TAMPERE UNIVERSITY OF TECHNOLOGY

PATTERN RECOGNITION AND MACHINE LEARNING

Slide Set 2: Estimation Theory

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Classical Estimation and Detection Theory

- Before the machine learning part, we will take a look at classical estimation theory.
- Estimation theory has many connections to the foundations of modern machine learning.
- Outline of the next few hours:
  1. Estimation theory: Fundamentals
  2. Estimation theory: Maximum likelihood
  3. Estimation theory: Examples
  4. Detection theory: Fundamentals
  5. Detection theory: Error metrics
  6. Estimation theory: Examples

Introduction - estimation

- Our goal is to estimate the values of a group of parameters from data.
- Examples: radar, sonar, speech, image analysis, biomedicine, communications, control, seismology, etc.
- *Parameter estimation*: Given an N-point data set $\mathbf{x} = \{x[0], x[1], \dots, x[N-1]\}$ which depends on the unknown parameter $\theta \in \mathbb{R}$, we wish to design an *estimator* $g(\cdot)$ for θ

$$\hat{\theta} = g(x[0], x[1], \dots, x[N-1]).$$

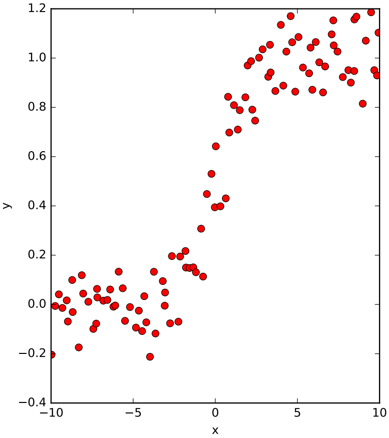
- The fundamental questions are:
  1. What is the model for our data?
  2. How to determine its parameters?

Introductory Example – Straight line

- Suppose we have the illustrated time series and would like to approximate the relationship of the two coordinates.
- The relationship looks linear, so we could assume the following model:

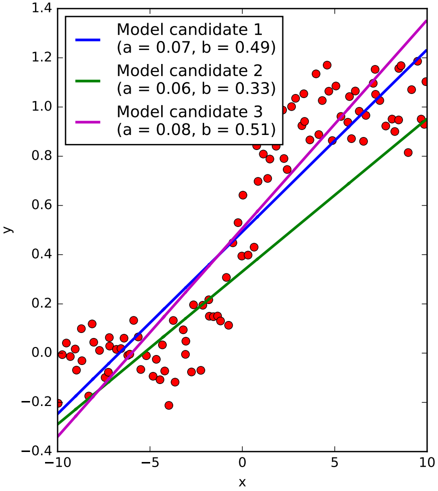
$$y[n] = ax[n] + b + w[n],$$

  with $a \in \mathbb{R}$ and $b \in \mathbb{R}$ unknown and $w[n] \sim \mathcal{N}(0, \sigma^2)$
- $\mathcal{N}(0, \sigma^2)$ is the normal distribution with mean 0 and variance σ^2.



Introductory Example – Straight line

- Each pair of *a* and *b* represent one line.
- Which line of the three would best describe the data set? Or some other line?



Introductory Example – Straight line

- It can be shown that the best solution (in the *maximum likelihood* sense; to be defined later) is given by

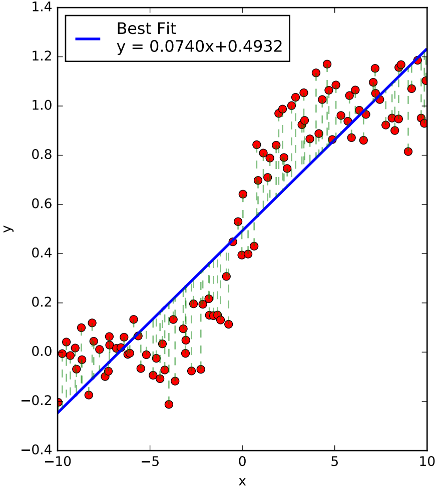
$$\begin{aligned}\hat{a} &= -\frac{6}{N(N+1)}\sum_{n=0}^{N-1} y(n) + \frac{12}{N(N^2-1)}\sum_{n=0}^{N-1} x(n)y(n)\\ \hat{b} &= \frac{2(2N-1)}{N(N+1)}\sum_{n=0}^{N-1} y(n) - \frac{6}{N(N+1)}\sum_{n=0}^{N-1} x(n)y(n).\end{aligned}$$

