Foundations of Machine Learning
AI2000 and AI5000

FoML-04
Maximum Likelihood Principle

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భారతీయ సాంకేతిక విజ్ఞాన సంస్థ హైదరాబాద్
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So far in FoML

- What is ML and the learning paradigms
- Probability refresher
    - Random variables, Bayes Theorem, Independence, Expectation, Variance

Maximum Likelihood Principle

Maximum Likelihood Principle

- Widely used technique for optimizing model parameters

Maximum Likelihood Principle

- Given - Dataset of N independent observations D $= \{x_1, x_2 \ldots x_N\}$

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Maximum Likelihood Principle

- Goal: recover the probability distribution that may have generated this dataset

Maximum Likelihood Principle

- Goal: recover the probability distribution that may have generated this dataset
- Likelihood of the dataset $p(D|w)$

Maximum Likelihood Principle

- The most likely 'explanation' of D is given by w_{ML} that maximizes the likelihood function

$$\mathbf{w}_{ML} = \underset{w}{\arg\max}\; p(D|w)$$

Maximum Likelihood Principle

- The iid assumption - each $x_i \epsilon D$ is independently distributed according to the same distribution conditioned on w

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Maximum Likelihood Principle

- The iid assumption - each $x_i \epsilon$ D is independently distributed according to the same distribution conditioned on w

The joint distribution $$P(D|\omega) = P(x_1, x_2 \dots x_N|\omega) = \prod_{i=1}^{N} P(x_i|\omega)$$

Maximum Likelihood Principle

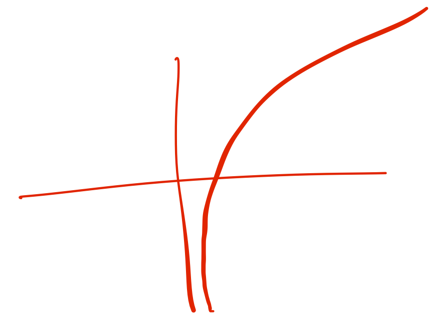
$$\mathbf{w}_{ML} = \arg\max_{\mathbf{w}} \; p(D|\mathbf{w}) = \arg\max_{\mathbf{w}} \; \prod_{i=1}^{N} p(x_i|\mathbf{w})$$

Maximum Likelihood Principle

$$\mathbf{w}_{ML} = \arg\max_{\mathbf{w}} \; p(D|\mathbf{w}) = \arg\max_{\mathbf{w}} \; \prod_{i=1}^{N} p(x_i|\mathbf{w})$$

- Numerical underflow

Maximum Likelihood Principle



$$\mathbf{w}_{ML} = \arg\max_{\mathbf{w}} \; p(D|\mathbf{w}) = \arg\max_{\mathbf{w}} \; \prod_{i=1}^{N} p(x_i|\mathbf{w})$$

- Numerical underflow
- Maximize the log-likelihood →

$$\log \prod_{i=1}^{N} p(x_i|w)$$

Maximum Likelihood Principle

P

x_1

x_2

x_N

$$\mathbf{w}_{ML} = \arg\max_{\mathbf{w}} \; p(D|\mathbf{w}) = \arg\max_{\mathbf{w}} \; \prod_{i=1}^{N} p(x_i|\mathbf{w})$$

- Numerical underflow
- Maximize the log-likelihood

$$\mathbf{w}_{ML} = \arg\max_{\mathbf{w}} \; \log \prod_{i=1}^{N} p(x_i|\mathbf{w})$$

Error function:

$$E(D;\mathbf{w}) = -\log p(D|\mathbf{w}) = -\sum_{i=1}^{N} \log p(x_i|\mathbf{w})$$

NLL

MLE for Gaussian Distributions

- iid Gaussian distributed real variables D =

$$p(x|\mathbf{w}) = \mathcal{N}(x|\mu, \sigma^2) \qquad p(D|\mathbf{w}) = p(D|\mu, \sigma^2) = \frac{1}{(2\pi\sigma^2)^{1/2}} e^{-\frac{1}{2\sigma^2}(x-\mu)^2}$$

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MLE for Gaussian Distributions

