Introduction to Deep Generative Modeling

Lecture #3

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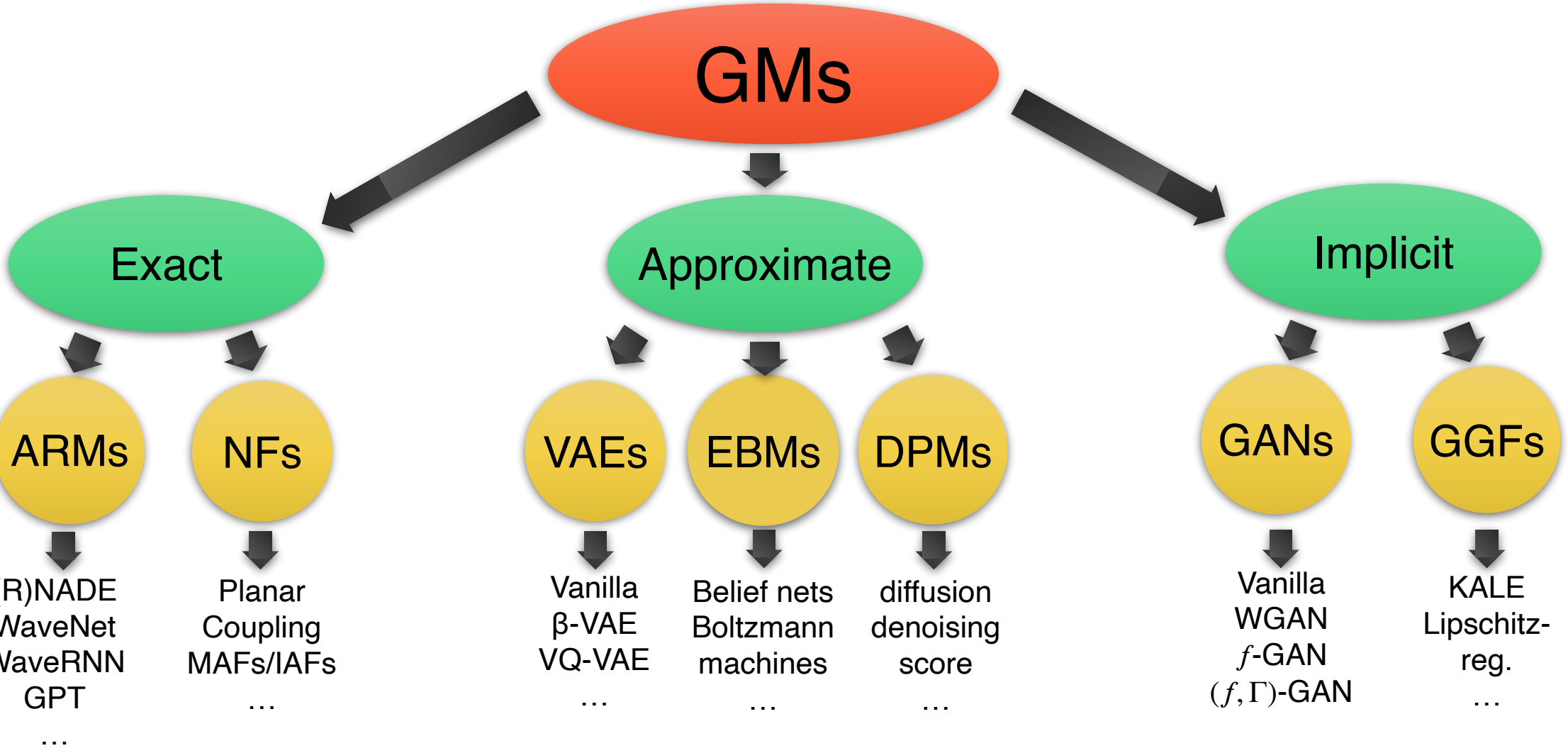
Taxonomy of Deep Generative Models According to the Likelihood Function