- Or, as we will later learn, in an easy matrix form:

$$\hat{\boldsymbol{\theta}} = \begin{pmatrix}\hat{a}\\ \hat{b}\end{pmatrix} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

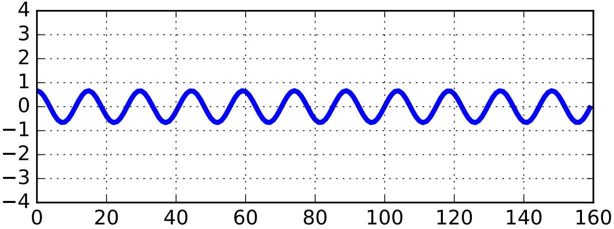
Introductory Example – Straight line

- In this case, $\hat{a} = 0.07401$ and $\hat{b} = 0.49319$, which produces the line shown on the right.
- The line also minimizes the squared distances (green dashed lines) between the model (blue line) and the data (red circles).



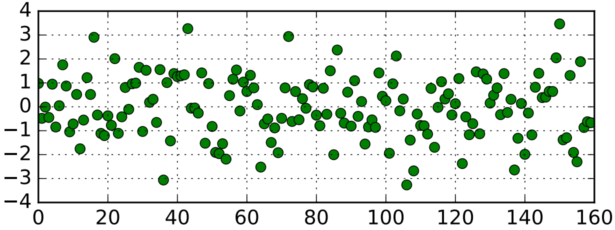
Introductory Example 2 – Sinusoid

- Consider transmitting the sinusoid below.



Introductory Example 2 – Sinusoid

- When the data
  is received, it is corrupted by noise and the received samples look like below.



- Can we recover the parameters of the sinusoid?

Introductory Example 2 – Sinusoid

- In this case, the problem is to find good values for A, f_0 and ϕ in the following model:

$$x[n] = A\cos(2\pi f_0 n + \phi) + w[n],$$

with $w[n] \sim \mathcal{N}(0, \sigma^2)$.

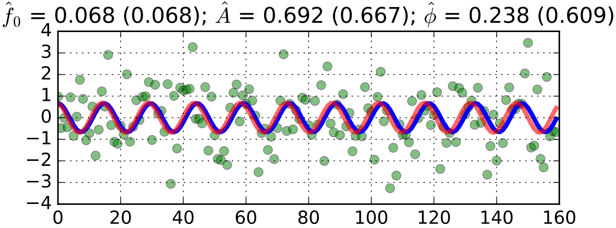
Introductory Example 2 – Sinusoid

- We will learn that the *maximum likelihood estimator; MLE* for parameters A, f_0 and ϕ are given by

$$
\begin{aligned}
\hat{f}_0 &= \text{value of } f \text{ that maximizes } \left| \sum_{n=0}^{N-1} x(n) e^{-2\pi i f n} \right|, \\
\hat{A} &= \frac{2}{N} \left| \sum_{n=0}^{N-1} x(n) e^{-2\pi i \hat{f}_0 n} \right| \\
\hat{\phi} &= \arctan \frac{-\sum_{n=0}^{N-1} x(n) \sin(2\pi \hat{f}_0 n)}{\sum_{n=0}^{N-1} x(n) \cos(2\pi \hat{f}_0 n)}.
\end{aligned}
$$