- iid Gaussian distributed real variables D =

$$p(x|\mathbf{w}) = \mathcal{N}(x|\mu, \sigma^2) \qquad p(D|\mathbf{w}) = p(D|\mu, \sigma^2) = \frac{1}{(2\pi\sigma^2)^{N/2}} \prod_{i=1}^{N} e^{-\frac{1}{2\sigma^2}(x_i-\mu)^2}$$

log likelihood = $-\frac{N}{2}\log 2\pi\sigma^2 - \frac{1}{2\sigma^2}\sum_{i=1}^{N}(x_i-\mu)^2$

MLE for Gaussian Distributions

- Estimate the model parameters $\mu_{ML}, \sigma^2_{ML} = \arg\max_{\mu,\sigma^2} \log p(D|\mu, \sigma^2)$

$$\frac{\partial}{\partial \mu}\left\{ \quad \right\} = 0 \qquad = \frac{-1}{\cancel{2}\sigma^2}(\cancel{2}) \sum_{i=1}^{N} (x_i - \mu)$$

$$\sum_{i=1}^{N} (x_i - \mu) = 0$$

$$\mu_{ML} = \frac{1}{N} \sum_{i=1}^{N} x_i$$

MLE for Gaussian Distributions

- Estimate the model parameters $\mu_{ML}, \sigma^2_{ML} = \underset{\mu, \sigma^2}{\arg\max} \; \log p(D|\mu, \sigma^2)$

$$\frac{\partial}{\partial \sigma^2}\left(\quad \right) = 0$$

$$-\frac{N}{2} \frac{1}{\cancel{2\pi}\sigma^2}(\cancel{2\pi}) + \frac{1}{2\sigma^4} \sum_{i=1}^{N} (x_i - \mu)^2 = 0$$

$$-\frac{N}{2} \sigma^2 + \frac{1}{2} \sum_{i=1}^{N} (x_i - \mu)^2 = 0$$

$$\sigma^2_{ML} = \frac{1}{N} \sum_{i=1}^{N} (x_i - \mu)^2$$

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MLE for Gaussian Distributions

$$\mu_{ML}, \sigma^2_{ML} = \arg\max_{\mu,\sigma^2} \log p(D|\mu, \sigma^2)$$

- How well do these estimates represent the true parameters?

MLE for Gaussian Distributions

$$\mu_{ML}, \sigma^2_{ML} = \arg\max_{\mu,\sigma^2} \; \log p(D|\mu, \sigma^2)$$

- How well do these estimates represent the true parameters?
- Note that these are functions of the data sample

$$D_1 = \{x_1 \cdots x_N\}^1 \longrightarrow {}^1\mu_{ML} \quad {}^1\sigma^2_{ML}$$

$$D_2 = \{x_1 \cdots x_N\}^2 \longrightarrow {}^2\mu_{ML} \quad {}^2\sigma^2_{ML}$$

$$\vdots$$

$$D_M = \{x_1 \cdots x_N\}^M \longrightarrow {}^M\mu_{ML} \quad {}^M\sigma^2_{ML}$$

MLE for Gaussian Distributions

$$\mu_{ML}, \sigma^2_{ML} = \arg\max_{\mu, \sigma^2} \; \log p(D|\mu, \sigma^2)$$

- How well do these estimates represent the true parameters?
- Note that these are functions of the data sample
    - → expected values of these estimates

$\mathbb{E}_D[\mu_{ML}]$ — ?

$\mathbb{E}_D[\sigma^2_{M}]$ — ?

$D \sim P(D|\mu, \sigma^2)$

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MLE for Gaussian Distributions

- ML estimate of the mean

$$\mathbb{E}_{D \sim p(D|\mu,\sigma^2)}\left[\frac{1}{N}\sum_{i=1}^{N} x_i\right] = \frac{1}{N}\sum_{i=1}^{N} \mathbb{E}_{D \sim p(D|\mu,\sigma^2)}\, x_i$$

$$= \frac{1}{N}\sum_{i=1}^{N} \mathbb{E}_{x_i \sim p(x|\mu,\sigma^2)}(x_i) = \frac{1}{N}\sum_{i=1}^{N} \mu = \mu$$

