# Concepts of Experiments at Future Colliders II

PD Dr. Oliver Kortner

06.06.2025

# Examples of important probability distributions

# Recapitulation of the previous lecture

## The binomial distribution

- The binomial distribution gives the probability of observing $n_k$ events out of a total of $N$ events when $\nu_k$ events are expected:

$$p(n_k;\nu_k) = \binom{N}{n_k}\left(\frac{\nu_k}{N}\right)^{n_k}\left(1-\frac{\nu_k}{N}\right)^{N-\nu_k}.$$

- With $p := \frac{\nu_k}{N}$, one obtains from

$$\begin{aligned}
0 &= \frac{d}{dp}1 = \frac{d}{dp}\sum_{n_k=0}^{N}\binom{N}{n_k}p^{n_k}(1-p)^{N-n_k} \\
&= \sum_{n_k=0}^{N}\binom{N}{n_k}\left[n_k p^{n_k-1}(1-p)^{N-n_k} - (N-n_k)p^{n_k}(1-p)^{N-n_k-1}\right] \\
&= \frac{1}{p} < n_k > - \frac{1}{1-p} < N - n_k > = \left(\frac{1}{p}+\frac{1}{1-p}\right) < n_k > + \frac{N}{1-p} \\
&= \frac{1}{p(1-p)} < n_k > + \frac{N}{1-p} \Leftrightarrow < n_k > = N\cdot p = N\cdot\frac{\nu_k}{N} = \nu_k.
\end{aligned}$$

- Using the same calculation trick, one obtains $Var(n_k) = \nu_k(1-\frac{\nu_k}{N})$.

## Transition to the Poisson distribution

If $\nu \gtrsim 10$, $\nu \ll N$ u=and $N$ are large, one can approximate it by the Poission distribution. The approximation is a results of the Stirling formula:

$$n! \approx \left(\frac{n}{e}\right)^n \sqrt{2\pi n} \; für \; n \to \infty.$$

$$\begin{aligned}
p(n_k;\nu_k) &= \frac{N!}{n_k!(N-n_k)!} p^{n_k}(1-p)^{N-n_k} \\
&\approx \frac{1}{n_k!} p^{n_k} \left(\frac{N}{e}\right)^N \sqrt{2\pi N} \frac{1}{\left(\frac{N-n_k}{e}\right)^{N-n_k} \sqrt{2\pi(N-n_k)}} (1-p)^{N-n_k} \\
&= \frac{1}{n_k} p^{n_k} e^{-n_k} \underbrace{\sqrt{\frac{N}{N-n_k}}}_{\to 1 \;\; f. \;\; N \to \infty} \frac{N^N}{(N-n_k)^{N-n_k}} (1-p)^{N-n_k} \\
&\approx \frac{1}{n_k!} e^{-n_k} p^{n_k} N^{n_k} N^{N-n_k} (1-p)^{N-n_k} \frac{1}{(N-n_k)^{N-n_k}} \\
&= \frac{\nu_k}{n_k!} e^{-n_k} \frac{(N-\nu_k)^{N-n_k}}{(N-n_k)^{N-n_k}} \approx \frac{\nu_k^{n_k}}{n_k!} e^{-\nu_k} \; \text{(Poisson distribution)}.
\end{aligned}$$

## Properties of the Poisson distribution

### Poisson distribution

$$p(n_k;\nu_k) = \frac{\nu_k^{n_k}}{n_k!} e^{-\nu_k}.$$

### Normalization

$$\sum_{n_k=0}^{\infty} p(n_k;\nu_k) = e^{-\nu_k} \sum_{n_k=0}^{\infty} \frac{\nu_k^{n_k}}{n_k!} = e^{-\nu_k} \cdot e^{\nu_k} = 1.$$

Expectation value: $\nu_k$, resulting from $0 = \frac{d}{d\nu_k} \sum_{n_k=0}^{\infty} p(n_k;\nu_k)$.

Variance: $\nu_k$, resulting from $0 = \frac{d^2}{d\nu_k^2} \sum_{n_k=0}^{\infty} p(n_k;\nu_k)$.

