In [2]:
```
# header: settings ↔
```

2. Useful concepts from Statistics

Important basic Datamining question: **Discrimination between *pattern* and *randomness***

- When can we call a discovered regularity statistically significant?
- How does a variable x depend from another variable y?
- Under what conditions can we state that there is a significant deviation from a norm?
  - (norm here means an average pattern or background pattern)

General Procedure

1. compute a statistic (an estimator) s, (in German: Prüfgröße)
2. derive (or compute) how s is distributed (as probability density distribution) under the assumption that a null hypothesis H_0 holds.

   - this may require definition (later: test for) assumptions on the sample pdf
3. compute then, what value $\hat{s}$ of s you obtain for the actual data set(s).
4. if $\hat{s}$ falls into an unlikely area: conclude, that H_0 can be rejected
5. if not, do **not** conclude that H_0 is valid, or is proven!

→ Statistics can never prove a null hypothesis, only reject it.

The result is often reported as p-value:

- $(p < 0.05)$ means, that the probability to find a value $\hat{s}$ like that or more extreme is smaller than 5%.

2.1 Detection of systematic deviations

Basic question: to judge whether two probability densities P_A, P_B are equal or different (at hand of limited samples)

- First we approach the 'weaker' question: are the means equal?
- Given: two 'unpaired' samples $\{x_i^A\},\ \{x_i^B\}$ of size N_A and N_B, drawn from unknown probability densities P_A and P_B.
  - note that unpaired means that the features x^A and x^B are not measurements from the same objects (e.g. the same test person), but totally independent measurements.

Empirical Means:

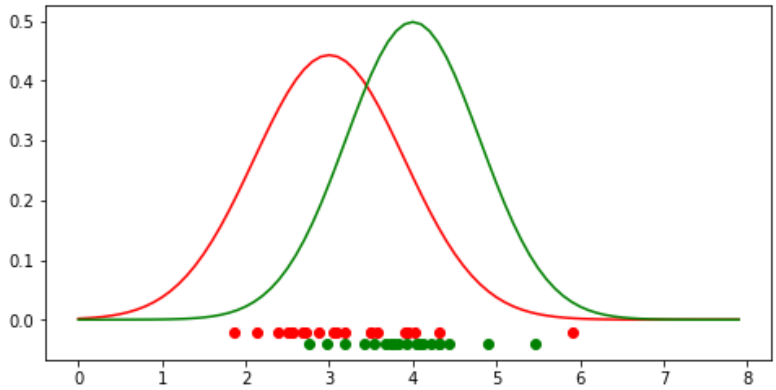
$$\hat{\mu}_A = \frac{1}{N_A}\sum_{i=1}^{N_A} x_i^A$$

$$\hat{\mu}_B = \frac{1}{N_B}\sum_{i=1}^{N_B} x_i^B$$

for the estimation of the actual mean values $\mu_A,\ \mu_B$ of $P_A,\ P_B$

- Null hypothesis: $\mu_A = \mu_B\ \ (H_0)$
  - these are the true means, not the sample means!
- We search a statistics (a data-derived feature) which varies systematically according to the likelihood that the null hypothesis holds.

In [17]:
```
# figure to illustrate 2 samples with underlying pdfs↔
```



Intuitive Selection for 'the statistics': Difference of the sample means

$$|\hat{\mu}_A - \hat{\mu}_B|$$

but then the value depends strongly on the width (i.e. the $\sqrt{\text{variance}}$) of the underlying distribution $P_{A/B}(x)$.

For that reason, a normalization is done:

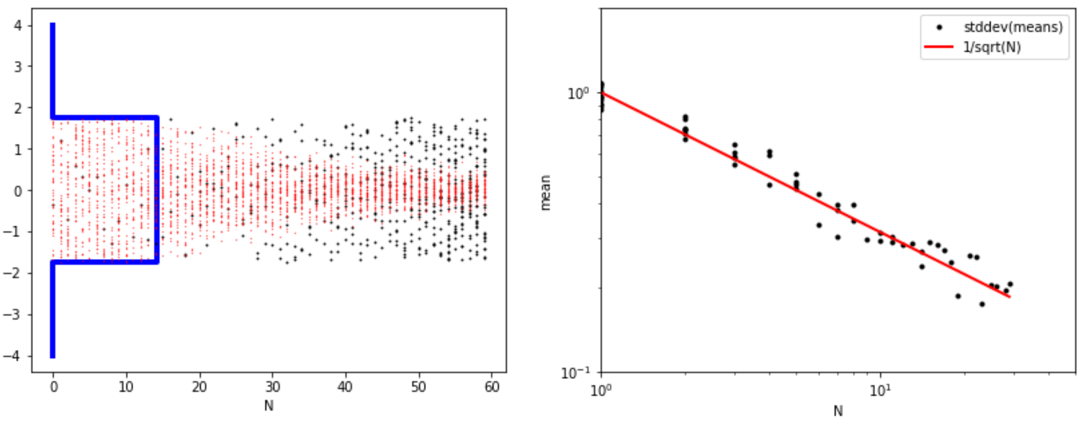
$$t = \frac{|\hat{\mu}_A - \hat{\mu}_B|}{\hat{\sigma}_{err}}$$

with

$$\hat{\sigma}_{err} = \sqrt{\left(\frac{1}{N_A} + \frac{1}{N_B}\right) \frac{\sum_{i=1}^{N_A}(x_i^A - \hat{\mu}_A)^2 + \sum_{i=1}^{N_B}(x_i^B - \hat{\mu}_B)^2}{N_A + N_B - 2}}$$

- note that the standard error is not the standard deviation but the standard deviation / $\sqrt{N}$. The reason is that the standard deviation of estimated means of a sample of size N scales with $1/\sqrt{N}$.

In [79]:
```
## quick test for that:↔
```



Explanation for the denominator

- If H_0 holds, $\mu_A - \mu_B = 0$ which we abbreviate as $\rightarrow \mu_{AB} = 0$
- Question: what is the variance of μ_{AB}?
- $\rightarrow$ the more samples we have, the better the empirical mean $\hat{\mu}_x$ approximates the real mean μ_x.

$$\sigma^2(\hat{\mu}_A) = \frac{\sigma^2(P_A)}{N_A}, \text{ (the same for B)}$$

$$\Rightarrow \sigma(\hat{\mu}_A) = \frac{\sigma(P_A)}{\sqrt{N_A}}$$

- Wanted: the variance of a linear combination
$$\sigma^2(\alpha x_1 + \beta x_2) = \alpha^2 \sigma^2(x_1) + \beta^2 \sigma^2(x_2)$$
- in our case with $\alpha = 1, \beta = -1$.

Since $\beta^2 = (-1)^2 = 1$ we can see:

$$\sigma^2(\hat{\mu}_A - \hat{\mu}_B) = \sigma^2(\hat{\mu}_A) + \sigma^2(\hat{\mu}_B)$$

- Inserting from above we find

$$\sigma^2(\hat{\mu}_A - \hat{\mu}_B) = \frac{\sigma^2(P_A)}{N_A} + \frac{\sigma^2(P_B)}{N_B}$$

Now we assume that $\sigma^2(P_A) = \sigma^2(P_B) = \sigma^2_{AB}$

$$\Rightarrow \sigma^2(\hat{\mu}_A - \hat{\mu}_B) = \sigma^2_{AB}\left(\frac{1}{N_A} + \frac{1}{N_B}\right)$$

- The standard deviation is $\sqrt{\sigma^2}$

$$\rightarrow \sigma(\hat{\mu}_A - \hat{\mu}_B) = \sqrt{\sigma^2_{AB}\left(\frac{1}{N_A} + \frac{1}{N_B}\right)}$$

- Last step: estimating the variance of σ^2_{AB} from the data

$$\sigma^2_{AB} = \frac{\sum_{i=1}^{N_A}(x_i^A - \hat{\mu}_A)^2 + \sum_{i=1}^{N_B}(x_i^B - \hat{\mu}_B)^2}{N_A + N_B - 2}$$

- The denominator has the sum of item minus 2, since both empirical means $\hat{\mu}_A$ and $\hat{\mu}_B$ are already estimated from the data.

