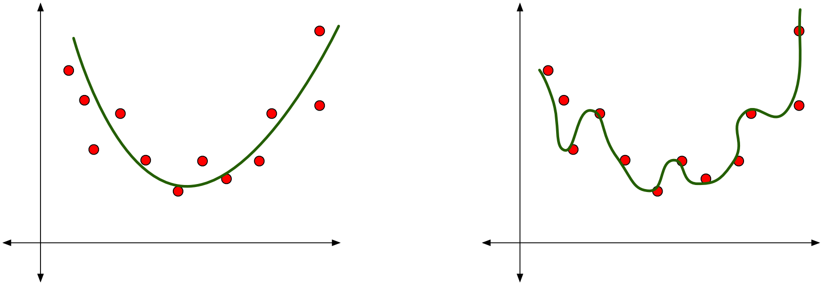

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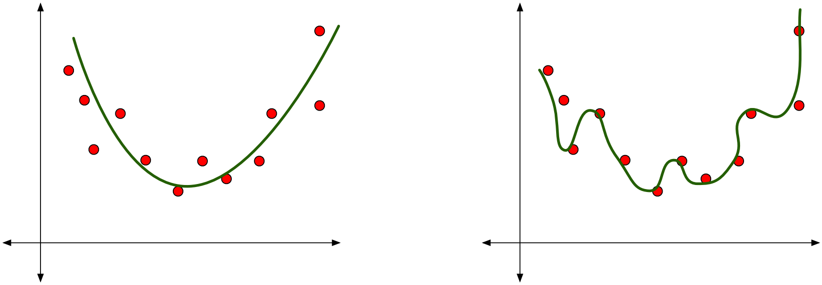

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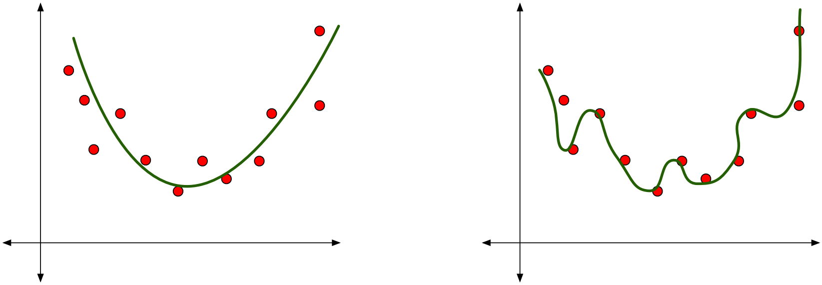

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Guessing points from curve

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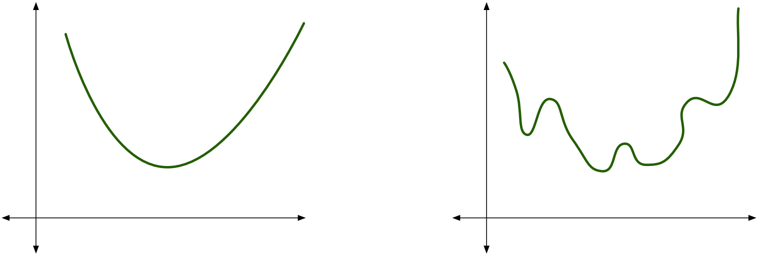

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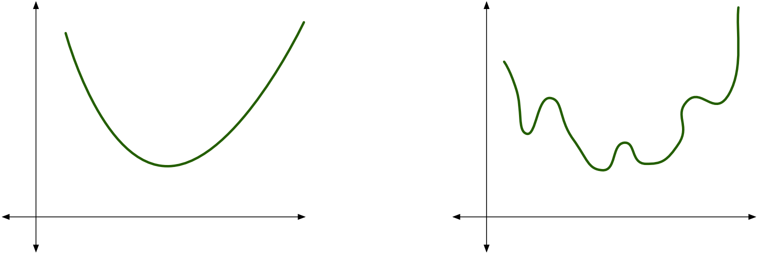

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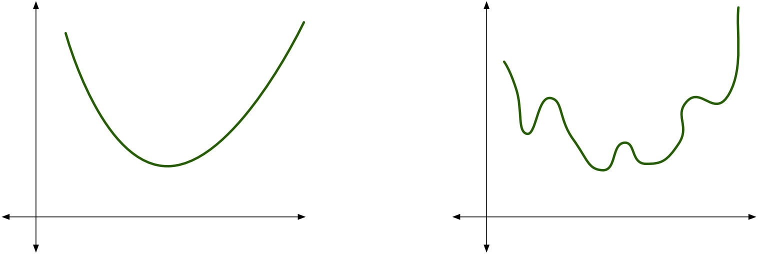

