approximate_cdf_with_hist

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1 Approximate_cdf_with_hist

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1.1 Introduction

This notebook approximates $\mathbb{P}(\lambda \leq \lambda_0|\theta) = \mathbb{E}(Z_0|\theta)$ by histogramming, where the indicator $Z_0 = \mathbb{I}[\lambda \leq \lambda_0]$ and $\lambda_0 = \lambda(D; \theta)$ is the observed value of a test statistic λ evaluated at the observed data D for a given parameter hypothesis θ. We use the following algorithm, where $\theta = (a, b)$ are two `Pythia8` tune parameters.

1. Create histogram $h_w \leftarrow \text{histogram}(a, b, \text{weight} = Z_0)$
2. Create histogram $h_u \leftarrow \text{histogram}(a, b, \text{weight} = 1)$
3. Approximate $\mathbb{P}(\lambda \leq \lambda_0|a, b)$ by $h_w \,/\, h_u$

A confidence set at confidence level (CL) $\tau = 1 - \alpha$, where α is the size of the test of the associated hypothesis about θ, is (by construction) the set of points (a, b) that satisfy the condition $\mathbb{P}(\lambda \leq \lambda_0|a, b) \leq \tau$.

[1]:
```python
import os, sys, re
import numpy as np
import pandas as pd
import matplotlib as mp
import matplotlib.pyplot as plt
import importlib

from glob import glob
from tqdm import tqdm
from yoda2numpy import Yoda2Numpy
```

[2]:
```python
# update fonts
FONTSIZE = 14
font = {'family' : 'serif',
        'weight' : 'normal',
        'size'   : FONTSIZE}
mp.rc('font', **font)

# set usetex = False if LaTex is not
# available on your system or if the
```

```
# rendering is too slow
mp.rc('text', usetex=True)
```

1.1.1 Get sim and new histograms as pandas dataframes

[3]:
```
yoda2numpy = Yoda2Numpy()

files = glob('rivet_histograms/newseeds/*.yoda')
M = len(files)

# --- SIM
print(f'looping over {M:d} sim yoda files...\n')
dfsims = []
for ii in tqdm(range(M)):
    dfsims.append( yoda2numpy.todf( yoda2numpy('sim', index=ii) ) )

# --- NEW
print(f'looping over {M:d} new yoda files...\n')
dfnews = []
for ii in tqdm(range(M)):
    dfnews.append( yoda2numpy.todf( yoda2numpy('new', index=ii) ) )

print()
key = '/ALEPH_1996_S3486095/d01-x01-y01'
dfsim = dfsims[0][key]
dfsim
```

```
looping over 1000 sim yoda files…

100%|                    | 1000/1000 [00:14<00:00, 67.69it/s]

looping over 1000 new yoda files…

100%|                    | 1000/1000 [00:15<00:00, 66.33it/s]
```

[3]:

	xlow	xhigh	sumw	sumw2	sumwx	sumwx2	numEntries
0	0.000	0.005	9.207162	4.709544	0.029255	0.021593	18.0
1	0.005	0.010	28.644500	14.651920	0.210193	0.317386	56.0
2	0.010	0.015	18.925832	9.680732	0.234288	0.586316	37.0
3	0.015	0.020	15.856778	8.110884	0.284102	1.023680	31.0
4	0.020	0.025	10.230180	5.232828	0.235225	1.085886	20.0
5	0.025	0.030	18.414322	9.419092	0.504793	2.773457	36.0
6	0.030	0.035	10.741688	5.494468	0.355455	2.357036	21.0

7	0.035	0.040	7.161126	3.662980	0.271840	2.065958	14.0
8	0.040	0.050	4.092072	1.046566	0.187649	0.864406	16.0
9	0.050	0.060	5.882353	1.504438	0.319918	1.743721	23.0
10	0.060	0.080	2.813299	0.359757	0.197314	0.695855	22.0
11	0.080	0.100	2.429667	0.310699	0.218462	0.985429	19.0
12	0.100	0.120	1.534527	0.196231	0.167965	0.921696	12.0
13	0.120	0.160	1.278772	0.081763	0.180299	0.638571	20.0
14	0.160	0.200	0.959079	0.061322	0.169320	0.750095	15.0
15	0.200	0.250	0.767263	0.039246	0.176224	0.812549	15.0
16	0.250	0.300	0.306905	0.015698	0.084873	0.470805	6.0
17	0.300	0.350	0.051151	0.002616	0.017546	0.120380	1.0
18	0.350	0.400	0.051151	0.002616	0.020255	0.160413	1.0
19	0.400	0.500	0.076726	0.001962	0.035161	0.161249	3.0
20	0.500	0.600	0.076726	0.001962	0.039292	0.201248	3.0
21	0.600	0.700	0.051151	0.001308	0.031580	0.194970	2.0
22	0.700	0.800	0.000000	0.000000	0.000000	0.000000	0.0