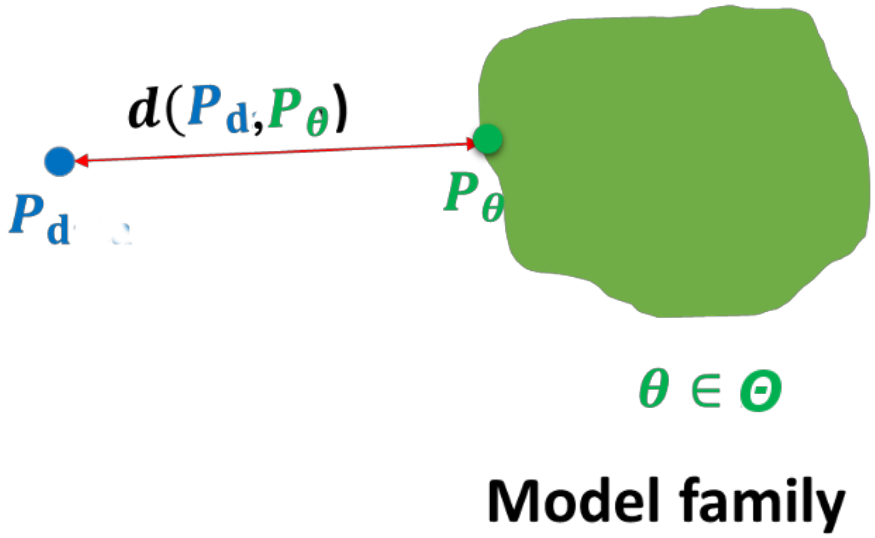
Introduction to Estimator Theory

- What is an estimator?

Let $\mathcal{D} = \{x_1, \ldots, x_n\}$ be a set of data drawn from $p_d(x)$, and $p_\theta(x)$ be a family of models with $\theta \in \Theta$. A point estimator $\hat{\theta} = \hat{\theta}(\mathcal{D})$ is a random variable for which we want:

$$p_{\hat{\theta}}(x) \approx p_d(x)$$

$x_i \sim P_d$
$i = 1, 2, \ldots, n$



Introduction to Estimator Theory

- How to construct an estimator?
  - Maximum Likelihood Estimation (MLE)
  - Maximum A Posteriory (MAP) Estimation
  - Based on a Probability Distance or a Divergence (implicit)
  - Bayesian Inference (learns a distribution for the estimator's parameters)

Maximum Likelihood Estimator

- Maximum Likelihood Estimator:

$$\hat{\theta}_{\mathrm{MLE}}(\mathcal{D}) = \arg\max_{\theta} p_\theta(\mathcal{D}) := p_\theta(x_1, \ldots, x_n).$$

- Equivalently, under the i.i.d. assumption:

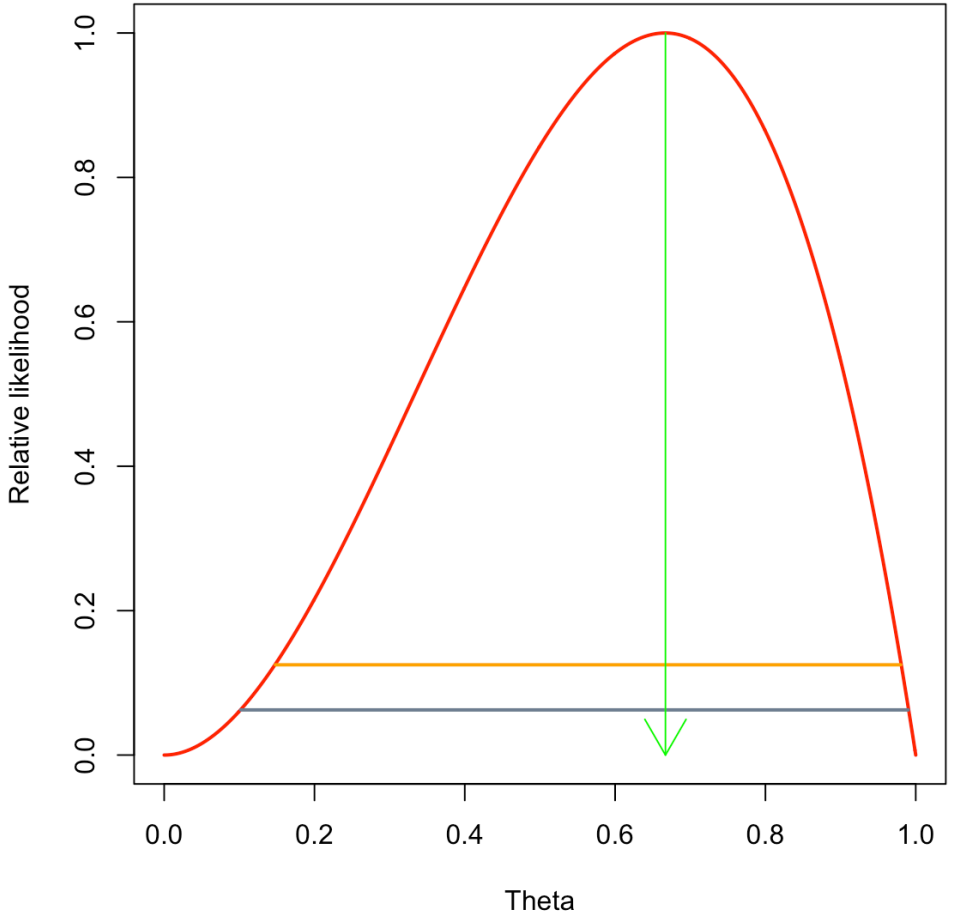
$$\hat{\theta}_{\mathrm{MLE}}(\mathcal{D}) = \arg\max_{\theta} \sum_{i=1}^{n} \log p_\theta(x_i) =: L(\theta; \mathcal{D}) \ \big(\equiv L_n(\theta) \big).$$

Maximum Likelihood Estimator

- MLE interpretation:

  – $L_n(\hat{\theta}_1) > L_n(\hat{\theta}_2)$ implies that $\hat{\theta}_1$ is *more likely* to have generated the observed samples $x_1, ..., x_n$.