Introductory Example 2 – Sinusoid

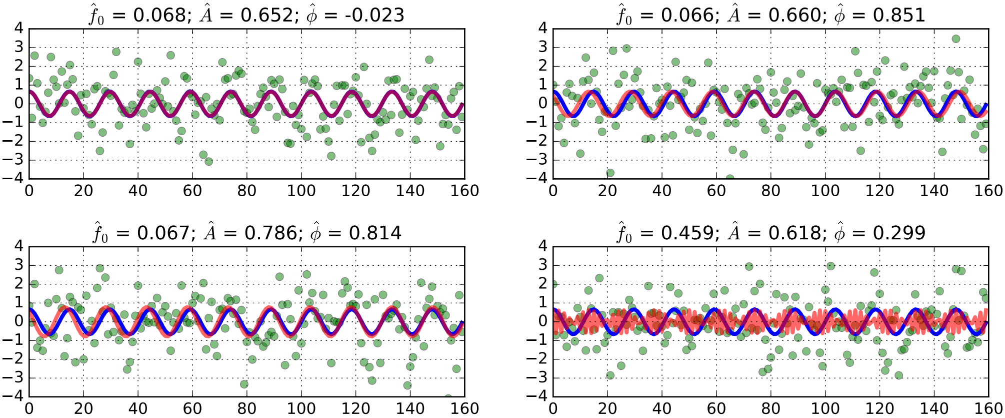
- It turns out that the sinusoidal parameter estimation is very successful:



- The blue curve is the original sinusoid, and the red curve is the one estimated from the green circles.
- The estimates are shown in the figure (true values in parentheses).

Introductory Example 2 – Sinusoid

- However, the results are different for each *realization* of the noise $w[n]$.



$\hat{f}_0$ = 0.068; $\hat{A}$ = 0.652; $\hat{\phi}$ = -0.023

$\hat{f}_0$ = 0.066; $\hat{A}$ = 0.660; $\hat{\phi}$ = 0.851

$\hat{f}_0$ = 0.067; $\hat{A}$ = 0.786; $\hat{\phi}$ = 0.814

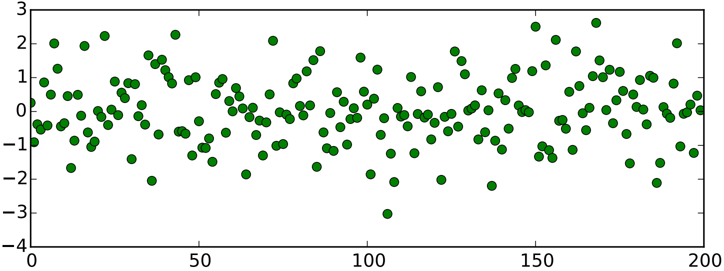
$\hat{f}_0$ = 0.459; $\hat{A}$ = 0.618; $\hat{\phi}$ = 0.299

Introductory Example 2 – Sinusoid

- Thus, we're not very interested in an individual case, but rather on the distributions of estimates
  - What are the expectations: $E[\hat{f}_0]$, $E[\hat{\phi}]$ and $E[\hat{A}]$?
  - What are their respective variances?
  - Could there be a better formula that would yield smaller variance?
  - If yes, how to discover the better estimators?

Example of the Variance of an Estimator

- Consider the estimation of the mean of the following measurement data:



Example of the Variance of an Estimator

- Now we're searching for the estimator $\hat{A}$ in the model

$$x[n] = A + w[n],$$

  with $w[n] \sim \mathcal{N}(0, \sigma^2)$ where σ^2 is also unknown.

- A natural estimator of A is the sample mean:

$$\hat{A} = \frac{1}{N} \sum_{n=0}^{N-1} x[n].$$

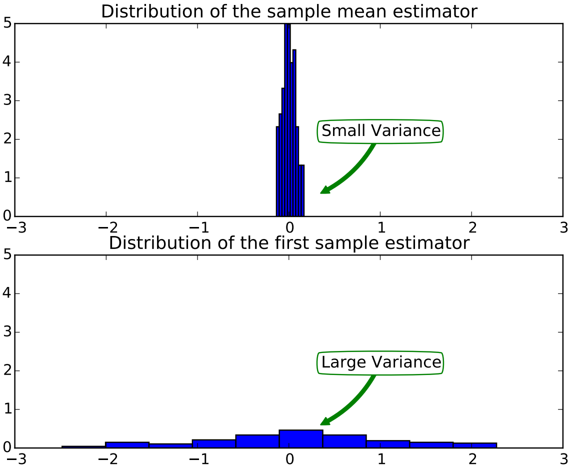
- Alternatively, one might propose to use only the first sample as such:

$$\check{A} = x[0].$$

- How to justify that the first one is better?