1.1.2 Get data histograms as pandas dataframes

[4]:
```python
dfdata = yoda2numpy.todf( yoda2numpy('dat') )

keydat = '/REF/ALEPH_1996_S3486095/d01-x01-y01'
dfdata[keydat]
```

[4]:

	xval	xerr-	xerr+	yval	yerr-	yerr+
0	0.0025	0.0025	0.0025	12.3600	0.407922	0.407922
1	0.0075	0.0025	0.0025	23.3300	0.254951	0.254951
2	0.0125	0.0025	0.0025	20.2300	0.156205	0.156205
3	0.0175	0.0025	0.0025	16.6900	0.120416	0.120416
4	0.0225	0.0025	0.0025	13.4100	0.100000	0.100000
5	0.0275	0.0025	0.0025	10.7900	0.098995	0.098995
6	0.0325	0.0025	0.0025	8.8700	0.094048	0.094048
7	0.0375	0.0025	0.0025	7.4080	0.089196	0.089196
8	0.0450	0.0050	0.0050	5.9220	0.069340	0.069340
9	0.0550	0.0050	0.0050	4.5080	0.052631	0.052631
10	0.0700	0.0100	0.0100	3.2580	0.030479	0.030479
11	0.0900	0.0100	0.0100	2.3170	0.023345	0.023345
12	0.1100	0.0100	0.0100	1.7420	0.022672	0.022672
13	0.1400	0.0200	0.0200	1.2110	0.018358	0.018358
14	0.1800	0.0200	0.0200	0.8132	0.015207	0.015207
15	0.2250	0.0250	0.0250	0.5626	0.012712	0.012712
16	0.2750	0.0250	0.0250	0.3973	0.010246	0.010246
17	0.3250	0.0250	0.0250	0.2903	0.007783	0.007783
18	0.3750	0.0250	0.0250	0.2224	0.006191	0.006191
19	0.4500	0.0500	0.0500	0.1476	0.003982	0.003982
20	0.5500	0.0500	0.0500	0.0861	0.002441	0.002441
21	0.6500	0.0500	0.0500	0.0447	0.001487	0.001487

```
 22  0.7500  0.0500  0.0500   0.0116  0.000781  0.000781
```

1.1.3 Determine which histograms to use

Criteria: 1. number of bins > 0 2. histogram exists in data and simulated samples 3. total cross section > 0.1 units

1.1.4 How to proceed?

Notice (unfortunately) that the total effective counts for every histogram is different! This is a huge complication because, in principle, we would need to generate different numbers of events for every histogram. But, as is true of much of what we do in science, we should make some simplifying assumptions to reduce to complexity of the problem.

Assumptions

1. Since we are not given correlation matrices for the measured cross sections, we assume that the bin-by-bin cross section measurements are conditionally independent: given fixed values of the tune parameters the measured cross sections are statistically independent.
2. The counts per bin are Poisson-distributed and the cross sections are just scaled values of the counts. We can, therefore, compute the effective count in each bin using the following *ansatz*

$$n_i = k_i \sigma_i, \tag{1}$$
$$\sqrt{n_i} = k_i \delta\sigma_i \quad \text{and, therefore,} \tag{2}$$
$$n_i = \left(\frac{\sigma_i}{\delta\sigma_i}\right)^2, \tag{3}$$

   where $\sigma_i \pm \delta\sigma_i$ is the measured cross section in bin i and k_i, the *effective integrated luminosity*, is the product $\epsilon_i L$ of the efficiency times acceptance, ϵ_i, and the integrated luminosity L. The total effective count for a histogram is then just $n = \sum_i n_i$.