  – Thus, it provides a ranking of model's fitness/accuracy/matching to the data.



MLE Example #1

- 1d Gaussian, unknown mean $\theta = \mu$, known variance σ^2:

Dataset: $\mathcal{D} = \{x_1, \ldots, x_n\}$,

Model family: $p_\theta(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\theta)^2}{2\sigma^2}}$.

$$L(\theta, \mathcal{D}) = \sum_{i=1}^{n} \log\left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i-\theta)^2}{2\sigma^2}}\right) = -\frac{n}{2}\log(2\pi\sigma^2) - \sum_{i=1}^{n} \frac{1}{2\sigma^2}(x_i - \theta)^2.$$

$$\frac{d}{d\theta} L(\theta; \mathcal{D}) = -\frac{1}{\sigma^2} \sum_{i=1}^{n} (x_i - \theta) \qquad \text{Thus, } \frac{d}{d\theta} L(\hat{\theta}; \mathcal{D}) = 0 \Longrightarrow \boxed{\hat{\theta} = \frac{1}{n} \sum_{i=1}^{n} x_i.}$$

MLE Example #2

- Exponential distribution:

$$p_\theta(x) = \begin{cases} \theta e^{-\theta x}, & x \geq 0 \\ 0, & x < 0. \end{cases}$$

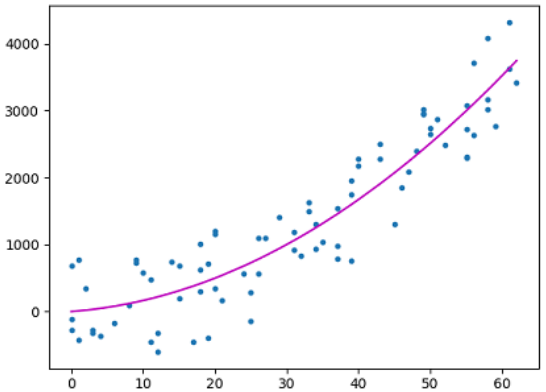
$$L(\theta, \mathcal{D}) = \sum_{i=1}^{n} (\log \theta - \theta x_i)$$

$$\frac{d}{d\theta} L(\theta; \mathcal{D}) = \sum_{i=1}^{n} \left(\frac{1}{\theta} - x_i\right)$$

$$\text{Thus, } \frac{d}{d\theta} L(\hat{\theta}; \mathcal{D}) = 0 \implies \boxed{\hat{\theta} = \frac{n}{\sum_{i=1}^{n} x_i}.}$$

MLE Example #3

- Linear model with Gaussian error:



Dataset: $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ with $x_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$,

Model family: $y_i = \theta^T x_i + e_i$ with $e_i \sim \mathcal{N}(0, \sigma^2)$ and $\theta \in \mathbb{R}^d$.

$$L(\theta, \mathcal{D}) = \sum_{i=1}^{n} \log\left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i - \theta^T x_i)^2}{2\sigma^2}}\right) = -\frac{n}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - \theta^T x_i)^2.$$

Partial derivative or gradient vector: $\frac{\partial}{\partial\theta} L(\theta; \mathcal{D}) = -\frac{1}{\sigma^2}\sum_{i=1}^{n}(y_i - \theta^T x_i)x_i^T.$

Thus, $\frac{\partial}{\partial\theta} L(\hat{\theta}; \mathcal{D}) = 0 \implies \hat{\theta} = \left(\sum_{i=1}^{n} x_i x_i^T\right)^{-1}\left(\sum_{i=1}^{n} x_i y_i\right).$

MLE Example #3

- In matrix form:

$$y = X\theta + e \text{ with } y = [y_1, ..., y_n]^T \in \mathbb{R}^n,\ X = \begin{bmatrix} x_1^T \\ \vdots \\ x_n^T \end{bmatrix} \in \mathbb{R}^{n \times d},$$

$$e = [e_1, ..., e_n]^T \in \mathbb{R}^n \text{ and } e \sim \mathcal{N}(0, \sigma^2 I_n).$$

$$L(\theta, \mathcal{D}) = C - \frac{1}{2\sigma^2}(y - X\theta)^T(y - X\theta).$$

Maximizing L(θ) is equivalent to minimizing the Sum of Squares (Least Squares)

$$\frac{\partial}{\partial\theta} L(\theta; \mathcal{D}) = -\frac{1}{\sigma^2} X^T(y - X\theta)$$

Exactly the same solution as LS!

$$\text{Thus, } \frac{\partial}{\partial\theta} L(\hat{\theta}; \mathcal{D}) = 0 \implies \hat{\theta} = (X^T X)^{-1} X^T y.$$

MLE Example #4

- Logistic regression with sigmoids a.k.a. binary classification.