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MLE for Gaussian Distributions

- Bias of the "ML estimate of the mean"

$x_i \sim p(x \mid \mu, \sigma^2)$

$$\mathbb{E}_D[\mu_{ML}] - \mu$$

$$\mu \quad - \mu$$

$$= 0$$

MLE for Gaussian Distributions

- ML estimate of the variance

$$\mathbb{E}\left[\frac{1}{N}\sum_{i=1}^{N}\left(x_i - \frac{1}{N}\sum_{j=1}^{N}x_j\right)^2\right]$$

$$= \frac{1}{N}\sum_{i=1}^{N}\mathbb{E}\left[\left(x_i - \frac{1}{N}\sum_{j=1}^{N}x_j\right)^2\right] = \frac{1}{N}\sum_{i=1}^{N}\mathbb{E}\left[x_i^2 - \frac{2}{N}x_i\sum_{j=1}^{N}x_j + \frac{1}{N^2}\sum_{l=1}^{N}\sum_{k=1}^{N}x_l x_k\right]$$

$$= \frac{1}{N}\sum_{i=1}^{N}\left[\mu^2+\sigma^2 - \frac{2}{N}\left(\sigma^2+\mu^2+(N-1)\mu^2\right) + \frac{1}{N^2}\left(N(\sigma^2+\mu^2)+N(N-1)\mu^2\right)\right]$$

$$= \frac{1}{N}\sum_{i=1}^{N}\left[\mu^2+\sigma^2 - \frac{2}{N}\left(\sigma^2+N\mu^2\right) + \frac{1}{N^2}\left(N\sigma^2+N^2\mu^2\right)\right]$$

$$= \mu^2\left[1-2+1\right]+\sigma^2\left[1-\frac{2}{N}+\frac{1}{N}\right] = \frac{N-1}{N}\sigma^2$$

$$\mathbb{E}[x_i x_j] = \mathrm{Cov}(x_i, x_j) + \mathbb{E}[x_i]\,\mathbb{E}[x_j]$$

$i=j \longrightarrow \sigma^2+\mu^2 \qquad i\neq j \quad \mu^2$

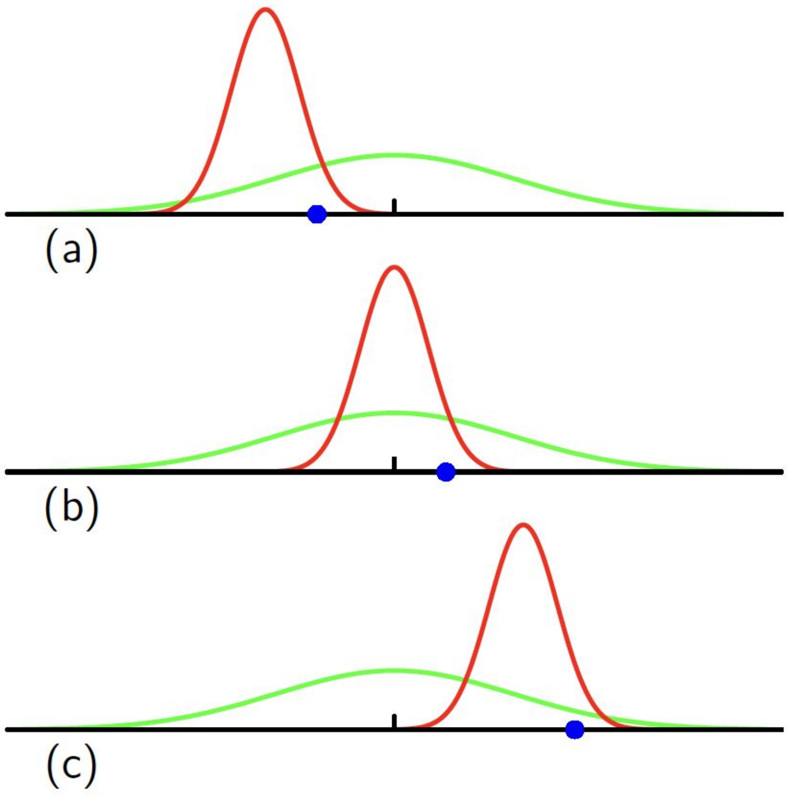
MLE for Gaussian Distributions

- Bias of the "ML estimate of the variance"