Therefore, for each tune parameter point, a sufficiently large sample of simulated events will result in histograms that serve both as the predictions as well as the basis for simulating events counts in all the simulated "observed" histograms. Given our assumptions, we can write down an approximation of the statistical model, $p(X|\theta)$, where X are *potentially observable* counts and θ are the tune parameters. With the assumptions above, the statistical model for the `ALEPH` data can be approximated as a product of either gamma or Gaussian densities depending on the size of the effective bin counts.

[21]:
```
keys = list(dfdata.keys())
keys.sort()

records = []
hist_names = []
for key in keys:
    dfdat = dfdata[key]
    yval  = dfdat['yval']
    yerr  = dfdat['yerr-']

    # ignore single count histograms
```

```
    if len(yval) < 2: continue

    mckey = key[4:]
    if not (mckey in dfsims[0]): continue

    dfMC  = dfsims[0][mckey]

    xlow  = dfMC.xlow
    xhigh = dfMC.xhigh
    dx = xhigh - xlow

    xsec = yval * dx
    total_xsec = xsec.sum()
    if total_xsec < 0.1: continue

    xsec_err = yerr * dx

    count = (xsec/xsec_err)**2  # count per bin
    total_count = count.sum()

    # cache histogram names
    hist_names.append(key)

    total_xsec_err = np.sqrt((xsec_err**2).sum())
    rel_err = 100 * total_xsec_err / total_xsec

    hname = key.split('/')[-1]
    records.append((total_count, hname, total_xsec, total_xsec_err, rel_err))

# sort according to total count
records.sort()

print('%s\t%10s     %6s %6s %10s' % \
          ('histogram', 'x-section', 'error', 'relerr', 'count'))
for total_count, hname, total_xsec, total_xsec_err, rel_err in records:
    print(f'{hname:s}\t{total_xsec:10.3f} +/- {total_xsec_err:6.3f} {rel_err:6.
 ↪2f}'\
          f' {total_count:10.0f}')
```

```
histogram        x-section      error relerr      count
d38-x01-y01          0.637 +/-  0.064   9.97        330
d37-x01-y01          1.444 +/-  0.118   8.20        348
d43-x01-y01          0.617 +/-  0.037   5.95        393
d39-x01-y01          0.827 +/-  0.057   6.89        415
d40-x01-y01          0.123 +/-  0.006   4.97        764
d18-x01-y01          2.001 +/-  0.075   3.75       1056
d30-x01-y01          0.282 +/-  0.015   5.19       2574
```

```
d29-x01-y01           4.802 +/-  0.143   2.97        2638
d26-x01-y01           1.279 +/-  0.018   1.43        9962
d27-x01-y01           0.605 +/-  0.012   1.95       10585
d28-x01-y01          12.505 +/-  0.371   2.97       14042
d33-x01-y01           0.374 +/-  0.003   0.84       20045
d06-x01-y01           1.000 +/-  0.010   0.97       28040
d32-x01-y01           2.051 +/-  0.014   0.69       31137
d05-x01-y01           1.001 +/-  0.006   0.56       36541
d02-x01-y01           0.992 +/-  0.007   0.66       63951
d03-x01-y01           1.000 +/-  0.004   0.42       71103
d07-x01-y01           1.002 +/-  0.006   0.62       81351
d04-x01-y01           0.999 +/-  0.004   0.42      116775
d08-x01-y01           1.001 +/-  0.003   0.28      149750
d01-x01-y01           1.000 +/-  0.003   0.34      149839
d10-x01-y01          20.870 +/-  0.076   0.36      205113
d12-x01-y01          20.868 +/-  0.071   0.34      367936
d25-x01-y01          11.172 +/-  0.021   0.19      477445
d11-x01-y01          20.889 +/-  0.056   0.27      522352
d09-x01-y01          20.063 +/-  0.100   0.50      785779
d17-x01-y01          19.824 +/-  0.076   0.38      957693
```

1.1.5 Define test statistic λ

$$\lambda(X;\theta) = \sqrt{\frac{1}{N}\sum_{\text{histograms}}\sum_{i}\left(\frac{D_i - T_i(\theta)}{\delta_i}\right)^2}, \tag{4}$$

where N is the total number of bins summed over histograms and δ_i^2 is the sum of the variances associated with the data D_i and the theoretical prediction T_i with the latter obtained via Monte Carlo simulation.