- Next step: compute the distribution function for the statistics t under the null hypothesis
  - = probability density $p(t)$ that this value of t is observed under valid H_0
- Assumption: $\sigma(P_A) = \sigma(P_B)$
  - we actually need first to verify this, for which the F-test is used (details: see NR in C, [http://www2.units.it/ipl/students_area/imm2/files/Numerical_Recipes.pdf (http://www2.units.it/ipl/students_area/imm2/files/Numerical_Recipes.pdf)](http://www2.units.it/ipl/students_area/imm2/files/Numerical_Recipes.pdf))

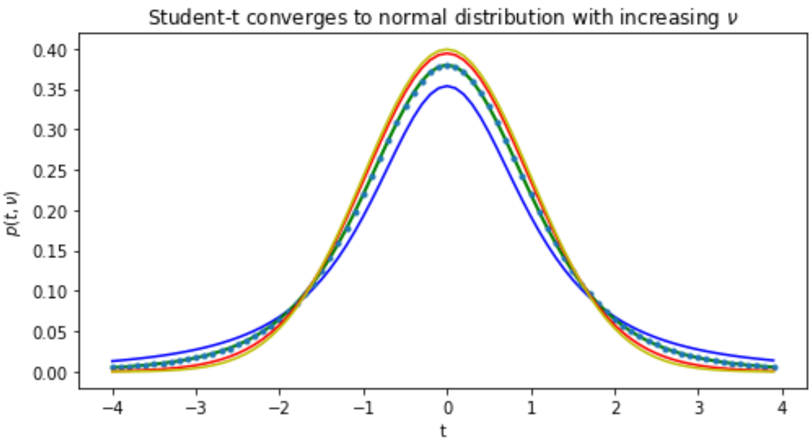
Result:

- If H_0 is true, t is distributed according to a so-called student-t-distribution with $\nu = N_A + N_B - 2$ degrees of freedoms
  - more about the t-distribution in Sec. 2.2.2
- The density function is

$$P(t, \nu) = \mathcal{N}_\nu \left(1 + \frac{t^2}{\nu}\right)^{-(\nu+1)/2}$$

- $\mathcal{N}_\nu$ is chosen so that $\int_{-\infty}^{\infty} P(t', \nu)dt' = 1$.

In [76]:
```
# plot t-distribution ↔
```

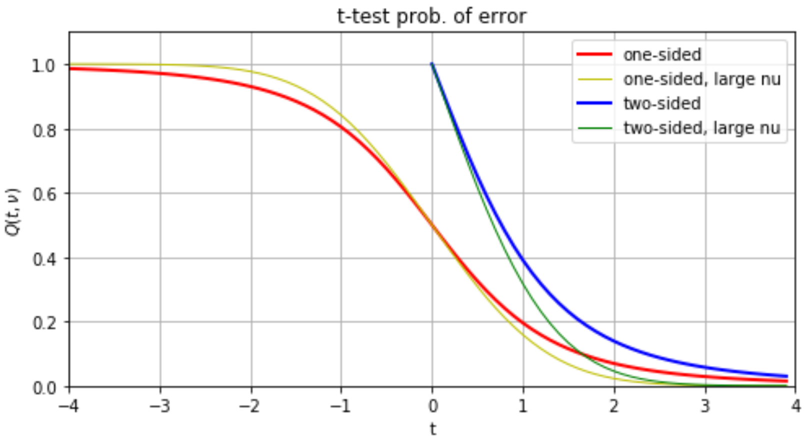


- **Wanted**: critical t_c, so that if $\hat{t}$ is equal to t_c or more extreme, H_0 can be rejected.
- Depends upon the wished significance level, e.g. 5%, 1% or 0.1%.
- In the one-sided test, we assume that $\mu_A > \mu_B$ (so positive t)
  - The area below the student-t density function from t_c to ∞ is the probability that a value $t > t_c$ occurs randomly.
- two-sided test: $|\mu_A - \mu_B| \neq 0$
  - $\Rightarrow$ area below the t-pdf from $[-\infty, -t_c]$ plus from $[t_c, \infty]$ wanted.
- We compute the cumulative density function (integral) $A(t, \nu)$

$$A(t, \nu) = \int_{-\infty}^{t} P(t', \nu)dt'$$

- $A(t, \nu)$ is a sigmoidal monotonously growing function with asymptodes 0 and 1, and $A(0) = 0.5$. So we take 2 steps:
- Step 1: select the level of significance α
  - also called *probability of error*
- Step 2: determine t_c at hand of $1 - A(t_c, \nu) = \alpha$
  - note that for the two-sided test the left side becomes $2 - 2A(t, \nu)$