Dataset: $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ with $x_i \in \mathbb{R}^d$ and $y_i \in \{0, 1\}$,

Model family: $p_\theta(y_i = 1|x_i) = \sigma(\theta^T x_i)$, $p_\theta(y_i = 0|x_i) = 1 - p_\theta(y_i = 1|x_i)$, $\theta \in \mathbb{R}^d$ and $\sigma(z) = \frac{1}{1+e^{-z}}$ be the sigmoid function.

Compact form: $p_\theta(y_i|x_i) = p_\theta(y_i = 1|x_i)^{y_i} p_\theta(y_i = 0|x_i)^{1-y_i}$.

$$L(\theta, \mathcal{D}) = \sum_{i=1}^{n} y_i \log \frac{1}{1 + e^{-\theta^T x_i}} + (1 - y_i) \log \frac{e^{-\theta^T x_i}}{1 + e^{-\theta^T x_i}}$$

Unfortunately, $\frac{\partial}{\partial \theta} L(\hat{\theta}; \mathcal{D}) = 0$ is a non-linear system of equations.

MLE Example #4

- Solution: Iteratively solve for the root of the system of equations.
- Gradient ascent.

  1. Randomly initialize $\theta^0 = (\theta_1^0, \ldots, \theta_d^0)$.
  2. Compute $\nabla_\theta L(\theta; \mathcal{D})$.
  3. Update $\theta^{t+1} = \theta^t + \alpha_t \nabla_\theta L(\theta; \mathcal{D})$.
  4. Repeat 2 & 3 until convergence.

  Learning rate

- Caution: MLE results in a non-convex optimization problem $\Rightarrow$ stack to a local maximum.

Maximum Likelihood Estimator

- We could obtain a histogram (i.e., empirical or sampling distribution) for the estimator as

$$\{\hat{\theta}(\mathcal{D}') : \mathcal{D}' \sim p_d(x)\}$$

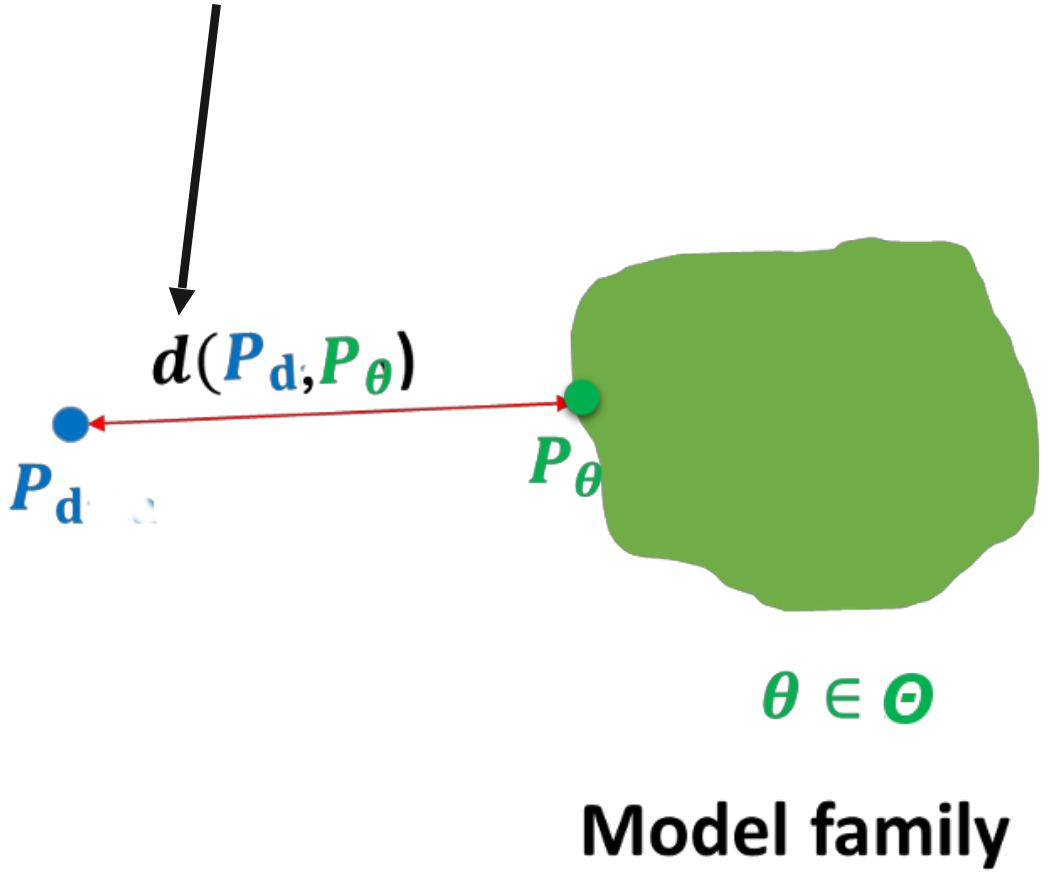
$\hookrightarrow$ The variance of the sampling distribution is a measure of uncertianty about $\hat{\theta}(\mathcal{D})$.