# Recapitulation of the previous lecture

When $\nu_k$ becomes large, the probability of the occurrence of small values of $n_k$ is small. Then $n_k$ can be considered large, and for $n_k!$ in the Poisson distribution, Stirling's approximation can be used:

$$
\begin{aligned}
\frac{\nu_k^{n_k}}{n_k!}e^{-\nu_k} &\approx \frac{\nu_k^{n_k}}{n_k^{n_k}}\frac{1}{\sqrt{2\pi n_k}}e^{n_k-\nu_k} \\
&\approx \frac{1}{\sqrt{2\pi\nu_k}}\exp\left(\ln\frac{\nu_k^{n_k}}{n_k^{n_k}}\right)\exp(n_k-\nu_k) \\
&= \frac{1}{\sqrt{2\pi\nu_k}}\exp\left(n_k\ln\frac{\nu_k}{\nu_k+n_k-\nu_k}\right)\exp(n_k-\nu_k) \\
&= \frac{1}{\sqrt{2\pi\nu_k}}\exp\left(n_k\ln\frac{1}{1-\frac{n_k-\nu_k}{\nu_k}}\right)\exp(n_k-\nu_k) \\
&\approx \frac{1}{\sqrt{2\pi\nu_k}}\exp\underbrace{\left[n_k\cdot\left(-\frac{n_k-\nu_k}{\nu_k}-\frac{1}{2}\frac{(n_k-\nu_k)^2}{\nu_k^2}\right)\right]}_{\approx-(n_k-\nu_k)-\frac{(n_k-\nu_k)^2}{2\nu_k}}\exp(n_k-\nu_k) \\
&\approx \frac{1}{\sqrt{2\pi\nu_k}}e^{-\frac{(n_k-\nu_k)^2}{2\nu_k}}.
\end{aligned}
$$

## The normal distribution

### Normal distribution of a one-dimensional random variable $x \in \mathbb{R}$

$$p(x;\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}.$$

- $< x >= \mu$, $Var(x) = \sigma^2$.
- The Poisson distribution approaches a normal distribution in the limit $\nu_k \to \infty$ with the expected value $\nu_k$ and the variance $\nu_k$.

### Normal distribution of a $d$-dimensional random variable $x \in \mathbb{R}^d$

$$p(x;\mu,\Sigma) = \frac{1}{(2\pi)^{d/2}} \frac{1}{\det(\Sigma)} \exp\left(-\frac{1}{2}(x-\mu)^t \Sigma (x-\mu)\right).$$

$$\Sigma \in \mathbb{R}^{d \times d}, \quad \mu \in \mathbb{R}^d.$$

- $< x >= \mu$.
- $cov(x_k, x_l) = \Sigma_{k,l}$.

# Recapitulation of the previous lecture

Properties of the one-dimensional normal distribution

$w_n :=$ Probability of observing a value $x \in [\mu - n\sigma, \mu + n\sigma]$.

| $n$ | $w_n$ |
|---|---|
| 1 | 0.6827 |
| 2 | 0.9545 |
| 3 | 0.9973 |
| 4 | $1 - 6.3 \cdot 10^{-5}$ |
| 5 | $1 - 5.7 \cdot 10^{-7}$ |

| $w_n$ | $n$ |
|---|---|
| 0.900 | 1.645 |
| 0.950 | 1.960 |
| 0.990 | 2.576 |
| 0.999 | 3.290 |

Concept of stochastic convergence

$(t_n)$ is a sequence of random variables and $T$ is also a random variable. We say $t_n$ converges stochastically to $T$ if for every $p \in [0, 1[$ and $\epsilon > 0$, there exists an $N$ such that the probability $P$ that $|t_n - T| > \epsilon$ is less than $p$ for all $n > N$:

$$P(|t_n - T| > \epsilon) < p \ (n > N).$$

In other words: The probability of observing a value $t_n$ different from $T$ vanishes as $n \to \infty$.

# Recapitulation of the previous lecture

## Law of large numbers. Central limit theorem

### The law of large numbers

$(x_n)$ is a sequence of independent random variables, each following the same distribution function. $\mu$ denotes the expected value of $x_n$. Then the arithmetic mean

$$\frac{1}{N}\sum_{n=1}^{N} x_n$$

converges stochastically to $\mu$.

