In [1]:

```
import scanpy as sc
import pandas as pd
from sccoda.util import cell_composition_data as dat
from sccoda.util import comp_ana as mod
from sccoda.util import data_visualization as viz
import matplotlib.pyplot as plt
import numpy as np
```

```
2025-05-08 12:19:07.566052: I tensorflow/core/util/port.cc:110] oneDNN
custom operations are on. You may see slightly different numerical resu
lts due to floating-point round-off errors from different computation o
rders. To turn them off, set the environment variable `TF_ENABLE_ONEDNN
_OPTS=0`.
2025-05-08 12:19:07.567807: I tensorflow/tsl/cuda/cudart_stub.cc:28] Co
uld not find cuda drivers on your machine, GPU will not be used.
2025-05-08 12:19:07.606680: I tensorflow/tsl/cuda/cudart_stub.cc:28] Co
uld not find cuda drivers on your machine, GPU will not be used.
2025-05-08 12:19:07.607548: I tensorflow/core/platform/cpu_feature_guar
d.cc:182] This TensorFlow binary is optimized to use available CPU inst
ructions in performance-critical operations.
To enable the following instructions: AVX2 AVX512F AVX512_VNNI FMA, in
other operations, rebuild TensorFlow with the appropriate compiler flag
s.
2025-05-08 12:19:09.533438: W tensorflow/compiler/tf2tensorrt/utils/py_
utils.cc:38] TF-TRT Warning: Could not find TensorRT
```

In [2]:

```
#read in adata file from analysis.ipynb
adata = sc.read("refs/adata.h5ad")
```

```
/projectnb/bf528/students/npetruni/.conda/envs/sccoda_env/lib/python3.
8/site-packages/anndata/_core/anndata.py:1838: UserWarning: Observation
names are not unique. To make them unique, call `.obs_names_make_unique
`.
  utils.warn_names_duplicates("obs")
```

In [3]:

```
#create cell counts matrix
counts_df = (
    adata.obs
    .groupby(['sample', 'manual_labels'])
    .size()
    .unstack(fill_value=0)
)

# Optional: View summary
counts_df
```

Out[3]:

manual_labels sample	Endothelial cells	Epithelial cells	Erythroids	Fibroblasts	ILC	Macrophag
Case1_YF	123	6731	2	674	429	578
Case1_ZY	2047	4741	1	512	69	159
Case2_ZC	0	433	4509	1	2	
Case2_YF	176	179	9	5261	3112	129
Case2_ZY	2752	474	1	2330	100	184
Case3_YF	3207	61	0	4117	565	8
Case3_ZY	2022	47	0	2671	866	7
Case4_ZY	804	8	0	662	0	

In [4]:

```
#create covariate df

covariates_df = pd.DataFrame({
    'sample': [
        'Case1_YF', 'Case1_ZY', 'Case2_ZC', 'Case2_YF',
        'Case2_ZY', 'Case3_YF', 'Case3_ZY', 'Case4_ZY'
    ],
    'tissue_type': [
        'PDAC', 'Metastasis', 'Normal', 'PDAC',
        'Metastasis', 'PDAC', 'Metastasis', 'Metastasis'
    ]
}).set_index('sample')
```

In [5]:

```
#reorders and filters the rows in counts_df to match exactly the sampl
counts_df = counts_df.loc[covariates_df.index]
#add pseudo count of 1 to prevent issues
counts_df += 1
```

In [6]:

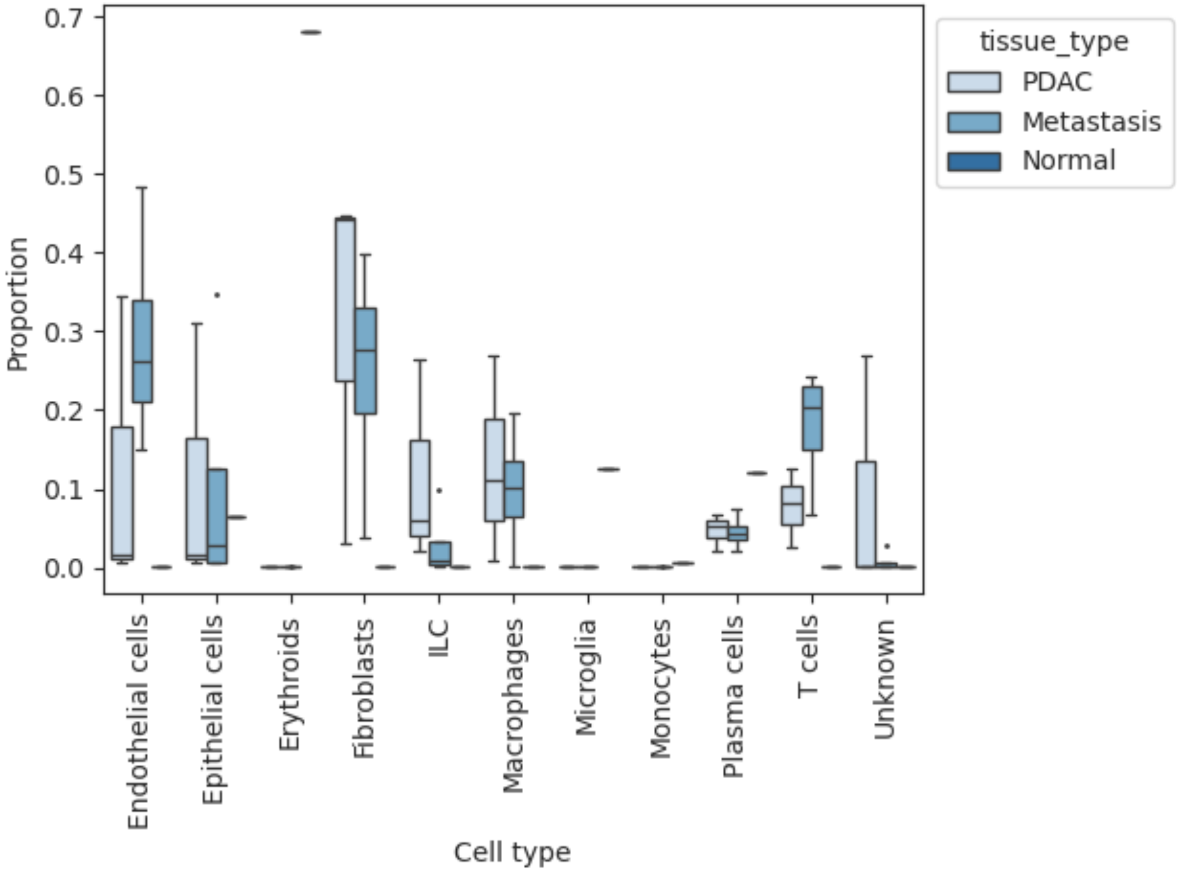
```
#convert to scCODA object
counts_df = counts_df.merge(covariates_df, left_index=True, right_inde
data_all = dat.from_pandas(counts_df, covariate_columns=['tissue_type'

print(data_all)
```

```
AnnData object with n_obs × n_vars = 8 × 11
    obs: 'tissue_type'
```

In [7]:

```
viz.boxplots(data_all, feature_name="tissue_type")
plt.show()
```

```
/projectnb/bf528/students/npetruni/.conda/envs/sccoda_env/lib/python3.
8/site-packages/sccoda/util/data_visualization.py:335: UserWarning: Fix
edFormatter should only be used together with FixedLocator
  ax.set_xticklabels(cell_types, rotation=90)
```



```
In [8]: #run scCODA
        model = mod.CompositionalAnalysis(data_all, formula="tissue_type", ref
        sim_results = model.sample_hmc()
```

```
2025-05-08 12:19:38.836612: I tensorflow/compiler/xla/service/service.c
c:168] XLA service 0x14c1c0009230 initialized for platform Host (this d
oes not guarantee that XLA will be used). Devices:
2025-05-08 12:19:38.836663: I tensorflow/compiler/xla/service/service.c
c:176]   StreamExecutor device (0): Host, Default Version
  0%|          | 0/20000 [00:00<?, ?it/s]2025-05-08 12:19:38.885590: I
tensorflow/compiler/mlir/tensorflow/utils/dump_mlir_util.cc:255] disabl
ing MLIR crash reproducer, set env var `MLIR_CRASH_REPRODUCER_DIRECTORY
` to enable.
2025-05-08 12:19:39.352290: I ./tensorflow/compiler/jit/device_compile
r.h:186] Compiled cluster using XLA!  This line is logged at most once
for the lifetime of the process.
100%|██████████| 20000/20000 [02:33<00:00, 130.45it/s]
MCMC sampling finished. (194.383 sec)
Acceptance rate: 63.2%
```

```
In [9]: #view results
        summary_df = sim_results.summary()
```