$\hookrightarrow$ One standard approach to approximate the sampling distribution is the bootstrap algorithm.

Kullback-Leibler Divergence (KLD)

- Geometric interpretation:
  MLE is equivalent to minimizing the KLD of $p_d(x)$ w.r.t. $p_\theta(x)$

$x_i \sim P_d$
$i = 1, 2, \ldots, n$



Maximum Likelihood Estimator

- MLE asymptotics:

$$L_n(\theta) \overset{n\to\infty}{\longrightarrow} \int \log p_\theta(x) p_d(x) dx = \mathbb{E}_{p_d}[\log p_\theta(x)] =: L(\theta; p_d) \ \big(\equiv L(\theta) \big).$$

- MLE is equivalent to minimizing the cross entropy!

$$\arg\max_\theta \ L(\theta; p_d) = \arg\min_\theta \ H^\times(p_d || p_\theta).$$

where the cross entropy of probability P with PDF $p(x)$ with respect to probability Q with PDF $q(x)$ is defined as

$$H^\times(P||Q) := \int \log \frac{1}{q(x)} p(x) dx = -\int \log q(x) p(x) dx.$$

Kullback-Leibler Divergence

- MLE is also equivalent to minimizing the KLD of $p_d(x)$ w.r.t. $p_\theta(x)$

$$\arg\max_\theta L(\theta; p_d) = \arg\min_\theta D_{KL}(p_d||p_\theta)$$

- The Kullback-Leibler divergence (KLD) of P w.r.t. Q is defined as

$$D_{\mathrm{KL}}(P||Q) := \int \log \frac{p(x)}{q(x)} p(x)dx = \underbrace{\int \log p(x)p(x)dx}_{-H(P)} \underbrace{- \int \log q(x)p(x)dx}_{H^\times(P||Q)}$$

- Thus,

$$D_{\mathrm{KL}}(P||Q) = -H(P) + H^\times(P||Q)$$

Entropy

Cross Entropy

Kullback-Leibler Divergence

- KLD satisfies the divergence property:

$$D_{\mathrm{KL}}(P||Q) \geq 0 \text{ and } D_{\mathrm{KL}}(P||Q) = 0 \iff P = Q.$$

Proof

Jensen's inequality

$$\mathbb{E}_P\left[-\log\frac{q(x)}{p(x)}\right] \geq -\log\left(\mathbb{E}_P\left[\frac{q(x)}{p(x)}\right]\right) = -\log\left(\int\frac{q(x)}{p(x)}p(x)dx\right) = 0$$

- KLD is asymmetric, i.e., $D(P||Q) \neq D(Q||P)$.
- Nevertheless, it offers a notion of a (pseudo-)distance.

Maximum A Posteriori Estimator

$$\hat{\theta}_{\mathrm{MAP}} = \arg\max_{\theta} p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}|\theta)p(\theta)}{p(\mathcal{D})}.$$

1. $p(\mathcal{D}|\theta) = p_\theta(\mathcal{D})$: likelihood.
2. $p(\theta)$: prior probability (prior knowledge).
3. $p(\mathcal{D}) = \int p(\theta')p(\mathcal{D}|\theta')d\theta'$: evidence (usually intractable but with tractable approximations).

Maximum A Posteriori Estimator

$$\hat{\theta}_{\mathrm{MAP}} = \arg\max_{\theta} \{\log p_\theta(\mathcal{D}) + \log p(\theta)\}.$$

- 1d Gaussian: $\mathcal{D} = \{x_1, \ldots, x_n\}$, $p_\theta(x) = \mathcal{N}(\theta, \sigma^2)$, $p(\theta) = \mathcal{N}(\theta_0, \sigma_0^2)$.

$$\frac{d}{d\theta} L_{\mathrm{MAP}}(\theta) = -\frac{1}{\sigma^2} \sum_{i=1}^{n} (x_i - \theta) - \frac{1}{\sigma_0^2}(\theta - \theta_0) = 0$$

$$\Longrightarrow \hat{\theta}_{\mathrm{MAP}} = \frac{\sum_{i=1}^{n} x_i - \rho\theta_0}{n - \rho}, \quad \rho = \frac{\sigma^2}{\sigma_0^2}.$$

$\hookrightarrow$ What happens as n increases?