### The central limit theorem

$(x_n)$ is a sequence of identically distributed random variables with mean $\mu$ and standard deviation $\sigma$. Then as $N \to \infty$, the standardized random variable

$$Z_N := \frac{\sum\limits_{n=1}^{N} x_n - N\mu}{\sigma\sqrt{N}}$$

converges pointwise to a normal distribution with mean 0 and standard deviation 1.

## Point estimation

Let $\alpha$ be a parameter of a probability distribution. The goal of point estimation is to find the best estimate (the best measurement in the terminology of physicists) of $\alpha$.

$x$: Random variable corresponding to the experimental measurements.
$p(x;\alpha)$: Probability density for the measurement of $x$ as a function of the parameter $\alpha$.

$x$ and $\alpha$ can be multidimensional.

Definition. A point estimator $\mathcal{E}_\alpha$ is a function of $x$ used to estimate the value of the parameter $\alpha$. Let $\hat{\alpha}$ denote this estimate. Thus, $\hat{\alpha} = \mathcal{E}_\alpha(x)$.

Goal is to find a function $\mathcal{E}_\alpha$ such that $\hat{\alpha}$ is as close as possible to the true value of $\alpha$.

Since $\hat{\alpha}$ is a function of random variables, $\hat{\alpha}$ itself is a random variable.

$$p(\hat{\alpha}) = \int_D \mathcal{E}_\alpha(x) p(x;\alpha) dx,$$

where $\alpha$ denotes the true value of the parameter.

## Quality criteria for point estimators

### Consistency

$n$: Number of measurements used for the point estimation.

$\hat{\alpha}_n$: Corresponding estimate.

$\alpha_0$: True value of $\alpha$.

$\mathcal{E}_\alpha$ is called a consistent point estimator if $\hat{\alpha}_n$ converges stochastically to $\alpha_0$. This means that the probability of estimating a value different from $\alpha_0$ goes to 0 as $n \to \infty$.

### Unbiasedness

The bias of an estimate $\hat{\alpha}$ is defined as

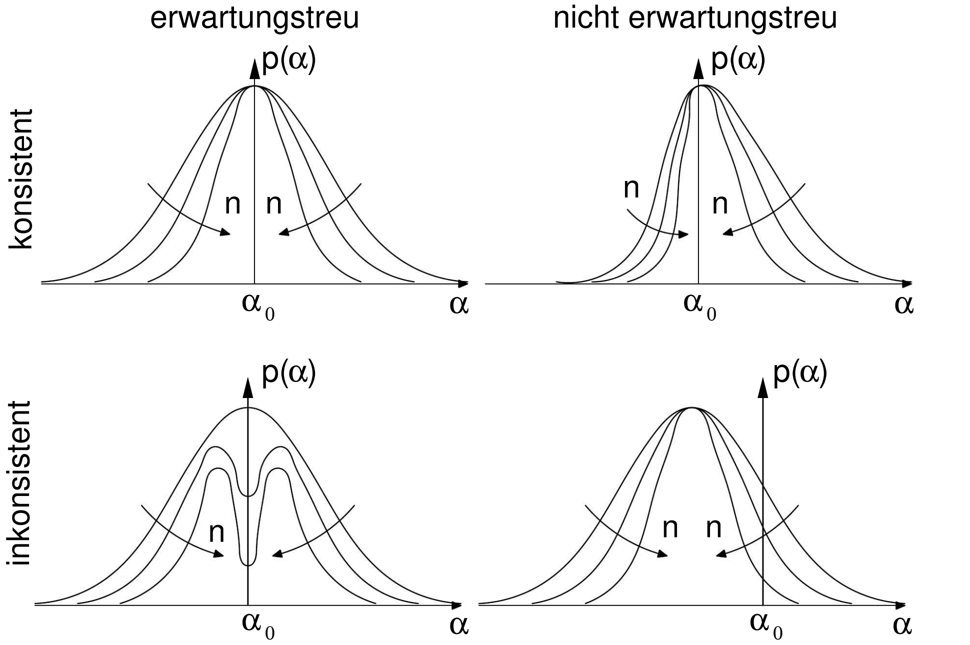
$$b_n(\hat{\alpha}) := E(\hat{\alpha}_n - \alpha_0) = E(\hat{\alpha}_n) - \alpha_0.$$

The point estimator is unbiased if

$$b_n(\hat{\alpha}) = 0, \text{ or } E(\hat{\alpha}_n) = \alpha_0$$

for all $n$.