σ_{ML}^2 is biased $\quad \frac{N-1}{N}\sigma^2$

$$\sigma_{ML\text{-}UB}^2 = \frac{N}{N-1}\sigma_{ML}^2$$

Bias in variance estimate



Regression example

MLE for Regression (curve fitting)

- Given data D $\quad D = \{(x_1, t_1), (x_2, t_2), \ldots (x_N, t_N)\} = \{\mathbf{x}, \mathbf{t}\}$

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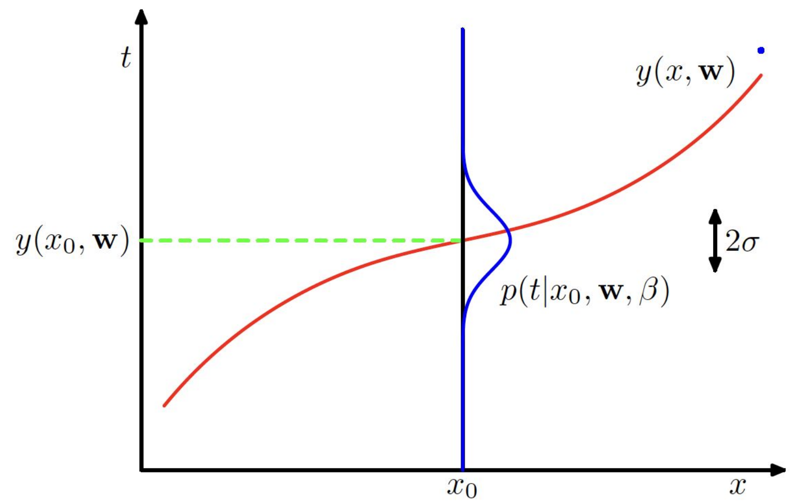
MLE for Regression (curve fitting)

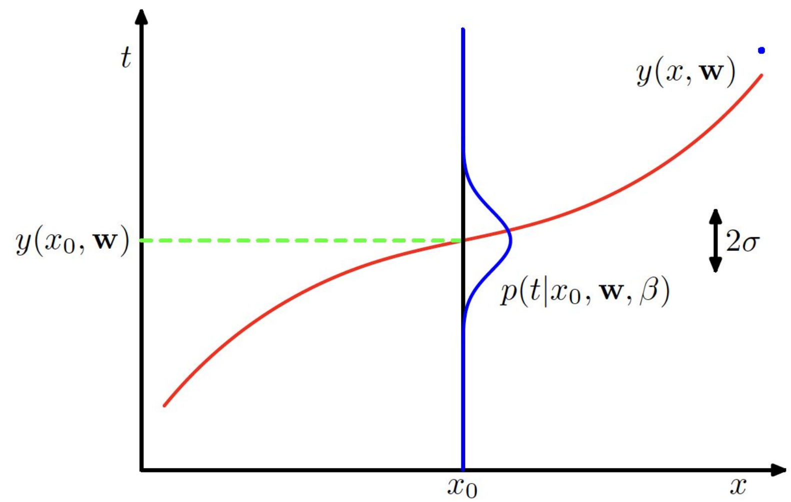
- Given data D $D = \{(x_1, t_1), (x_2, t_2), \dots (x_N, t_N)\} = \{\mathbf{x}, \mathbf{t}\}$
- Assume the data is generated by

$$t = y(x, \mathbf{w}) + \sigma \cdot \epsilon, \quad \epsilon \in \mathcal{N}(0, 1)$$



MLE for Regression (curve fitting)

- Target distribution $$p(t|x, \mathbf{w}, \beta) = \mathcal{N}(t|y(x, \mathbf{w}), \beta^{-1})$$