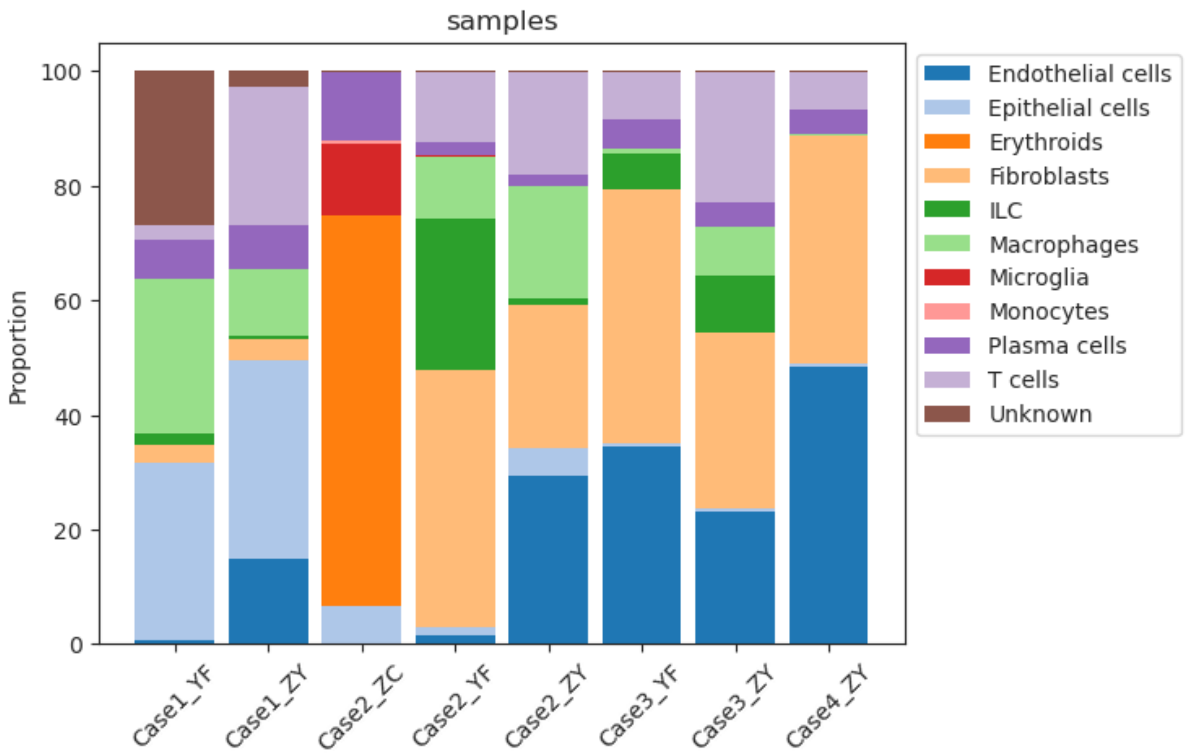
```
summary_df
```

```
Compositional Analysis summary:

Data: 8 samples, 11 cell types
Reference index: 3
Formula: tissue_type

Intercepts:
                   Final Parameter  Expected Sample
Cell Type
Endothelial cells            0.343      1992.435473
Epithelial cells            -0.562       806.023602
Erythroids                  -1.917       207.911607
Fibroblasts                  0.479      2282.697246
ILC                         -0.779       648.792553
Macrophages                 -0.309      1038.064318
Microglia                   -1.929       205.431578
Monocytes                   -1.925       206.254950
Plasma cells                -0.412       936.465822
T cells                      0.194      1716.620867
Unknown                     -1.546       301.301982


Effects:
                                         Final Parameter  Expected Samp
le  \
Covariate             Cell Type
tissue_type[T.Normal] Endothelial cells         0.000000           4.3136
82
                      Epithelial cells          5.956606         674.1131
37
                      Erythroids                9.659506        7053.6286
68
                      Fibroblasts               0.000000           4.9421
07
                      ILC                       0.000000           1.4046
55
                      Macrophages               0.000000           2.2474
40
                      Microglia                 7.975856        1294.1998
33
                      Monocytes                 4.881416          58.8627
34
                      Plasma cells              6.419230        1243.9188
79
                      T cells                   0.000000           3.7165
35
                      Unknown                   0.000000           0.6523
28
tissue_type[T.PDAC]   Endothelial cells         0.000000        1992.4354
73
                      Epithelial cells          0.000000         806.0236
```

```
02
                      Erythroids                0.000000        207.9116
07
                      Fibroblasts               0.000000       2282.6972
46
                      ILC                       0.000000        648.7925
53
                      Macrophages               0.000000       1038.0643
18
                      Microglia                 0.000000        205.4315
78
                      Monocytes                 0.000000        206.2549
50
                      Plasma cells              0.000000        936.4658
22
                      T cells                   0.000000       1716.6208
67
                      Unknown                   0.000000        301.3019
82

                                         log2-fold change
Covariate             Cell Type
tissue_type[T.Normal] Endothelial cells         -8.851397
                      Epithelial cells          -0.257831
                      Erythroids                 5.084323
                      Fibroblasts               -8.851397
                      ILC                       -8.851397
                      Macrophages               -8.851397
                      Microglia                  2.655331
                      Monocytes                 -1.809002
                      Plasma cells               0.409594
                      T cells                   -8.851397
                      Unknown                   -8.851397
tissue_type[T.PDAC]   Endothelial cells          0.000000
                      Epithelial cells           0.000000
                      Erythroids                 0.000000
                      Fibroblasts                0.000000
                      ILC                        0.000000
                      Macrophages                0.000000
                      Microglia                  0.000000
                      Monocytes                  0.000000
                      Plasma cells               0.000000
                      T cells                    0.000000
                      Unknown                    0.000000
```