Example of the Variance of an Estimator

- Method 1: estimate variances **empirically**.
- Histograms of the estimates over 100 data realizations are shown on the right.
- In other words, we synthesized 100 versions of the data with the same statistics.
- Each synthetic sample produces one estimate of the mean for both estimators.



Example of the Variance of an Estimator

- Attached is the code for the experiment of previous slide.
- Code available at **https://github.com/mahehu/SGN-41007/blob/master/code/Two_Estimators.ipynb**
- Requires the following imports:

```python
import numpy as np
import matplotlib.pyplot as plt
```

```python
mean_estimates_1 = []
mean_estimates_2 = []
numSamples = 100

for iteration in range(100):

    # Create a random sample of data from N(0,1)
    x = np.random.randn(numSamples)

    # Compute the estimate of the mean using
    # the sample mean
    aHat_1 = x.mean() # or np.mean(x)

    # Compute the "first sample estimator"
    aHat_2 = x[0]

    # Append the computed values to our lists:
    mean_estimates_1.append(aHat_1)
    mean_estimates_2.append(aHat_2)

# Plot the empirical distributions
fig, axes = plt.subplots(2, 1, sharex=True)

axes[0].hist(mean_estimates_1, normed = True)
axes[1].hist(mean_estimates_2, normed = True)

plt.show()
```

Example of the Variance of an Estimator

- Method 2: estimate variances **analytically**.
- Namely, it is easy to compute variances in a closed form:

$$\begin{aligned}
\textbf{Estimator 1:}\ \mathrm{var}(\hat{A}) &= \mathrm{var}\left(\frac{1}{N}\sum_{n=0}^{N-1} x[n]\right)\\
&= \frac{1}{N^2}\sum_{n=0}^{N-1}\mathrm{var}(x[n])\\
&= \frac{1}{N^2}N\sigma^2 = \frac{\sigma^2}{N}.\\
\textbf{Estimator 2:}\ \mathrm{var}(\check{A}) &= \mathrm{var}(x[0]) = \sigma^2.
\end{aligned}$$

Example of the Variance of an Estimator

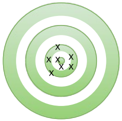
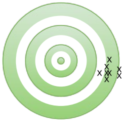
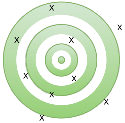
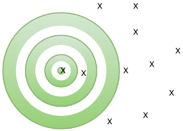
- Compared to the "First sample estimator" $\check{A} = x[0]$, the estimator variance of $\hat{A}$ is one N'th.
- The analytical approach is clearly the desired one whenever possible:
  - Faster, more elegant and less prone to random effects.
  - Often also provides proof that there exists no estimator that would be more efficient.
- Usually can be done for easy cases.
- More complicated scenarios can only be studied empirically.

Estimator Design

- There are a few well established approaches for estimator design:
  - **Minimum Variance Unbiased Estimator (MVU):** Analytically discover the estimator that minimizes the output variance among all *unbiased* estimators.
  - **Maximum Likelihood Estimator (ML):** Analytically discover the estimator that maximizes the likelihood of observing the measured data.
  - Others: **Method of Moments (MoM)** and **Least Squares (LS)**.
- Our emphasis will be on Maximum Likelihood, as it appears in the machine learning part as well.
- Note, that different methods often (not always) result in the same estimator.
- For example, the MVU, ML, MoM and LS estimators for the mean parameter all end up at the same formula: $\hat{A} = \frac{1}{N}\sum x_n$.

Minimum Variance Unbiased Estimator

- Commonly the MVU estimator is considered optimal.
- However, finding the MVU estimator may be difficult. The MVUE may not even exist.
- We will not concentrate on this estimator design approach. Interested reader may consult, *e.g.*, S. Kay: *Fundamentals of Statistical Signal Processing: Volume 1* (1993).
- For an overview, read Wikipedia articles on *Minimum-variance unbiased estimator* and *Lehmann–Scheffé theorem*.