## Illustration of Consistency and Unbiasedness



## Further quality criteria for point estimators

### Efficiency

Let $V_{min}$ be the minimum possible variance among all point estimators of a real-valued parameter. The efficiency of a particular point estimator is given by the ratio $\frac{V_{min}}{Var(\hat{\alpha})}$, where $Var(\hat{\alpha})$ is the variance of $\hat{\alpha}$ for that point estimator.

### Sufficiency

Any function of data $x$ is called a statistic. A sufficient statistic for $\alpha$ is a function of the data that contains all the information about $\alpha$.

# Point estimators used in high energy physics

## Maximum likelihood method

$p(x;\alpha)$: Probability of obtaining the measured values $x$ given a parameter $\alpha$.

- Substituting the measured values $x$ into the function $p(x;\alpha)$ yields a statistic of $x$, which is called the likelihood or the likelihood function $L(x;\alpha)$.
- The term likelihood is used to indicate the relationship with the probability density $p(x;\alpha)$ while making it clear that $L$ is not a probability function.

Let $f(x_k;\alpha)$ be the probability density for the outcome of a single measurement $x_k$. With $n$ independent measurements $x = (x_1, \ldots, x_n)$, we have

$$L(x_1, \ldots, x_n; \alpha) = \prod_{k=1}^{n} f(x_k; \alpha).$$

In the method of maximum likelihood, the estimate for $\alpha$ is taken as the value of $\alpha$ that maximizes $L(x;\alpha)$.

# Recapitulation of the previous lecture

## Asymptotic behavior of maximum likelihood

$n \to \infty$

- The point estimator is consistent.
- The point estimator is efficient.
- $\hat{\alpha}$ is normally distributed.
- Due to consistency, the point estimator is asymptotically unbiased.

## Finite $n$

To determine the behavior of the point estimator with limited data size $n$, experimental practice uses ensembles of randomly generated simulated data to which the point estimator is applied.

## Method of least squares

$n$ measurements $x_1, \ldots, x_n$.

$E(x_k; \alpha)$: Expectation value of $x_k$ given $\alpha$ (ttheoretical predictionffor the value of $x_k$).

$V = (cov(x_k, x_\ell))$: Covariance matrix. In general, $V$ is also a function of $\alpha$.

$$Q^2 := \sum_{k,\ell=1}^{n} [x_k - E(x_k; \alpha)]\, V_{k\ell}^{-1}(\alpha)\, [x_\ell - E(x_\ell; \alpha)]\,.$$

In the method of least squares, the estimate for $\alpha$ is chosen as the value for which $Q^2$ is minimized.

Remark. If $V_{k\ell}(\alpha)$ is unbounded, we may obtain nonsensical results for $\alpha$. For example, if $V_{k\ell}(\alpha) \to \infty$ as $\alpha \to \alpha_{\text{non-sense}}$ and $x_k - E(x_k; \alpha)$ remains bounded, the minimization yields $\alpha_{\text{non-sense}}$. In practice, $Q^2$ is often minimized iteratively. One starts with an estimate for $V$ and varies $V$ during the minimization of $Q^2$. Then, $V$ is recalculated for the obtained estimate of $\alpha$, and the minimization is repeated with $V$ fixed until $\hat{\alpha}$ no longer changes significantly.

Goal: Determination of an interval which contains the true value of a parameter with a given probability.