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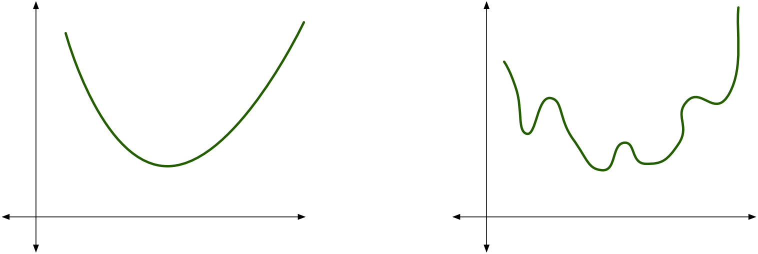

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- Curve contains more information about dataset

This talk

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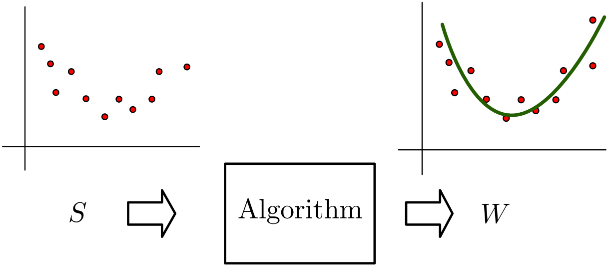
- Speculations, open problems, etc.

Learning algorithm as a channel



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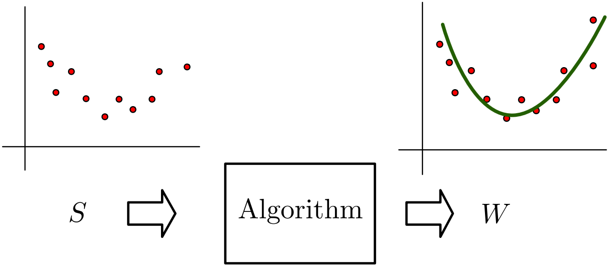

- Input: Dataset S with N i.i.d. samples $(X_1, X_2, \ldots, X_n) \sim \mu^{\otimes n}$
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- Algorithm equivalent to designing $\mathbb{P}_{W|S}$. Very different from channel coding!

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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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- 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:

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

Bounding generalization error using $I(W; S)$

Theorem (Xu & Raginsky (2017))

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

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- Notion of stability different from traditional notions

Proof sketch

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Lemma (Key Lemma in Raginsky & Xu (2017))

If $f(X, Y)$ is σ-subgaussian under $\mathbb{P}_X \times \mathbb{P}_Y$, then

$$|\mathbb{E}f(X, Y) - \mathbb{E}f(\bar{X}, \bar{Y})| \leq \sqrt{2\sigma^2 I(X; Y)},$$

where $(X, Y) \sim \mathbb{P}_{XY}$ and $(\bar{X}, \bar{Y}) \sim \mathbb{P}_X \times \mathbb{P}_Y$.

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- Recall $I(X; Y) = KL(\mathbb{P}_{XY} || \mathbb{P}_X \times \mathbb{P}_Y)$
- Follows directly by alternate characterization of $KL(\mu||\nu)$ as

$$KL(\mu||\nu) = \sup_F \left(\int F d\mu - \log \int e^F d\nu \right)$$

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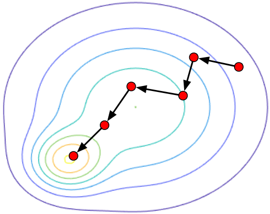

Figure: Update W_t using some update rule to generate W_{t+1}

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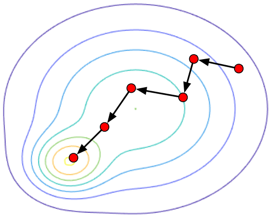

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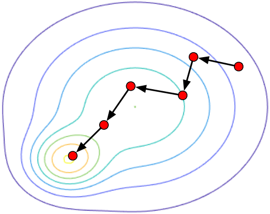

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- Bound $I(W; S)$ by controlling information at each iteration

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

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

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

Graphical model

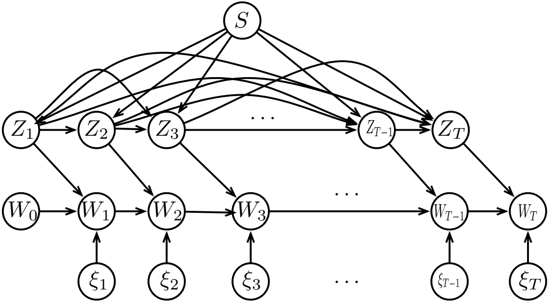

Figure: Graphical model illustrating Markov properties among random variables in the algorithm