	Small Bias	Large Bias
Small Variance		
Large Variance		

Maximum Likelihood Estimation

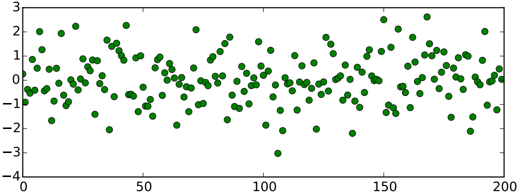
- Maximum likelihood (ML) is the most popular estimation approach due to its applicability in complicated estimation problems.
- Maximization of likelihood also appears often as the optimality criterion in machine learning.
- The method was proposed by Fisher in 1922, though he published the basic principle already in 1912 as a third year undergraduate.
- The basic principle is simple: find the parameter θ that is the most probable to have generated the data $\mathbf{x}$.
- The ML estimator may or may not be optimal in the minimum variance sense. It is not necessarily unbiased, either.

The Likelihood Function

- Consider again the problem of estimating the mean level A of noisy data.
- Assume that the data originates from the following model:

$$x[n] = A + w[n],$$

where $w[n] \sim \mathcal{N}(0, \sigma^2)$: Constant plus Gaussian random noise with zero mean and variance σ^2.



The Likelihood Function

- For simplicity, consider the first sample estimator for estimating A.
- We assume normally distributed $w[n]$, *i.e.,* the following probability density function (PDF):

$$p(w[n]) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{1}{2\sigma^2}(w[n])^2\right]$$

- Since $x[n] = A + w[n]$, we can substitute $w[n] = x[n] - A$ above to describe the PDF of $x[n]$[1]:

$$p(x[n];A) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{1}{2\sigma^2}(x[n]-A)^2\right]$$

[1] We denote $p(x[n];A)$ to emphasize that p depends on A.

The Likelihood Function

- Thus, our first sample estimator has the PDF

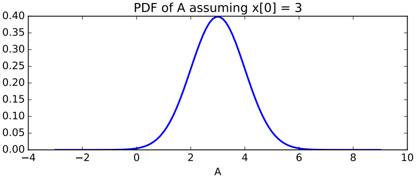
$$p(x[0];A) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{1}{2\sigma^2}(x[0]-A)^2\right]$$

- Now, suppose we have observed $x[0]$, say $x[0] = 3$.
- Then some values of A are more likely than others and we can derive the complete PDF of A easily.

The Likelihood Function

- Actually, the PDF of A has the same form as the PDF of $x[0]$:

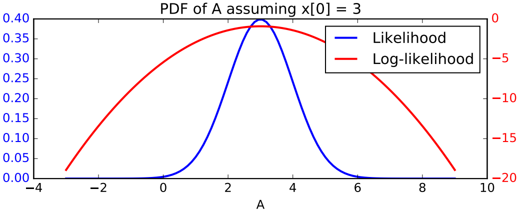
$$\text{pdf of } A = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{1}{2\sigma^2}(3-A)^2\right]$$



- This function is called *the likelihood function* of A, and its maximum the *maximum likelihood estimate*.

The Likelihood Function

- In summary: If the PDF of the data is viewed as a function of the unknown parameter (with fixed data), it is called the *likelihood function*.
- Often the likelihood function has an exponential form. Then it's usual to take the natural logarithm to get rid of the exponential. Note that the maximum of the new *log-likelihood* function does not change.



ML Example

- Consider the familiar example of estimating the mean of a signal:

$$x[n] = A + w[n], \qquad n = 0, 1, \ldots, N-1,$$

  with $w[n] \sim \mathcal{N}(0, \sigma^2)$.