## Limit case of the normal distribution

Let us assume the variable $x \in \mathbb{R}$ is normally distributed, i.e.

$$p(x) = N(x; \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}}.$$

If $\mu$ and $\sigma$ are known, then

$$p(a < x < b) = \int_a^b N(x; \mu, \sigma) dx =: \beta.$$

If $\mu$ is unknown, one can calculate $p(\mu + c < x < \mu + d)$:

$$\begin{aligned} \beta = p(\mu + c < x < \mu + d) &= \int_{\mu+c}^{\mu+d} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}} dx = \int_c^d \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\frac{y^2}{\sigma^2}} dy \\ &= p(c - x < -\mu < d - x) = p(x - d < \mu < x - c). \end{aligned}$$

# Interval estimation with the normal distribution

$$\beta = p(\mu + c < x < \mu + d) = \int_{\mu+c}^{\mu+d} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}} dx = \int_{c}^{d} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\frac{y^2}{\sigma^2}} dy$$
$$= p(c - x < -\mu < d - x) = p(x - d < \mu < x - c).$$

That is, if $x$ has been measured, the probability that the desired value of $\mu$ lies between $x - d$ and $x - c$ is equal to $\beta$.

- If $x$ is a parameter $\hat{\alpha}$ from a point estimation conducted using the method of maximum likelihood or the method of least squares, then $\hat{\alpha}$ is asymptotically normally distributed, and the above formulas can be applied for interval estimation.
- The intervals $[a, b]$ or $[x - d, x - c]$ are called confidence intervals. $\beta$ is the confidence level corresponding to the confidence level.

# Generalization to the multidimensional case

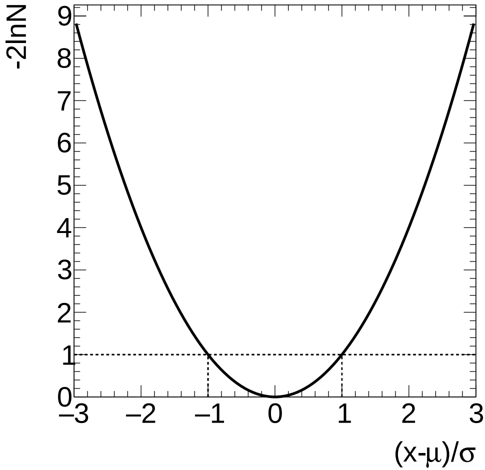
$$Q(x;\mu,\Sigma) := (x-\mu)^t\Sigma^{-1}(x-\mu),\;\; x,\mu \in |\mathsf{R}.$$
$$p(Q) = \frac{1}{(2\pi)^{d/2}} \cdot \frac{1}{\sqrt{det(\Sigma)}} \exp\left(-\frac{1}{2}Q(x;\mu,\Sigma)\right).$$

In multiple dimensions, the confidence interval becomes a confidence region corresponding to the confidence level $\beta$:

$$p(Q(x;\mu,\Sigma) < K_\beta^2) = \beta.$$

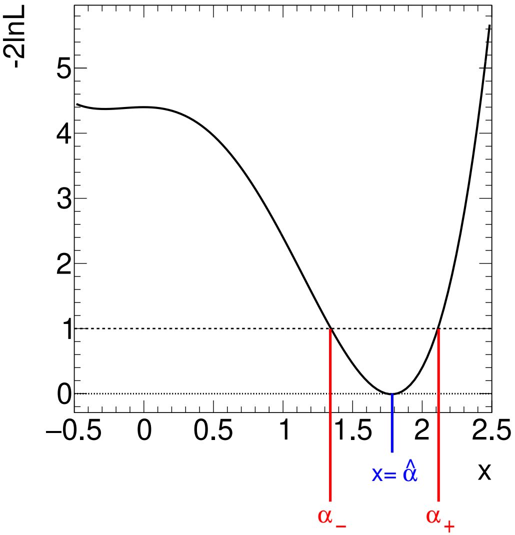
# Likelihood-based confidence intervals

$$-2\ln N(x=\mu\pm\sigma;\mu,\sigma)-[-2\ln N(x=\mu;\mu,\sigma]=1.$$



# Likelihood-Based Confidence Intervals

Generalization




Confidence Interval: $[\alpha_-, \alpha+]$.

# Hypothesis testing

Goal, to determine which hypothesis (for a probability distribution) describes the recorded data point distributions (data).

Nomenclature. $H_0$: null hypothesis.
$H_1$: alternative hypothesis.

Simple and Composite Hypotheses

- When the hypotheses $H_0$ and $H_1$ are given completely without free parameters, the hypotheses are called simple hypotheses.
- If a hypothesis contains at least one free parameter, it is referred to as a composite hypothesis.