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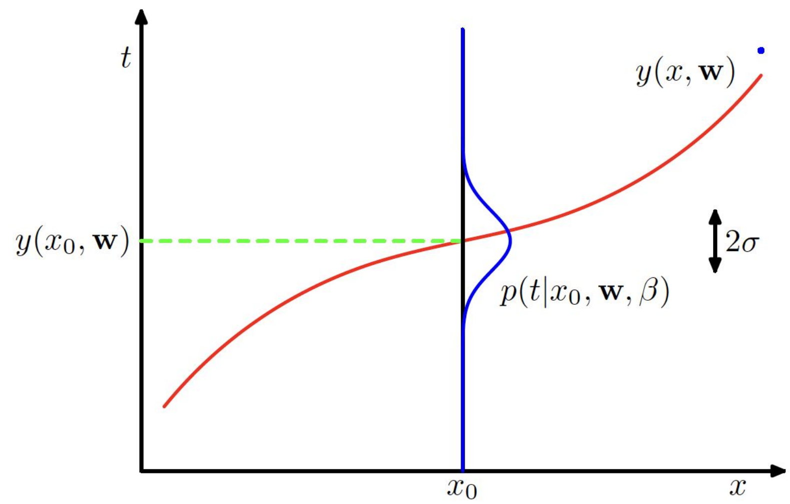
MLE for Regression (curve fitting)

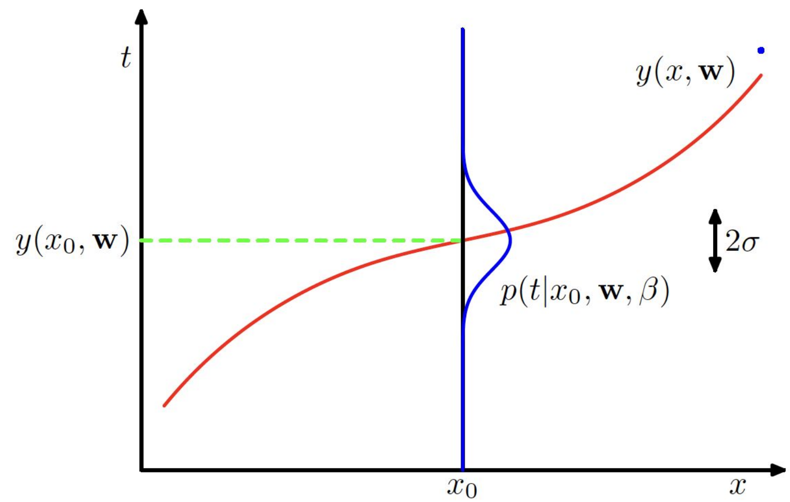
- Target distribution $$p(t|x, \mathbf{w}, \beta) = \mathcal{N}(t|y(x, \mathbf{w}), \beta^{-1})$$
- log likelihood

$$\log p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta^{-1})$$



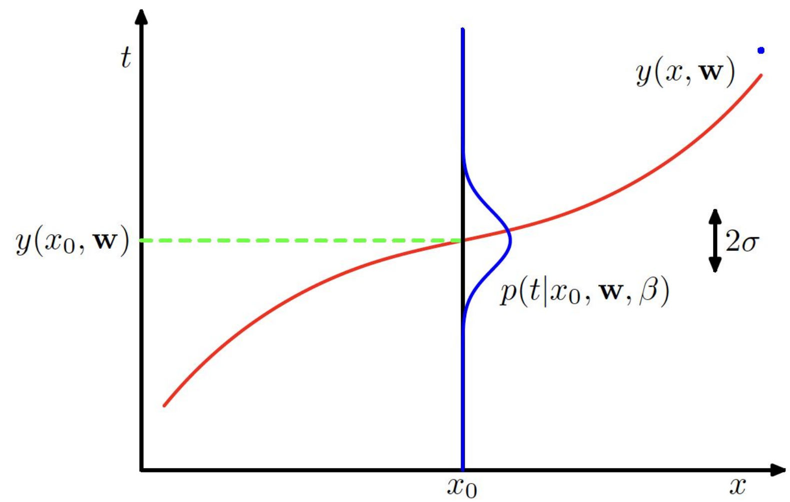
MLE for Regression (curve fitting)

- Minimize the NLL w.r.t the parameters w and β



MLE for Regression (curve fitting)

- The predictive distribution



Rough work

Next
MAP