[22]:
```python
def test_statistic(names, dfdata, dfpred, which=0):
    Y = 0.0
    nbins = 0

    for name in names:

        # get data
        if which == 0:
            # ALEPH data
            df   = dfdata[name]
            data = df['yval']
            derr = df['yerr-']
        else:
            # Simulated data
            df   = dfdata[name[4:]]
            data = df['sumw']
            derr = np.sqrt(df['sumw2'])
```

```
        ndat = len(df)

        # get predictions
        df    = dfpred[name[4:]]
        npred= len(df)

        assert ndat == npred

        pred = df['sumw']
        perr2= df['sumw2']

        stdv = np.sqrt(derr**2 + perr2)
        stdv = np.where(stdv < 1e-3, 1, stdv)

        X   = (((data - pred)/stdv)**2).sum()

        # accumulate test statistic
        Y += X
        # accumulate total bin count
        nbins += ndat

    return np.sqrt(Y/nbins)
```

1.1.6 Compute test statistic using observed data

[23]:
```
X0 = []
for ii in tqdm(range(M)):
    X0.append( test_statistic(hist_names, dfdata, dfnews[ii], which=0) )
X0 = np.array(X0)
```

```
100%|                     | 1000/1000 [00:04<00:00, 249.93it/s]
```

1.1.7 Get best fit values of a and b

We get the best fit value by finding the point (a, b) yielding the smallest value of the test statistic.

[24]:
```
df = pd.read_csv('a_b_samples_uniform_1.csv')

K_best = np.argmin(X0)    # file with minimum value of test statistic
dfbest = dfnews[K_best]

a_best = df.a.iloc[K_best]
b_best = df.b.iloc[K_best]
count  = dfbest[hist_names[0][4:]].numEntries.sum()
print(f'k: {K_best:5d}\ta: {a_best:10.3f}\tb: {b_best:10.3f}\ttotal count:␣
 ↪{count:10.0f}')
```

```
dfbest[hist_names[0][4:]][:10]
```

```
k:   408        a:      0.741    b:      0.988    total count:      49999
```

[24]:

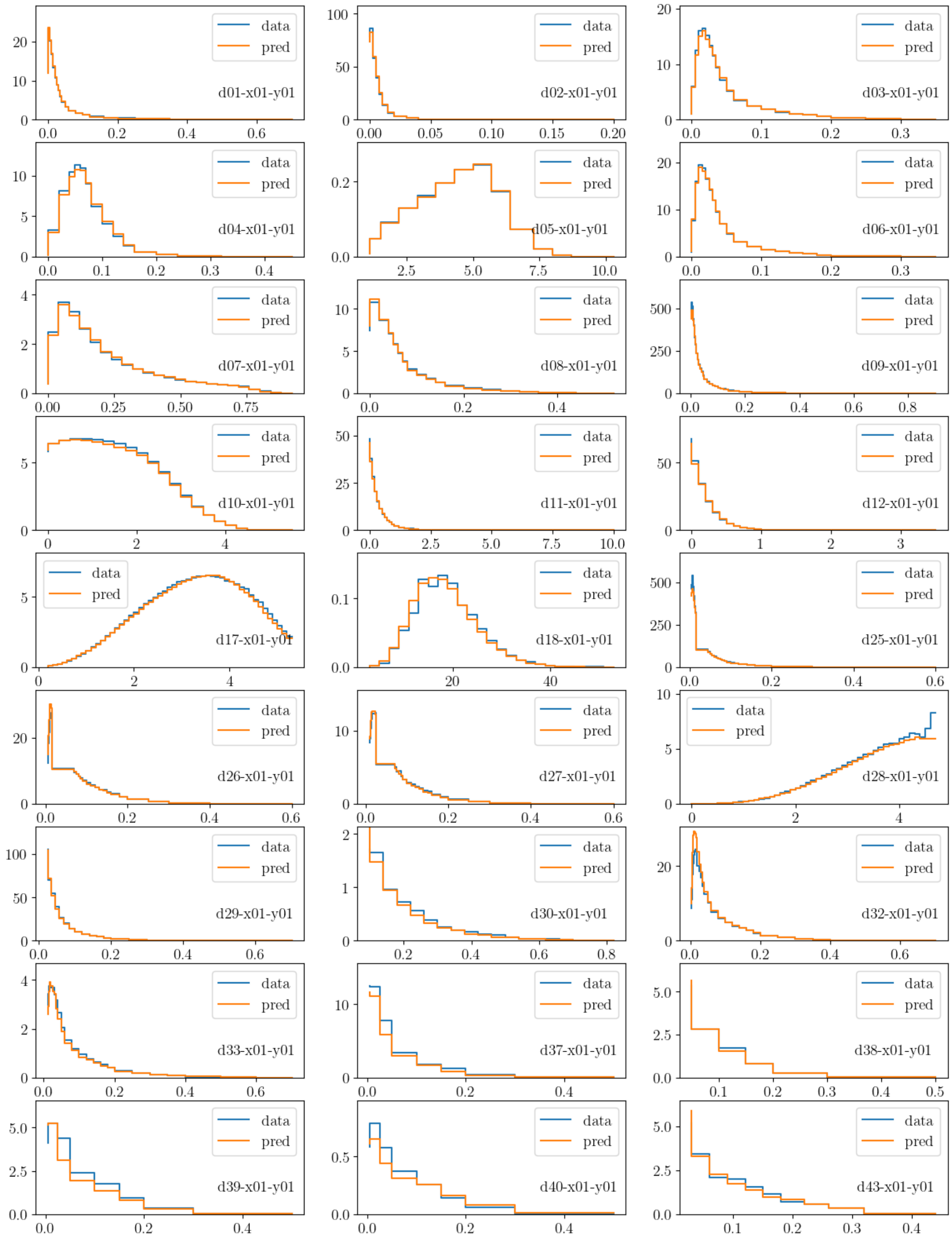
	xlow	xhigh	sumw	sumw2	sumwx	sumwx2	numEntries
0	0.000	0.005	11.824	0.047296	0.040673	0.030584	2956.0
1	0.005	0.010	23.464	0.093856	0.176105	0.273884	5866.0
2	0.010	0.015	20.396	0.081584	0.253187	0.637155	5099.0
3	0.015	0.020	16.940	0.067760	0.294970	1.034157	4235.0
4	0.020	0.025	13.688	0.054752	0.306313	1.376525	3422.0
5	0.025	0.030	10.976	0.043904	0.301065	1.656309	2744.0
6	0.030	0.035	8.996	0.035984	0.291708	1.895592	2249.0
7	0.035	0.040	7.464	0.029856	0.279606	2.097975	1866.0
8	0.040	0.050	6.060	0.012120	0.270879	1.215698	3030.0
9	0.050	0.060	4.594	0.009188	0.251323	1.378791	2297.0

1.1.8 Plot best-fit distributions

[25]:
```
hists = []
for name in hist_names:
    data = dfdata[name]
    yval = data['yval']
    yerr = data['yerr-']

    # get predictions
    key  = name[4:]

    pred = dfbest[key]
    pval = pred['sumw']
    perr = np.sqrt(pred['sumw2'])
    edges= dfbest[key]['xlow']

    name = name.split('/')[-1]
    hists.append((name, edges, yval, pval))
```

[26]:
```
def plot_dist(hist_names, hists, filename='fig_bestfit_dist.png'):

    def plt_sim_data_hist(ax, hist):
        name, edges, hdat, hsim = hist

        xmin = 0
        xmax = edges.max()
        ax.set_ylim(xmin, xmax)

        ymin = 0
        ymax = 1.25 * hdat.max()
        ax.set_ylim(ymin, ymax)
```

```
        ax.text(xmin + 0.7*(xmax-xmin), ymin + 0.2*(ymax-ymin), name)

        ax.step(y=hdat, x=edges, label='data')
        ax.step(y=hsim, x=edges, label='pred')
        ax.legend()

    nhists= len(hist_names)
    ncols = 3
    nrows = nhists // ncols
    nhists= nrows * ncols

    fig, ax = plt.subplots(nrows, ncols, figsize=(15, 20), edgecolor='k')
    ax = ax.ravel()
    for hist_ind, hist in enumerate(hists[:nhists]):
        plt_sim_data_hist(ax[hist_ind], hist)

    plt.savefig(filename)

plot_dist(hist_names, hists)
```



1.1.9 Compute the 3 test statistics

To test the procedure, we'll use the simulated data corresponding to the best fit point as the "observed" data in lieu of the ALEPH data. We do this so that the simulated data have the same statistical power as the *fixed* "observed" data since they have the same integrated luminosity. To use the ALEPH data the simulated data needs to match the statistical power of the former, that is, the simulated data must be sampled from the same distribution as the observed data except that the simulated data, necessarily, are sampled using different hypotheses for the tune parameters.