Procedure

For hypothesis testing, $W$ must be chosen such that

$$p(\text{data} \in W|H_0) = \alpha$$

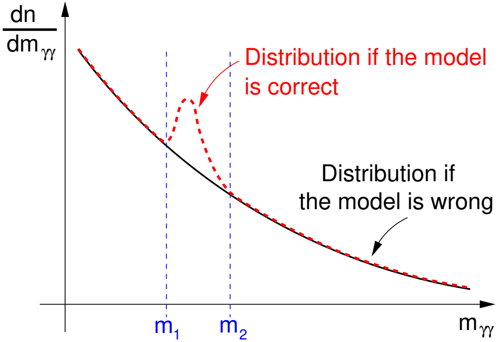
with a small value of $\alpha$ and simultaneously

$$p(\text{data} \in D\backslash W|H_1) = \beta$$

with the smallest possible $\beta$.

# Introductory example of hypothesis testing

A theoretical model predicts the existence of a particle with mass $M$, the production cross-section, and the partial width for decay into a photon pair. To confirm or refute this model, one must examine the distribution of $m_{\gamma\gamma}$.



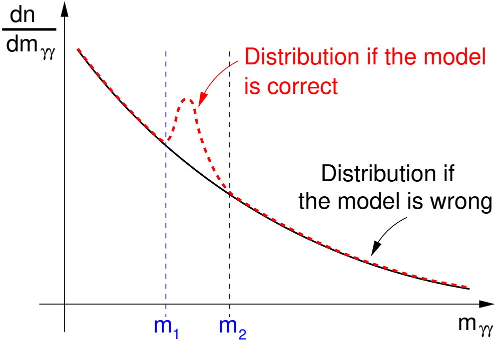

In the interval $[m_1, m_2]$, one is sensitive to the model's prediction. There are two hypotheses, namely that the theory is correct or incorrect.

$H_0$: Null hypothesis: TTheory is incorrect.“

$H_1$: Alternative hypothesis: TTheory is correct.“

With a sufficiently large amount of data, the probability that the measured $m_{\gamma\gamma}$ distribution looks like $H_0$ is small if the theory is correct. At the same time, the probability that the measured mass distribution looks like $H_1$ is large.

# Introductory example of hypothesis testing




$n$: Number of events measured in the interval $[m_1, m_2]$.
One must now choose a threshold value $N$ such that

$$p(n > N|H_0) = \alpha$$

with a small value of $\alpha$ and

$$p(n \leq N|H_1) = \beta$$

is as small as possible if the theory, i.e., $H_1$, is correct.

$n$: Number of events measured in the interval $[m_1, m_2]$.
One must now choose a threshold value $N$ such that

$$p(n > N|H_0) = \alpha$$

with a small value of $\alpha$ and

$$p(n \leq N|H_1) = \beta$$

is as small as possible if the theory, i.e., $H_1$, is correct.

## Experimental Practice

- $\alpha = 5.7 \cdot 10^{-7}$, which corresponds to 5$\sigma$ of a normal distribution, to claim the discovery of a particle.
- With a value of $\alpha = 0.3\%$, which corresponds to 3$\sigma$ of a normal distribution, one says there is evidence for the existence of a new particle.

# Type I and type II errors

The confidence level $\alpha$ is defined as the probability that $x \in W$ if the null hypothesis $H_0$ is correct:

$$p(x \in W | H_0) = \alpha.$$

The probability $\beta$ represents the likelihood of incorrectly rejecting the alternative hypothesis $H_1$:

$$p(x \in D \backslash W | H_1) = \beta.$$

| Approach | $H_0$ correct | $H_1$ correct |
|---|---|---|
| $x \notin W \Rightarrow H_0$ is considered correct | Good acceptance, since $p(x \in D \backslash W \| H_0) = 1 - \alpha$ is large | Contamination<br>Type II error<br>$p(x \in D \backslash W \| H_1) = \beta$. |
| $x \in W \Rightarrow H_0$ is rejected, $H_1$ is considered correct | Wrong decision<br>Type I error<br>$p(x \in W \| H_0) = \alpha$ is small | Rejecting $H_0$ good, since $p(x \in W \| H_1) = 1 - \beta$ is large. |