In [81]:
```
# plot 1-A as function of t for nu dofs↔
```



- the above figure depicts the probability $P(\hat{t} \geq t_c)$ that the empirical value $\hat{t}$ is t_c or greater, blue for the two-sided, red for the one-sided t-test
  - yellow resp. green plots are for large nu (converges to normal pdf)
- if $\hat{t} \geq t_c$: reject H_0
  - ... it is just unlikely that such a large value of t occurs under H_0
- but if $\hat{t} < t_c$:→ no statement about H_0 can be made.

Remarks:

- valid only under the assumption of equal variances $\sigma^2(P_A) = \sigma^2(P_B)$
  - if not the case, a different test is needed (the Welch's t-test)
- Note that the two-sided level of significance is exactly doubled compared to the one-sided test. The reason is that

$$P = \int_{-\infty}^{-t} P(t', \nu)dt' + \int_{t}^{+\infty} P(t', \nu)dt' = 2\int_{t}^{\infty} P(t', \nu)dt'$$

- Usually the critical values t_c are looked up in tables:

ν	$t_{0.01}$	$t_{0.001}$
10	2.76	4.14
60	2.39	3.23
∞	2.33	3.09

In [58]:
```
# compute values with inverse survival function isf↔
```

```
nu\alpha [0.05, 0.01, 0.005, 0.001, 0.0001]
-------------------------------------------
10       1.81     2.76     3.17     4.14     5.69
20       1.72     2.53     2.85     3.55     4.54
50       1.68     2.40     2.68     3.26     4.01
99       1.66     2.36     2.63     3.17     3.86
999      1.65     2.33     2.58     3.10     3.73
```

2.2. Excursion: χ^2- und Student-t-distribution

2.2.1 χ^2-distribution

Let $X_1, X_2, \ldots, X_n$ be pairwise independent normal distributed random variables with variance $\sigma_i^2 = 1$ and mean $\mu_i = 0$.

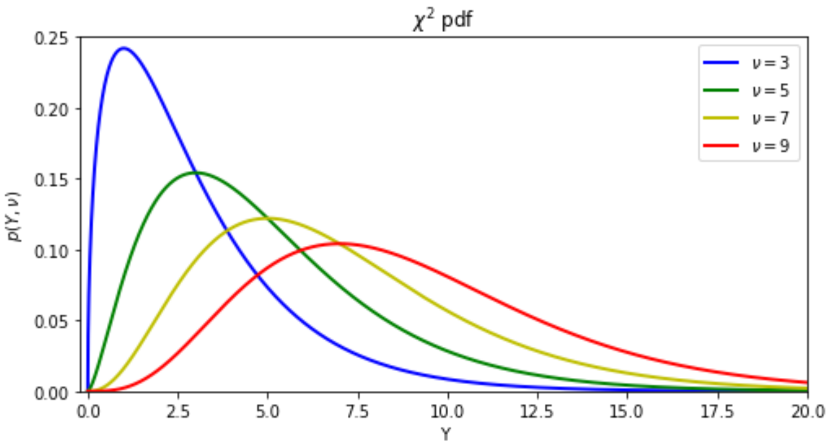
Then the sum Y of their squares

$$Y = \sum_{i=1}^{N} X_i^2$$

is χ^2-distributed with $\nu = N$ degrees of freedom.