- The noise samples $w[n]$ are assumed independent, so the distribution of the whole batch of samples $\mathbf{x} = (x[0], \ldots, x[N-1])$ is obtained by multiplication:

$$p(\mathbf{x}; A) = \prod_{n=0}^{N-1} p(x[n]; A) = \frac{1}{(2\pi\sigma^2)^{\frac{N}{2}}} \exp\left[-\frac{1}{2\sigma^2} \sum_{n=0}^{N-1} (x[n] - A)^2 \right]$$

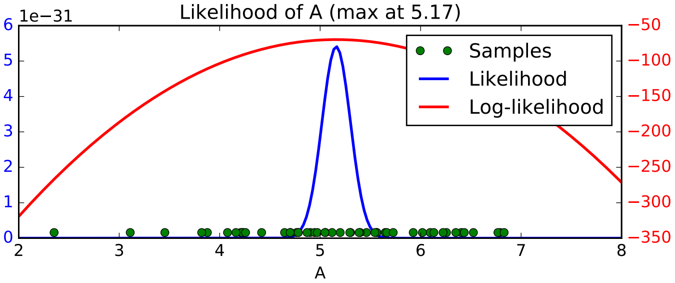
ML Example

- When we have observed the data $\mathbf{x}$, we can turn the problem around and consider what is the most likely parameter A that generated the data.
- Some authors emphasize this by turning the order around: $p(A; \mathbf{x})$ or give the function a different name such as $L(A; \mathbf{x})$ or $\ell(A; \mathbf{x})$.
- So, consider $p(\mathbf{x}; A)$ as a function of A and try to maximize it.

ML Example

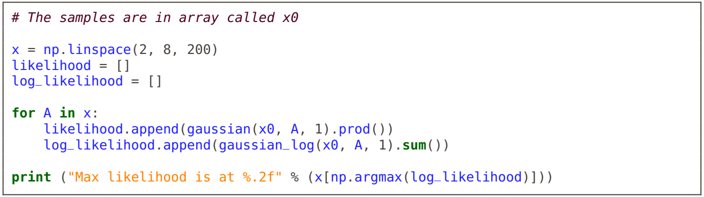
- The picture below shows the likelihood function and the log-likelihood function for one possible realization of data.
- The data consists of 50 points, with true $A = 5$.
- The likelihood function gives the probability of observing these particular points with different values of A.

ML Example


Likelihood of A (max at 5.17)
1e−31
6
5
4
3
2
1
0
−50
−100
−150
−200
−250
−300
−350
2
3
4
5
6
7
8
A
Samples
Likelihood
Log-likelihood

ML Example

- Instead of finding the maximum from the plot, we wish to have a closed form solution.
- Closed form is faster, more elegant, accurate and numerically more stable.
- Just for the sake of an example, below is the code for the stupid version.



```
# The samples are in array called x0

x = np.linspace(2, 8, 200)
likelihood = []
log_likelihood = []

for A in x:
    likelihood.append(gaussian(x0, A, 1).prod())
    log_likelihood.append(gaussian_log(x0, A, 1).sum())

print ("Max likelihood is at %.2f" % (x[np.argmax(log_likelihood)]))
```

ML Example

- Maximization of $p(\mathbf{x};A)$ directly is nontrivial. Therefore, we take the logarithm, and maximize it instead:

$$\begin{aligned} p(\mathbf{x};A) &= \frac{1}{(2\pi\sigma^2)^{\frac{N}{2}}} \exp\left[-\frac{1}{2\sigma^2}\sum_{n=0}^{N-1}(x[n]-A)^2\right] \\ \ln p(\mathbf{x};A) &= -\frac{N}{2}\ln(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{n=0}^{N-1}(x[n]-A)^2 \end{aligned}$$

- The maximum is found via differentiation:

$$\frac{\partial \ln p(\mathbf{x};A)}{\partial A} = \frac{1}{\sigma^2}\sum_{n=0}^{N-1}(x[n]-A)$$

ML Example

- Setting this equal to zero gives

$$\begin{aligned}
\frac{1}{\sigma^2}\sum_{n=0}^{N-1}(x[n]-A) &= 0 \\
\sum_{n=0}^{N-1}(x[n]-A) &= 0 \\
\sum_{n=0}^{N-1}x[n]-\sum_{n=0}^{N-1}A &= 0 \\
\sum_{n=0}^{N-1}x[n]-NA &= 0 \\
\sum_{n=0}^{N-1}x[n] &= NA \\
A &= \frac{1}{N}\sum_{n=0}^{N-1}x[n]
\end{aligned}$$

Conclusion

- *What did we actually do?*
  - We proved that the **sample mean** is the maximum likelihood estimator for the **distribution mean**.
- *But I could have guessed this result from the beginning. What’s the point?*
  - We can do the same thing for cases where you can not guess.