Maximum A Posteriori Estimator

- Often, the prior probability acts as regularization.

$$\hat{\theta}_{\text{MAP}} = \arg\max_{\theta} \{\log p_\theta(\mathcal{D}) + \log p(\theta)\}.$$

- Linear model: $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$, $x_i \in \mathbb{R}^d$, $y_i \in \mathbb{R}$, model: $y_i = \theta^T x_i + \epsilon_i$, $\epsilon_i \sim \mathcal{N}(0, 1)$

  – $p(\theta) = \mathcal{N}(0, \lambda^{-1} I_d) \Rightarrow$ rigde regression a.k.a. (Tikhonov) regularized Least Squares.

  – $p(\theta) = \text{Laplace}(0, \lambda^{-1}) \Rightarrow$ lasso regression (least absolute shrinkage and selection operator).

Estimator Assessment

- Basic toolkit to assess an estimator:
  1. Unbiasedness.
  2. Consistency.
  3. Bias-Variance Trade-Off.
  4. Efficiency.
  5. Fisher Information.
  6. Cramér-Rao Lower Bound (CRLB).

Estimator Assessment

1. Unbiasedness:

Key assumption: $\exists \theta^* \text{ s.t. } p_d(x) = p_{\theta^*}(x)$.

- An unbiased estimator is an estimator whose expected values (w.r.t. the data generation distribution) is equal to the parameter:

$$\text{Bias}(\hat{\theta}) = \theta^* - \mathbb{E}_{p_d}[\hat{\theta}].$$

- The *sample mean* $\hat{\theta} = \frac{1}{n}\sum_{i=1}^{n} x_i$ with $x_i \sim p_{\theta^*}(x) \equiv \mathcal{N}(\theta^*, \sigma^2)$, i.i.d., is an unbiased estimator.

  Proof:

$$\mathbb{E}_{p_d}[\hat{\theta}] = \frac{1}{n}\sum_{i=1}^{n} \mathbb{E}_{p_{\theta^*}}[x_i] = \frac{1}{n}\sum_{i=1}^{n} \theta^* = \frac{1}{n} n\theta^* = \theta^*.$$

Estimator Assessment

1. Unbiasedness:

- An asymptotically unbiased estimator is the least requirement for an estimator:

$$\lim_{n\to\infty} \text{Bias}(\hat{\theta}_n) = 0.$$

  - Example: Let $\theta = \mathbb{E}_{p_d}[g(x)]$ and $\hat{\theta}_n = \frac{1}{n}\sum_{i=1}^{n} g(x_i)$ its estimator.
    $\hookrightarrow$ $\hat{\theta}_n$ is unbiased and the basic idea of **Monte Carlo** methods.

  - Example: Let $\theta = g(\mathbb{E}_{p_d}[x])$ and $\hat{\theta}_n = g\left(\frac{1}{n}\sum_{i=1}^{n} x_i\right)$ its estimator.
    $\hookrightarrow$ $\hat{\theta}_n$ is biased, but asymptotically it is an unbiased estimator.

Estimator Assessment

2. Consistency:

- An unbiased estimator is said to be consistent if the difference between the estimator and the true value becomes smaller as we increase the sample size. Formally:

$$\lim_{n\to\infty} P_{p_d}(|\hat{\theta}_n - \theta^*| > \epsilon) = 0 \ , \quad \forall \epsilon > 0.$$

– Example (consistent): Sample mean $\hat{\theta}_n = \frac{1}{n}\sum_{i=1}^{n} x_i$ with $x_i \sim \mathcal{N}(\theta^*, \sigma^2)$, i.i.d.

Chebyshev's inequality

$$\mathrm{Var}_{p_d}(\hat{\theta}_n) = \frac{\sigma^2}{n} \Rightarrow P_{p_d}(|\hat{\theta}_n - \theta^*| > \epsilon) \leq \frac{\sigma^2}{n\epsilon^2}.$$

– Example (not consistent): $\hat{\theta}_{10} = \frac{1}{10}\sum_{i=1}^{10} x_i$.