Properties: $\langle Y \rangle = N, \quad \sigma^2(Y) = 2N$

In [61]:
```
y = np.arange(0, 20, 0.01)
for (nu, co)  in [[3, 'b'], [5, 'g'], [7, 'y'], [9,'r']]:↔
plt.xlabel(r'Y'); plt.ylabel(r'$p(Y, \nu)$'); plt.title(r'$\chi^2$ pdf');
plt.legend(); plt.axis([-0.20,20,0,0.25]);
```



- The above figure shows that
  - mean and variance grow with ν
  - small values become increasingly unlikely with large ν

[ws1819EOT2.1017]

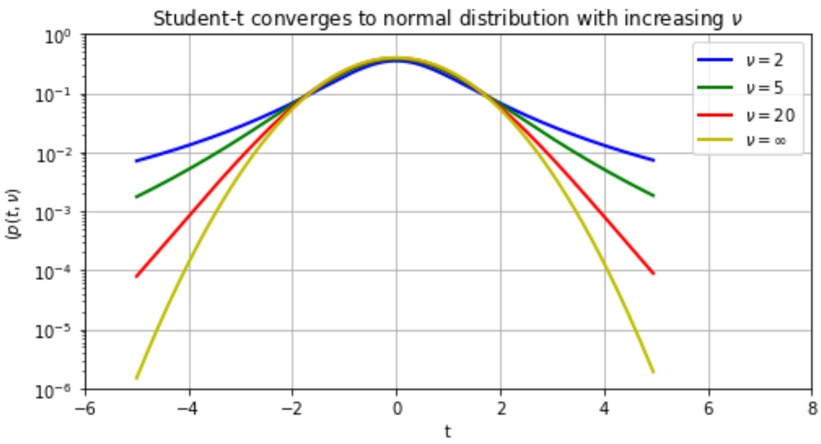
2.2.2. Student-t-distribution

Let X be normal distributed with mean 0 and variance 1, and Y an independent χ^2-distributed random variable with ν degrees of freedom. Then

$$t = \frac{X}{\sqrt{Y/\nu}}$$

is defined as Student-t-distributed with ν degrees of freedom

In [62]:
```
t = np.arange(-5, 5, 0.05)
plt.plot(t, sp.stats.t.pdf(t, 2), "b-",lw=2,label=r'$\nu=2$')
plt.plot(t, sp.stats.t.pdf(t, 5), "g-",lw=2,label=r'$\nu=5$')
plt.plot(t, sp.stats.t.pdf(t, 20),"r-",lw=2,label=r'$\nu=20$')
plt.plot(t, sp.stats.norm.pdf(t), "y-",lw=2,label=r'$\nu=\infty$')
plt.xlabel(r't'); plt.ylabel(r'$ (p(t, \nu)$')
plt.title(r'Student-t converges to normal distribution with increasing $\nu$')
plt.semilogy(); plt.legend(); plt.axis([-6,8, 1e-6, 1]); plt.grid();
```



Properties:

- For $\nu \gg 1$, the student-t resembles a normal distribution, however, the decay is only polynomial in the tails ($o(t^{-(2\nu+1)})$).

$$\langle T_\nu \rangle = 0, \quad \sigma^2(T_\nu) = \frac{\nu}{\nu - 2}, \quad \lim_{\nu\to\infty} T_\nu = \text{normal pdf}$$

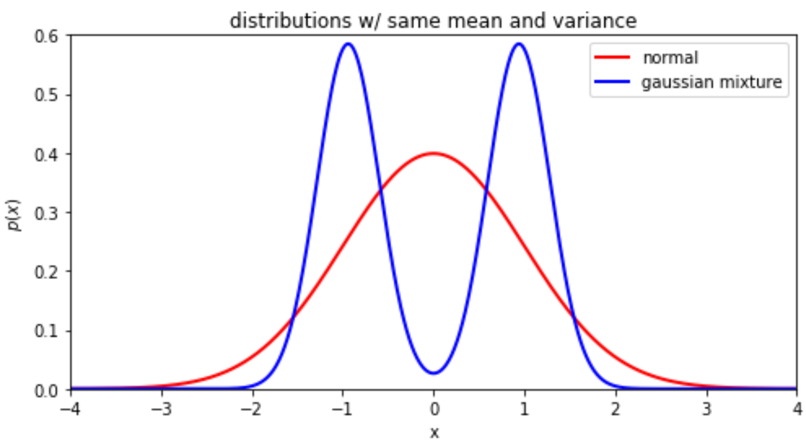
2.3. Tests to discriminate distributions