Example: Sinusoidal Parameter Estimation

- Consider the model

$$x[n] = A\cos(2\pi f_0 n + \phi) + w[n]$$

with $w[n] \sim \mathcal{N}(0, \sigma^2)$. It is possible to find the MLE for all three parameters: $\boldsymbol{\theta} = [A, f_0, \phi]^T$.

- The PDF is given as

$$p(\mathbf{x}; \boldsymbol{\theta}) = \frac{1}{(2\pi\sigma^2)^{\frac{N}{2}}} \exp\left[-\frac{1}{2\sigma^2}\sum_{n=0}^{N-1}(\underbrace{x[n] - A\cos(2\pi f_0 n + \phi)}_{w[n]})^2\right]$$

Example: Sinusoidal Parameter Estimation

- Instead of proceeding directly through the log-likelihood function, we note that the above function is maximized when

$$J(A, f_0, \phi) = \sum_{n=0}^{N-1} (x[n] - A\cos(2\pi f_0 n + \phi))^2$$

  is minimized.
- The minimum of this function can be found although it is a nontrivial task (about 10 slides).
- We skip the derivation, but for details, see Kay *et al.* "Statistical Signal Processing: Estimation Theory," 1993.

Sinusoidal Parameter Estimation

- The MLE of frequency f_0 is obtained by maximizing the *periodogram* over f_0:

$$\hat{f}_0 = \arg\max_f \left| \sum_{n=0}^{N-1} x[n] \exp(-j2\pi f n) \right|$$

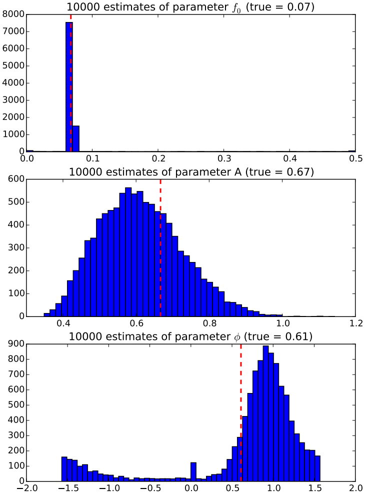
- Once $\hat{f}_0$ is available, proceed by calculating the other parameters:

$$\hat{A} = \frac{2}{N} \left| \sum_{n=0}^{N-1} x[n] \exp(-j2\pi \hat{f}_0 n) \right|$$

$$\hat{\phi} = \arctan\left(-\frac{\sum_{n=0}^{N-1} x[n] \sin 2\pi \hat{f}_0 n}{\sum_{n=0}^{N-1} x[n] \cos 2\pi \hat{f}_0 n} \right)$$

Sinusoidal Parameter Estimation—Experiments

- Four example runs of the estimation algorithm are illustrated in the figures.
- The algorithm was also tested for 10000 realizations of a sinusoid with fixed $\boldsymbol{\theta}$ and $N = 160$, $\sigma^2 = 1.2$.
- Note that the estimator is not unbiased.


10000 estimates of parameter f_0 (true = 0.07)

10000 estimates of parameter A (true = 0.67)

10000 estimates of parameter ϕ (true = 0.61)

Estimation Theory—Summary

- We have seen a brief overview of estimation theory with particular focus on Maximum Likelihood.
- If your problem is simple enough to be modeled by an equation, the estimation theory is the answer.
  - Estimating the frequency of a sinusoid is completely solved by classical theory.
  - Estimating the age of the person in picture can not possibly be modeled this simply and classical theory has no answer.
- **Model based** estimation is the best answer when a model exists.
- Machine learning can be understood as **a data driven approach**.