Estimator Assessment

2. Consistency and (asymptotic) unbiasedness:

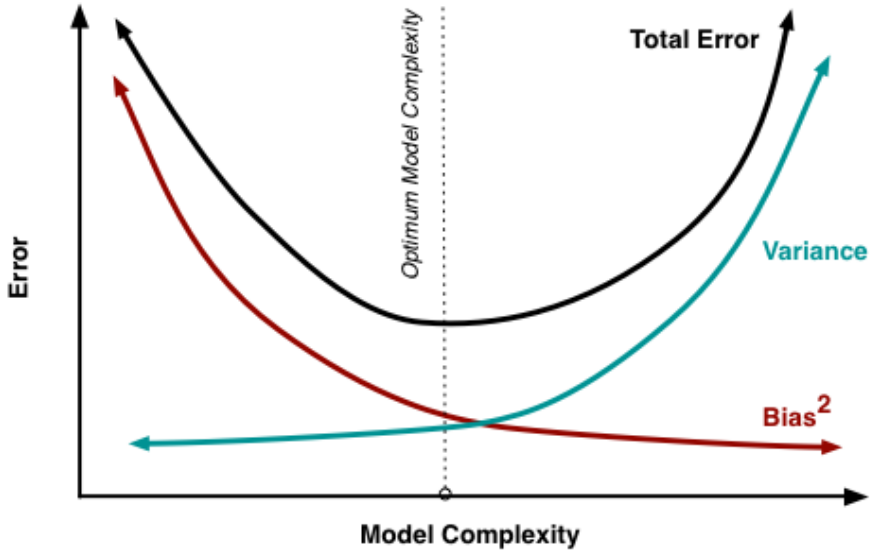
- *Proposition:* If $\mathrm{Var}_{p_d}(\hat{\theta}_n)$ is finite, then, consistency implies asymptotic unbiasness.
- *Proposition:* If $\mathrm{Var}_{p_d}(\hat{\theta}_n)$ tends to 0 as $n \to \infty$, then, asymptotic unbiasness implies consistency.
- *Proposition:* If the Mean Squared Error $\mathrm{MSE}(\hat{\theta}_n) := \mathbb{E}_{p_d}\left[(\hat{\theta}_n - \theta^*)^2\right]$ tends to 0 as $n \to \infty$, then, the estimator $\hat{\theta}_n$ is consistent.

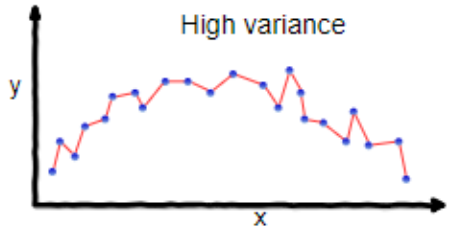
Estimator Assessment

3. Bias-variance trade-off in estimation theory:

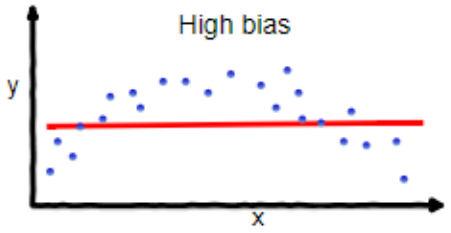
$$\mathrm{MSE}(\hat{\theta}) := \mathbb{E}_{p_d}\left[(\hat{\theta} - \theta^*)^2\right] = \mathrm{Bias}^2_{p_d}(\hat{\theta}) + \mathrm{Var}_{p_d}(\hat{\theta}).$$

Bias-variance trade-off in machine learning:

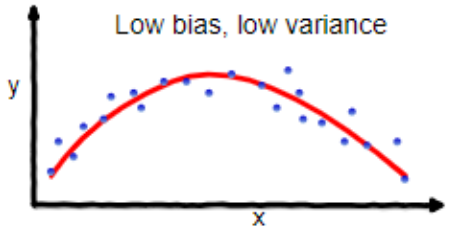




overfitting



underfitting

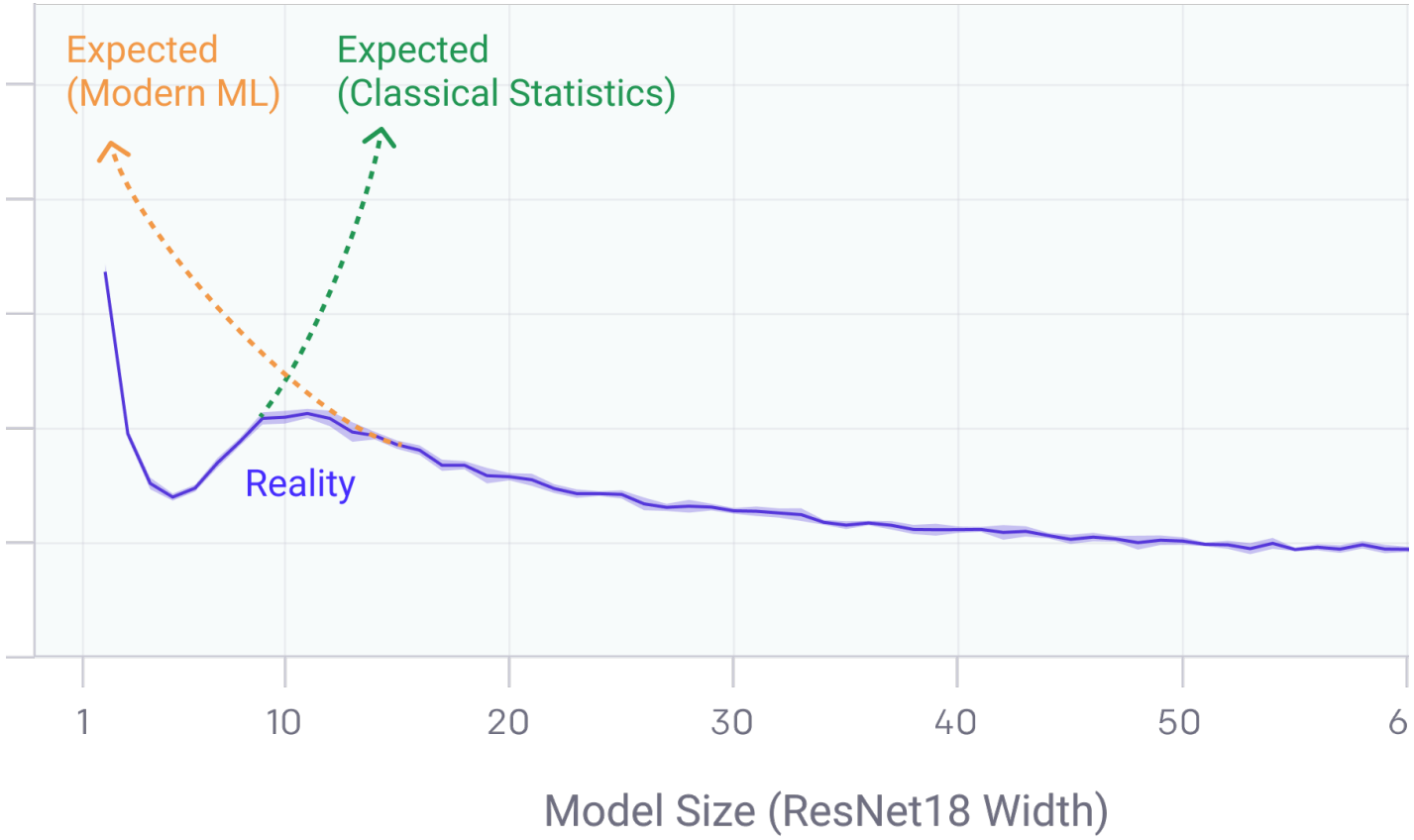


Good balance

Estimator Assessment - Caution

(Deep) Double Descent Phenomenon:

Double descent is a modern machine learning phenomenon where, contrary to classical statistical wisdom, increasing model complexity (parameters, training time) beyond the point of overfitting causes test error to decrease again.



Estimator Assessment

4. Efficiency:

- Let $\hat{\theta}_1$ and $\hat{\theta}_2$ be two unbiased estimators of θ^*. $\hat{\theta}_1$ is more efficient than $\hat{\theta}_2$ if and only if $\text{Var}(\hat{\theta}_1) < \text{Var}(\hat{\theta}_2)$.

- An estimator $\hat{\theta}$ is efficient if the variance of the estimator, $\text{Var}(\hat{\theta})$, equals the Cramér-Rao lower bound.

Estimator Assessment

5. Fisher Information:

$$I(\theta) = \mathbb{E}_{p_\theta}\left[\left(\frac{d}{d\theta}\log p_\theta(x)\right)^2\right].$$

$\hookrightarrow$ $I(\theta) = \mathrm{Var}_{p_\theta}\left(\frac{d}{d\theta}\log p_\theta(x)\right) = -\mathbb{E}_{p_\theta}\left[\frac{d^2}{d\theta^2}\log p_\theta(x)\right]$,

since $-\mathbb{E}_{p_\theta}\left[\frac{d}{d\theta}\log p_\theta(x)\right] = 0.$

– Example: $p_\theta(x) = \mathrm{Bernoulli}(\theta),\ \theta \in [0,1]$: success probability.

$I(\theta) = \cdots = \frac{1}{\theta(1-\theta)}.$

Estimator Assessment

6. Cramér-Rao Lower Bound (CRLB):

- The variance of any unbiased estimator $\hat{\theta}_n$ of θ^* is bounded by the reciprocal of the Fisher information:

$$\mathrm{Var}_{p_{\theta^*}}(\hat{\theta}_n) \geq \frac{1}{I_n(\theta^*)} = \frac{1}{nI(\theta^*)}, \quad \text{n: \# i.i.d. samples drawn from } p_{\theta^*}(x).$$

- MLE is asymptotically efficient!

References

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   `https://www.math.uwaterloo.ca/~hwolkowi/matrixcookbook.pdf`

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