A Data and Code availability

The data and code for fully reproducing all results presented in this manuscript are available at Zenodo at https://doi.org/10.5281/zenodo.4734527. The simulation code has been tested on R version 4.0. The trac R package is available at https://github.com/jacobbien/trac. A vignette describing key functionalities of the package and an archetypical workflow are available at https://jacobbien.github.io/trac/articles/trac-example.html. The c-lasso Python package [1] is available at https://github.com/Leo-Simpson/c-lasso and can be installed via pip.
B Derivation of Optimization Problem

We design a convex tree-based penalty $\mathcal{P}_T(\beta)$ that promotes $\beta$ to be constant along branches of $T$. We encode $T$ through a binary matrix $A \in \{0, 1\}^{p \times (|T| - 1)}$ indicating whether feature $j$ is a leaf of each non-root node $u \in T - \{r\}$, that is $A_{ju} = 1\{j \in \mathcal{L}(u)\}$ where $\mathcal{L}(u)$ is the set of leaves that descend from $u$. In particular, we take

$$\mathcal{P}_T(\beta) = \min_{\gamma \in \mathbb{R}^{|T| - 1}} \{ \|\gamma\|_1 \text{ s.t. } \beta = A\gamma \}.$$  

![Figure 1: Schematic of the tree aggregation process.](image)

Figure 1 shows a schematic of the tree aggregation idea. The vector $\gamma \in \mathbb{R}^{|T| - 1}$ can be thought of as a latent parameter vector with an entry associated with each node of the tree (see Figure 1). We associate a $\beta_j$ to each leaf of $T$, and the constraint $\beta = A\gamma$ expresses a particular relationship between these, namely that each coefficient $\beta_j$ is the sum of the $\gamma_u$ for which $j \in \mathcal{L}(u)$ (i.e., each $\beta_j$ is the sum of its ancestor $\gamma$-values in the tree). This relationship implies that when all the $\gamma$-values in a subtree are zero (denoted by crossed out nodes in the figure), then all the $\beta$ coefficients within the subtree are equal. Thus, the sparsity inducing $\ell_1$-norm on $\gamma$ in $\mathcal{P}_T(\beta)$ induces $\beta$ to tend to be constant within subtrees of $T$. Using this penalty in Eq. (1) in the main paper leads to the trac method, which is computed by solving

$$\minimize_{\beta \in \mathbb{R}^p, \gamma \in \mathbb{R}^{|T| - 1}} \; L(y - \log(X)\beta) + \lambda \|\gamma\|_1 \text{ s.t. } 1^T_p \beta = 0, \; \beta = A\gamma. \; (1)$$

This estimator is built on the tree-based aggregation penalty in [2], developed for general situations in which features are rare and a tree relating the features is available. In their setting, features are not compositional, so they do not introduce a sum-to-zero constraint or take the log of the features. The trac problem can be written more simply, entirely in terms of $\gamma$, as

$$\minimize_{\gamma \in \mathbb{R}^{|T| - 1}} \; L(y - \log(X)A\gamma) + \lambda \|\gamma\|_1 \text{ s.t. } 1^T_pA\gamma = 0.$$
The $n \times (|T| - 1)$ matrix $\log(X)A$ has the sum of the log counts of each of the $|T| - 1$ subtrees of $T$ (excluding $T$ itself). Changing variables to $\alpha_u = \gamma_u \cdot |\mathcal{L}(u)|$ and using properties of logarithms establishes the equivalence with problem Eq. (2) in the main paper.

## C Extended Results

We provide extended results, including an in-depth analysis of \text{trac} prediction of BMI from American Gut Project data, moisture prediction in Central Park soil, and leucine prediction in the Fram Strait.

### Immune marker sCD14 prediction in HIV patients

For the sCD14 data, we provide coefficient tables learned by \text{trac} ($a = 1$), \text{trac} ($a = 1/2$), and the sparse log-contrast model on the first random train-test data split (of ten) in Section D. This complements the tree visualizations shown in the main manuscript. We also include the results on the family base level (corresponding to panels C and D of Figure 3 in the main paper).

### BMI prediction from American Gut microbiome profiles

Finding consistent gut microbial signatures that are predictive of a person’s body mass index (BMI) remains a non-trivial problem. Several early studies argued that obesity is associated with phylum-level changes in the microbiome [3], including increased Firmicutes to Bacteroidetes phyla ratios [4], often referred to as a hallmark predictor of obesity. The authors in [5] and [6] were among the first to identify a small set of microbial genera that were (moderately) predictive of host BMI using sparse log-contrast models on the COMBO microbiome dataset [7].

Using \text{trac}, we revisit BMI prediction from microbial abundance data using a subset of the American Gut Project (AGP) data comprising $p = 1387$ OTUs across $n = 6266$ participants in the lean to obese BMI range. The standard \text{trac} model ($a = 1$) with the 1SE rule identified a model with 132 predictors, consisting of aggregations across all taxonomic levels. Table II summarizes the 15 strongest predictors which include the kingdom Bacteria (vs. Archaea) as negative baseline, the phylum Bacteroidetes and several families and genera in the class Clostridia (which belongs to the Firmicutes phylum) with positive associations. The strongest positive OTU level predictor is an unknown species belonging to the Ruminococcaceae family. Figure 2 shows the corresponding \text{trac} model BMI predictions (with 1SE rule) vs. measured BMI on the test set (split 1). The out-of-sample test error on this split is 15.31, and roughly 16 on average across all ten splits (see Table I). Standard \text{trac}, weighted \text{trac}, and sparse log-contrast models show similar performance in terms of test error ($16 - 17$) across all taxon base levels, with sparsity levels between 73 and 122 on OTU and genus level, and about 23-27 on the family level.