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

Implications for gen($\mu, \mathbb{P}_{W|S}$)

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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* $n > \frac{8R^2}{\alpha^2}\left(\frac{\epsilon}{\beta} + \log(\frac{2}{\beta})\right)$, *we have*

$$\mathbb{P}_{S,W}\left(|L_\mu(W) - L_S(W)| > \alpha\right) \leq \beta, \tag{2}$$

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

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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

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- Similar to SGLD, but different noise distribution:

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- Bounds in expectation and high probability follow directly from this bound

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- Same bound also holds for "noisy" Nesterov's accelerated gradient descent method (1983)

Proof sketch

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

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- Bottom line: Bound "one step" information between W_t and Z_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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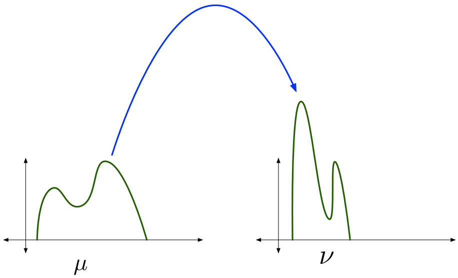
- "Noisy" algorithms are *essential* for using mutual information based bounds

Wasserstein metric



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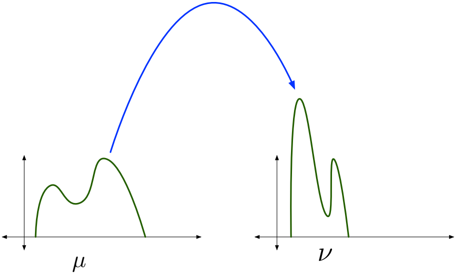

- Wasserstein distance given by

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

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

W_p for $p = 1$ and 2

- W_1 also called "Earth Mover distance" or Kantorovich-Rubinstein distance

$$W_1(\mu, \nu) = \sup \left\{ \int f(d\mu - d\nu) \middle| f \text{ continuous and } 1-\text{Lipschitz} \right\}$$

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- Optimal coupling in $\Pi(\mu, \nu)$ is a function T such that $T_{\#\mu} = \nu$
- For μ and ν in $\mathbb{R}$,

$$W_2^2(\mu, \nu) = \int |F^{-1}(x) - G^{-1}(x)|^2 dx$$

where F and G are cdf's of μ and ν

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Wasserstein bounds on 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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Theorem (Tovar-Lopez & J., (2018))

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)

Wasserstein and KL

Definition

We say μ satisfies a $T_p(c)$ transportation inequality with constant $c > 0$ if for all ν, we have

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- Transport inequalities used to show concentration phenomena
- For $p \in [1, 2]$ this inequality tensorizes! This means $\mu^{\otimes n}$ satisfies inequality $T_p(cn^{2/p-1})$

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

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Theorem (Tovar-Lopez & J., (2018))

Suppose $p = 1$, then

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and so

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Coupling based bound on gen($\mu, \mathbb{P}_{W|S}$)

- Recall generalization error expression:

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

where $(\bar{S}, \bar{W}) \sim \mathbb{P}_S \times \mathbb{P}_W$ and $(S, W) \sim \mathbb{P}_{WS}$.

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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

Proof sketch

- We have

$$\begin{aligned}\text{gen}(\mu, \mathbb{P}_{W|S}) &= \left| \int \ell_N(s, w) d\mathbb{P}_{SW} - \int \ell_N(\bar{s}, \bar{w}) d\mathbb{P}_{\bar{S}\times\bar{W}} \right| \\ &= \left| \mathbb{E}_{SW\bar{S}\bar{W}} \ell_N(S, W) - \ell_N(\bar{S}, \bar{W}) \right|\end{aligned}$$

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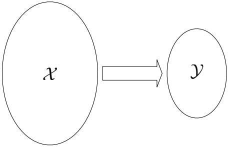
- Pre-process data to deliberately make backward channel noisy (data augmentation, smoothing, etc.)

Speculations: Relation to rate distortion theory

- Branch of information theory dealing with lossy data compression



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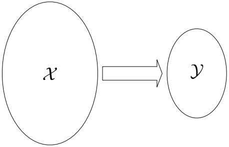

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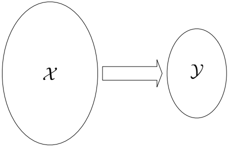

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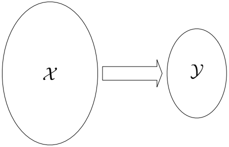

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- Essentially same problem, but connections still unclear

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- Chain rule? Data processing?

Thank you!