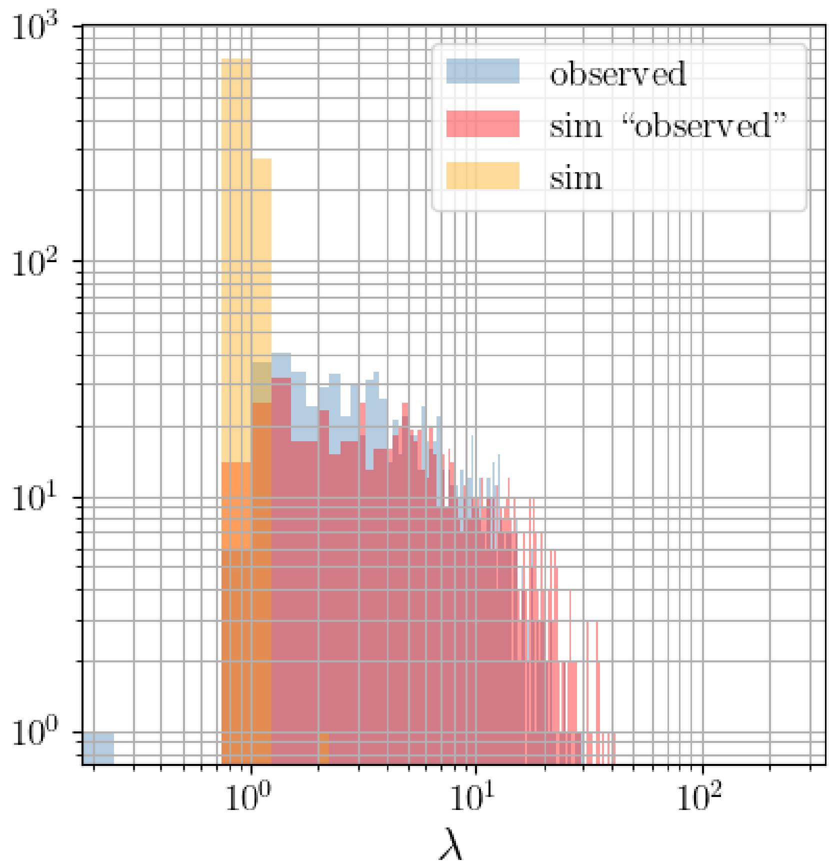
1. `l0` $= \lambda_0(D; \theta)$ computed with *fixed* "observed" data and predictions at θ_i.
2. `lp` $= \lambda'(D'; \theta)$ computed with simulated data at θ_i' and predictions at θ_i.
3. `l` $= \lambda(D; \theta)$ with simulated data and predictions both at θ_i.

[27]:
```
# randomly shuffle integers 0 to M-1
jj = np.array(list(range(M)))
np.random.shuffle(jj)

# 1. test statistic with "observed" data
l0 = []
for ii in tqdm(range(M)):
    l0.append( test_statistic(hist_names, dfbest, dfnews[ii], which=1) )
l0 = np.array(l0)

# 2. test statistic with simulated "observed" data
lp = []
for ii in tqdm(range(M)):
    lp.append( test_statistic(hist_names, dfsims[jj[ii]], dfnews[ii], which=1) )
lp = np.array(lp)

# 3. test statistic with simulated data and predictions at the same parameter␣
↪point
l  = []
for ii in tqdm(range(M)):
    l.append( test_statistic(hist_names, dfsims[ii], dfnews[ii], which=1) )
l  = np.array(l)

print(f'{l0.mean():10.3f}, {lp.mean():10.3f}, {l.mean():10.3f}')
```

```
100%|                    | 1000/1000 [00:04<00:00, 226.09it/s]
100%|                    | 1000/1000 [00:04<00:00, 221.07it/s]
100%|                    | 1000/1000 [00:04<00:00, 227.14it/s]

     7.506,     10.235,      0.979
```