Motivation:

- t-test/F-test merely look on mean resp. variance of a distribution, which are only very coarse features of a detailed distribution.
- The following example depicts two distributions of equal mean and equal variance:

In [3]:
```
# plot↔
```

```
normal: mean = -0.00000, variance = 0.999985
2-gaus: mean =  0.00000, variance = 0.999949
```



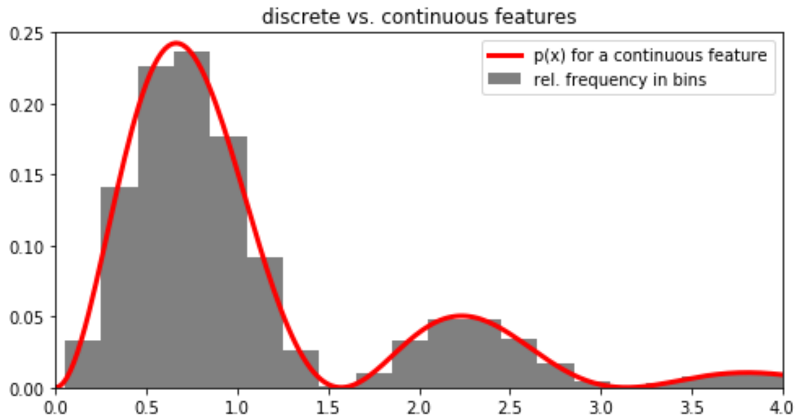
Wanted: methods that allow to uncover differences between such distributions.

- **Null hypothesis** H_0: Two data sets are samples from an identical probability distribution
  - here, again, it is only possible to reject H_0
  - no sample size, however large, will suffice to uncover a real existent yet very small difference (e.g. think of 10^{-10}...)

Test on distributions has two aspects:

- **A1. Variable type: Continuous vs. Discrete**
  - continuous features lead to density functions
  - discrete features lead to frequency distributions (histograms), where A_i is the number of instances in bin i
  - continuous features can always be reduced to discrete features by quantization. This, however, destroys information.

In [4]:
```
# histogram figure↔
```



A2. Comparison target: against data vs. against reference

We wish to compare the underlying (unknown) distribution of the observed data with

1. a given distribution (expectation, norm, reference)
   - Are all stars at the sky uniformly distributed?
2. the distribution of another dataset (e.g. data under a different condition)
   - Is the grade distribution in biology the same as in law?

Methods:

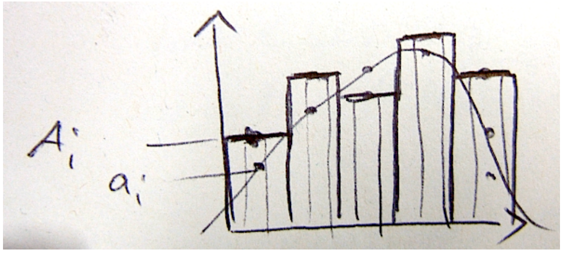
- for discrete distributions: → χ^2 **test**
- for continuous distributions: → **Kolmogorov-Smirnov test**
- There are two variants according to A2

2.3.1. χ^2-test

- We start with A2 case 1 (i.e. discrete binning)

Given:

- Dataset as discrete distribution with $i = 1, \dots, M$ bins
- $A_i \hat{=}$ number of events in bin i
- a_i is the expected number <contiuous, coming from model/hypothesis>

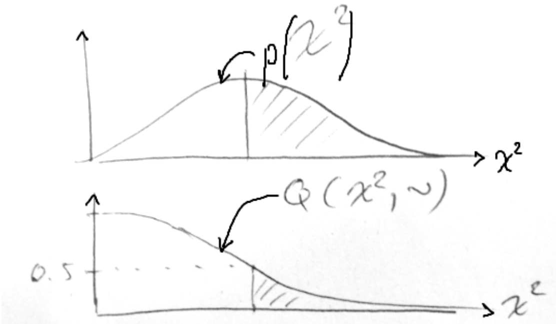


Case 1: Comparison of the a dataset with a given distribution

Statistics:

$$\chi^2 = \sum_{i=1}^{M} \frac{(A_i - a_i)^2}{a_i}$$

- Note that the denominator is the variance of the numerator
- You can regard the measurement as 'throwing a dart arrow on the wall of bins':
  - bin i will be realized with probability
    $$p = \frac{a_i}{\sum a_i}$$
  - Then the expected number (in n trials) is $\mu = np = a_i$.
  - The variance is in such Bernoulli-experiments
    $$\sigma^2 = npq = np(1-p)$$
  - approximately this is $np = a_i$. This motivates the denominator.
- For large $\chi^2 \Rightarrow$ large deviations between the distributions
- Ignore all terms with $a_i = 0$ (division by zero problem)
- From Pearson we know: for large M, the denominator will be normal distributed.
- If H_0 holds, $\rightarrow \quad a_i - A_i = \epsilon_i$, so errors are normal distributed.
- thus (according to the definition) the sum is χ^2-distributed with M degrees of freedom, independent from the distributions in the bins.
- Distribution of the statistics χ^2 with pdf $p(x)$ under the assumption that H_0 holds is the integral of the χ^2-density from χ^2 to ∞.
  $$\int_0^{\chi^2} p(\chi^2) d(\chi^2) = P(\chi^2) = 1 - Q(\chi^2)$$
- probability that an observed value $\hat{\chi}^2$ is larger ($\hat{\chi}^2 > \chi_c^2$) just by accident is $Q(\chi_c^2, \nu)$.



$$Q(\chi^2, \nu) = \frac{1}{\Gamma(\frac{\nu}{2})} \int_{\chi^2}^{\infty} e^{-t} t^{\frac{\nu}{2}-1} dt$$

In [5]:
```
# significance level figure↔
```

A Jupyter widget could not be displayed because the widget state could not be found. This could happen if the kernel storing the widget is no longer available, or if the widget state was not saved in the notebook. You may be able to create the widget by running the appropriate cells.

Remark:

- $\Gamma(x+1) = x!$, if $x \in N$
- degrees of freedom ν:
  - $\nu = M$ if the a_is were not normalized
  - $\nu = M - 1$ if $\sum a_i = \sum A_i$ was used for normalization.
  - Each boundary condition eliminates one degree of freedom.

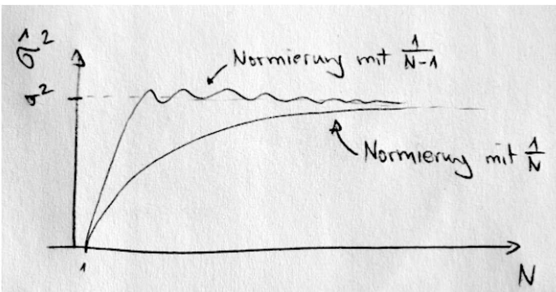
Case 2: Comparison of two datasets

- New statistics:
$$\chi^2 = \sum_{i=1}^{M} \frac{(A_i - B_i)^2}{A_i + B_i}$$
- Variance:
$$\sigma^2(A_i - B_i) = \sigma^2(A_i) + \sigma^2(B_i) \approx A_i + B_i$$
under the assumption of large sample size and small probability of the bins
  - The variance of the difference is the added variances of the summands!
- The terms of the sum are again approximately normal distributed with mean 0 and variance 1.
- Therefore the statistic χ^2 is again approximately χ^2-distributed.
- The degrees of freedom are, as above: $\nu = M$ minus the number of boundary conditions.

Remark concerning the degrees of freedom:

Example: draw a sample $\{v_1, \ldots, v_N\}$ from a random variable and compute the empiric mean
$$\hat{\mu}_v = \frac{1}{N} \sum_{i=1}^{N} v_i$$

- Estimating the variance by
$$\sigma^2(v) = \frac{1}{N} \sum_{i=1}^{N} (v_i - \hat{\mu}_v)^2$$
will underestimate the true variance.
- The cause is that $\hat{\mu}_v$ is not the true mean, but a value that is computed from the sample itself.
  - **it thus lies also closer to the concrete data**
- to improve the estimate, particularly for small N, we can change the factor 1/N to 1/(N-1)
$$\hat{\sigma}^2(v) = \frac{1}{N-1} \sum (v_i - \hat{\mu}_v)^2$$
- Mathematical Analysis shows: on average, the $N - 1$ norm is optimal. The estimator is said to be unbiased.