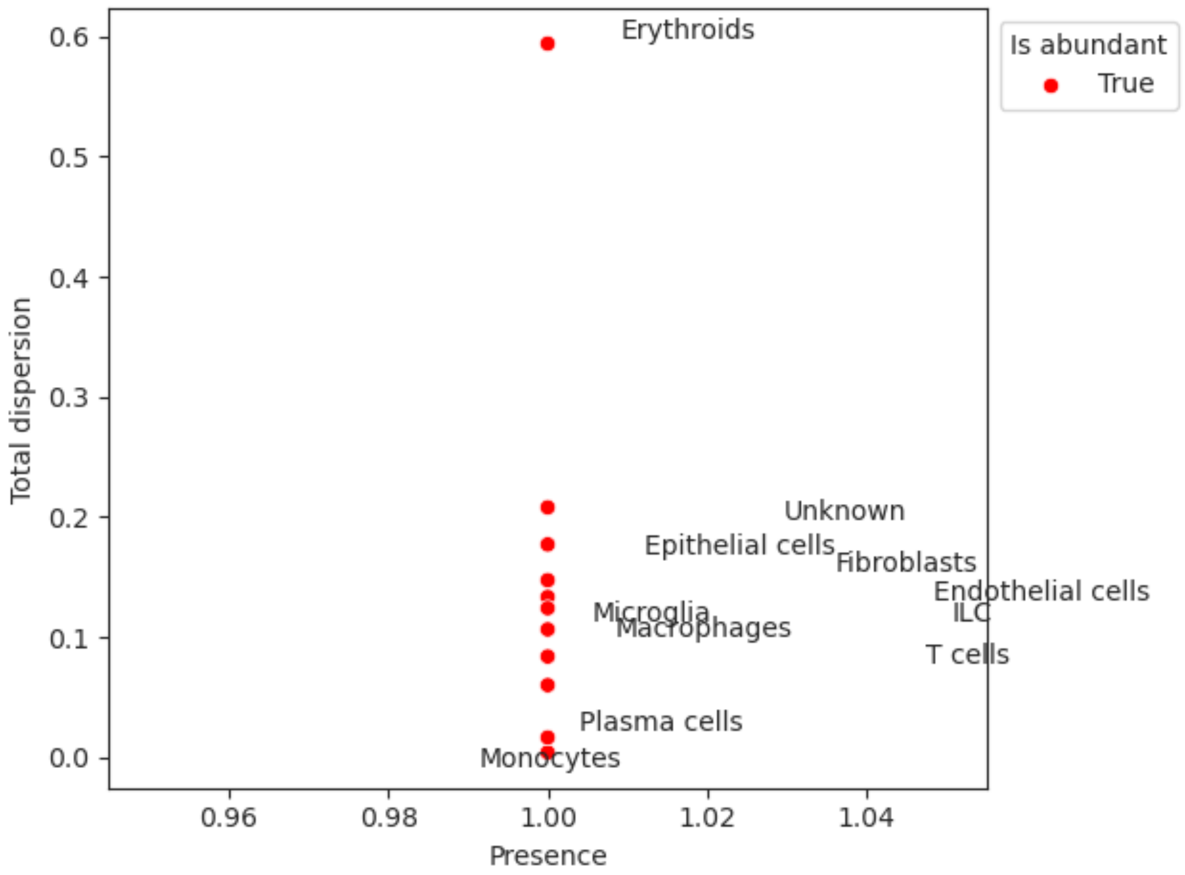
In [10]:

```
viz.stacked_barplot(data_all, feature_name="samples")
plt.show()
```



In [11]:

```
# Relative abundance vs dispersion
viz.rel_abundance_dispersion_plot(data=data_all, abundant_threshold=0.

# Jitter text labels
ax = plt.gca()
for text in ax.texts:
    x, y = text.get_position()
    text.set_position((x + np.random.uniform(-0.03, 0.03), y + np.rand

plt.show()
```



Discussion

As an additional analysis, I applied scCODA, a Bayesian compositional model, to identify shifts in cell type proportions across PDAC, metastatic, and normal tissues. By choosing fibroblasts as a stable reference cell type, I was able to model relative changes while accounting for the compositional nature of single-cell data. My results show a depletion of epithelial cells and erythroids in PDAC compared to normal tissue, and an expansion of endothelial cells and T cells in metastatic samples. These shifts are consistent with literature showing epithelial plasticity and immune infiltration during tumor progression (Dongre & Weinberg, 2019). This analysis highlights cell types that may play a role in tumor development and dissemination, offering targets for future mechanistic studies or therapeutic intervention.