[28]:
```
def plot_test_statistics(x0, xo, x,
              xbins=1000, xmin=0, xmax=250,
              ymin=0, ymax=800, ftsize=18):

    # create an empty figure
    fig = plt.figure(figsize=(5, 5))
    fig.tight_layout()
```

```
    # add a subplot to it
    nrows, ncols, index = 1,1,1
    ax  = fig.add_subplot(nrows, ncols, index)
    #ax.set_xlim(xmin, xmax)
    ax.set_xlabel('$\lambda$', fontsize=ftsize)
    ax.set_xscale('log')
    ax.set_yscale('log')

    ax.hist(x0, bins=xbins, range=(xmin, xmax), color='steelblue', alpha=0.4,␣
 ↪label='observed')
    ax.hist(xo, bins=xbins, range=(xmin, xmax), color='red', alpha=0.4,␣
 ↪label='sim ``observed"')
    ax.hist(x,  bins=xbins, range=(xmin, xmax), color='orange', alpha=0.4,␣
 ↪label='sim')

    ax.legend()

    ax.grid(True, which="both", linestyle='-')

    plt.show()

plot_test_statistics(l0, lp, l)
```



1.1.10 Compute indicators $Z_0 = \mathbb{I}[\lambda \leq \lambda_0]$ and $Z' = \mathbb{I}[\lambda \leq \lambda']$

[29]:
```
df['l0'] = l0
df['lp'] = lp
df['l']  = l
df['Z0'] = (l <= l0).astype(int)
df['Zp'] = (l <= lp).astype(int)

print(f'{df.l0.mean():10.2f}, {df.lp.mean():10.2f}, {df.l.mean():10.2f}')
print(f'{df.Z0.mean():10.4f}, {df.Zp.mean():10.4f}')

df[:10]
```

```
      7.51,      10.24,       0.98
    0.9960,     0.9940
```

[29]:

	Unnamed: 0	a	b	l0	lp	l	Z0	Zp
0	0	0.890731	1.773921	4.893057	14.840858	2.199495	1	1
1	1	1.306220	1.490305	1.312000	11.018291	1.001977	1	1

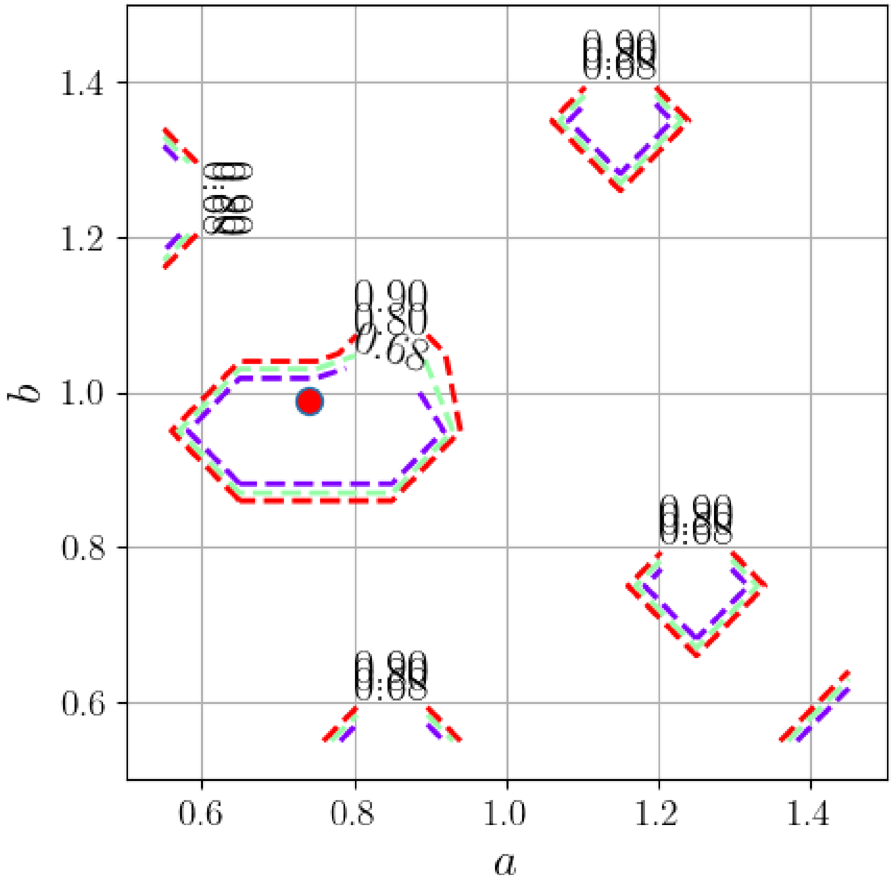
2	2	1.653587	0.538929	16.438451	26.601965	0.954788	1	1
3	3	0.666805	1.375998	4.338279	3.324299	0.982656	1	1
4	4	1.105232	1.243956	1.470954	1.041777	1.061903	1	0
5	5	1.663316	0.514966	17.059907	16.762613	0.926968	1	1
6	6	0.020567	0.917892	9.064542	12.246315	0.959049	1	1
7	7	0.838095	1.297131	2.178625	7.177722	0.961769	1	1
8	8	1.597502	1.513509	3.029759	4.141842	0.972587	1	1
9	9	0.330494	0.874556	3.988953	7.089688	1.010666	1	1