2.3.2 Kolmogorov-Smirnov Test

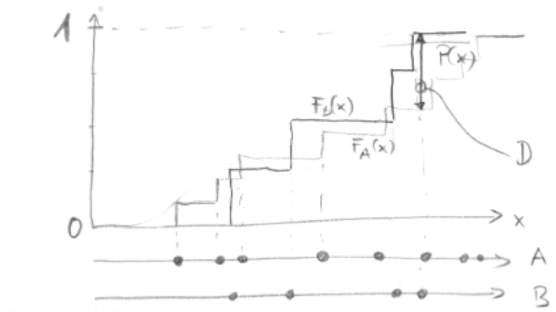
Given:

- two samples
$$\{x_i^A\}_{i=1,\dots,N_A}, \{x_i^B\}_{i=1,\dots,N_B}$$
- optionally: Comparison with a hypothetical distribution
$$P(x) = \int_{-\infty}^{x} p(x')dx'$$

Goal:

- to check, whether the distributions differ significantly
- Calculation of the empiric cumulative distribution

$$F_A(x) = \frac{1}{N_A}\sum_i \Theta(x - x_i^A) \text{ with } \Theta(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{else} \end{cases}$$



2. Computation of the statistics
$$D = \max_x |F_A(x) - F_B(x)|$$
3. respective: $D = \max_x |F_A(x) - P(x)|$ in case of the comparison agains a reference distribution

[ws1819EOT3.1024]

Announcement:

- aus raumorganisatorischen Gründen musste folgender Veranstaltung ein neuer Raum zugeteilt werden:
- VA 392123 | wöchentlich Mi 12:00-14:00 Uhr 23.01.2019-30.01.2019: Introduction to Data mining
- Der neue Raum ist H1.

Alternative Statistic:

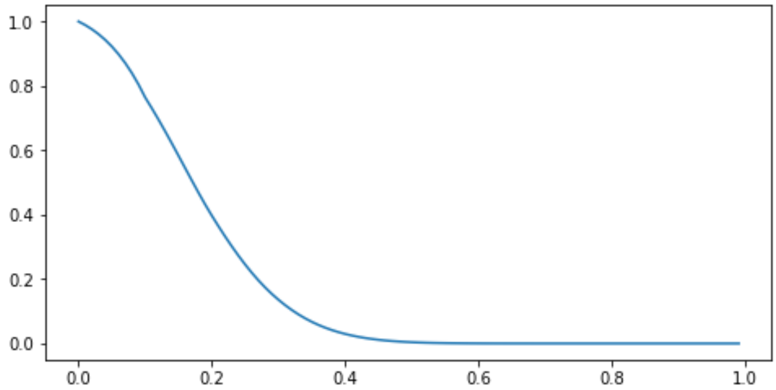
- Difference area between the distribution functions
  - yet this is not invariant on scaling or warping of the variables
- Derive the distribution of D under the assumption that H_0 is true

$$P(D \geq \hat{D}) \cong Q_{KS}\left(\sqrt{\frac{N_A N_B}{N_A + N_B}}\hat{D}\right)$$
$$\text{where } Q_{KS}(\lambda) = 2\sum_{j=1}^{\infty}(-1)^{j-1}e^{-2j^2\lambda^2}$$

In [25]:
```
sp.stats.ks_2samp(np.random.randn(200), np.random.randn(200)+0.5) # D_KS and p v
```

Out[25]:
```
Ks_2sampResult(statistic=0.28500000000000003, pvalue=1.1477873287896804e-07)
```

In [24]:
```
t = np.arange(0, 1, 0.01); plt.plot(t, 1-sp.stats.ksone(10).cdf(t));
```



- The approximation is already good, if the root is larger than 4
- again: H_0 can only be rejected, never be proven
- practical solution: table for $D_{crit}(\alpha)$ for level of significance α
- Advantage against χ^2-test:
  - no need for condensing data into histograms
  - no artificial quantization (which destroys information)