1.1.11 Plot confidence set based on histogramming

[30]:
```
def plot_cdf(df, a=None, b=None,
             xbins=10, xmin=0.5, xmax=1.5,
             ybins=10, ymin=0.5, ymax=1.5,
             filename='fig_cdf_via_hist.png',
             fgsize=(5, 5),
             ftsize=18):

    # approximate cdf via histogramming
    xrange = (xmin, xmax)
    yrange = (ymin, ymax)

    # weighted histogram   (count the number of ones per bin)
    hw, xe, ye = np.histogram2d(df.a, df.b,
                                bins=(xbins, ybins),
                                range=(xrange, yrange),
                                weights=df.Z0)

    # unweighted histogram (count number of ones and zeros per bin)
    hu, _, _ = np.histogram2d(df.a, df.b,
                              bins=(xbins, ybins),
                              range=(xrange, yrange))
    P =  hw / (hu + 1.e-10)

    # flatten arrays so that p, x, and y are 1d arrays
    # of the same length.
    # get bin centers
    x   = (xe[1:] + xe[:-1])/2
    y   = (ye[1:] + ye[:-1])/2
    X,Y = np.meshgrid(x, y)
    x   = X.flatten()
    y   = Y.flatten()

    # WARNING: must transpose P so that X, Y, and P have the
    # same shape
    P   = P.T
    p   = P.flatten()
```

```
    # Now make plots
    fig, ax = plt.subplots(nrows=1, ncols=1, figsize=fgsize)

    ax.set_xlim(xmin, xmax)
    #ax.set_xticks(np.linspace(xmin, xmax, 6))
    ax.set_xlabel(r'$a$', fontsize=ftsize)

    ax.set_ylim(ymin, ymax)
    #ax.set_yticks(np.linspace(xmin, xmax, 9))
    ax.set_ylabel(r'$b$',  fontsize=ftsize)

    mylevels = np.array([0.68, 0.8, 0.9])

    colormap = 'rainbow'

    cs = ax.contour(X, Y, P,
                    extent=(xmin, xmax, ymin, ymax),
                    levels=mylevels,
                    linewidths=2,
                    linestyles='dashed',
                    cmap=colormap)

    ax.clabel(cs, cs.levels,
              inline=True,
              fontsize=18, fmt='%4.2f',
              colors='black')

    if a != None:
        if b != None:
            print(f'a(best): {a_best:10.3f} b(best): {b_best:10.3f}')
            ax.plot([a_best], [b_best],
                    markerfacecolor='red',
                    markersize=20,
                    marker='.')

    ax.grid()

    plt.tight_layout()
    plt.savefig(filename)
    plt.show()


plot_cdf(df, a_best, b_best)
```

```
a(best):      0.741 b(best):      0.988
```



0.90
0.80
0.68
1.4
1.2
1.0
0.8
0.6
b
a


```
[ ]:
```