The standard \text{trac} model contains aggregations across all taxonomic levels. For instance, on the genus level, \text{trac} selects Blautia, Dorea, and Ruminococcus as positive predictors.
Figure 2: A scatter plot of measured BMI (y-axis) vs. trac model BMI predictions on a test set of $n = 2088$ AGP participants shows that predicted BMIs largely cover the “normal” BMI range between 20 and 28 with an overall test set correlation of 0.33. This model has 132 selected taxa, ranging from Kingdom to OTU levels. Table 11 shows the top 15 aggregations with largest $\alpha$-coefficients.
| Base Level | $p$ | trac ($a = 1$) | trac ($a = 1/2$) | Sparse Log-Contrast |
|------------|-----|---------------|-----------------|--------------------|
| OTU        | 1387 | 16 (115)      | 16 (100)        | 16 (81)            |
| Genus      | 824  | 16 (73)       | 16 (111)        | 16 (122)           |
| Family     | 199  | 17 (27)       | 17 (23)         | 17 (24)            |

Table 1: Average out-of-sample test errors (model sparsity in parenthesis) for trac ($a = \{1,1/2\}$) and sparse log-contrast models, respectively. Each row considers a different base level (OTU, genus, and family). Each number is averaged over ten different training/test splits of the Gut (AGP), BMI data.

The strongest overall positive predictors are the Bacteroidetes phylum, and the Ruminococcaceae, Lachnospiraceae, and Clostridiales families. The Lachnospiraceae/Bacteria ratio is also the first log-contrast to enter the trac aggregation path on the AGP data. The Erysipelotrichaceae and the Mogibacteriaceae families are the strongest negative predictors. Consistent with our model, Mogibacteriaceae were shown to be more abundant in lean individuals [8], and Erysipelotrichaceae were recently reported to be more abundant in normal compared to obese people or subjects with metabolic disorder [9]. However, the fact that standard trac could not identify a simple sparse predictive aggregation model for BMI suggests that more complex statistical models are required for predictive modeling, including adjustment for available covariates such as diet, sex, and overall lifestyle.
Predicting Central Park pH and soil moisture from microbial communities

Here, we complement the microbiome-pH analysis from the main text with an investigation of the relationship between soil microbiome and gravimetric moisture (% water) measurements in Central Park. Since pH and moisture measurements are uncorrelated in the Central Park dataset, we also investigated the similarity between the predictive aggregations for pH and moisture.

Standard trac inferred a predictive model of moisture consisting of 23 taxonomic aggregations, including the phylum Proteobacteria and the classes Alpha- and Deltaproteobacteria as strong positive predictors, and the phyla Verrucomicrobia, Actinobacteria, and the order Sphingobacteriales as strong negative predictors (see Table 15). On the test data (split 1), the correlation between model predictions and measurements was 0.42. Compared to pH, the reduced predictive power is in agreement with [10]'s observation about the smaller influence of SMD compared to pH on microbial composition. Nonetheless, trac's taxonomic groupings provide meaningful information about the taxonomic structure of soil microbiota along moisture gradients. For example, the model supports the positive association between Proteobacteria and moisture, as previously observed in a study along a vegetation gradient on the Loess Plateau in China [11], and the negative effect of moisture on the phylum Verrucomicrobia and the positive effect on Deltaproteobacteria in the Giessen free-air CO2 enrichment (Gi-FACE) experiment [12]. The Gi-FACE study, however, also reported several relationships between the microbiome and the soil moisture that are incongruent with our model, including the role of Acidobacteria.

Figure 3: Taxonomic aggregations (as highlighted by branch colors) inferred by trac (\(a = 1\)), that are predictive of Central Park soil pH and moisture, respectively. The color coding on the outermost ring corresponds to the estimated leaf coefficients \(\beta\) and are in units of the response (which differs in the two cases).

Figure 3 compares the aggregations across the taxonomic tree that were found by standard trac for soil pH and moisture prediction, respectively. We observe that only the phyla Bacteroidetes and Verrucomicrobia, and the order Acidobacteriales are common in both models, confirming that the relevant taxonomic aggregations depend on the response
Finally, we observe similar prediction performance in terms of test error (40 – 45), with standard trac being outperformed by the other methods across all base level aggregations. For moisture prediction, weighted trac provides an excellent trade-off between model interpretability and predictability.

| Base Level | p | trac (a = 1) | trac (a = 1/2) | Sparse Log-Contrast |
|------------|---|--------------|----------------|---------------------|
| OTU        | 3379 | 42 (8) | 40 (13) | 40 (23) |
| Genus      | 2779 | 42 (5) | 40 (17) | 41 (19) |
| Family     | 1492 | 45 (4) | 42 (12) | 41 (16) |

Table 2: Average out-of-sample test errors (model sparsity in parenthesis) for trac (a = \{1, 1/2\}) and sparse log-contrast models, respectively. Each row considers a different base level (OTU, genus, and family). Each number is averaged over ten different training/test splits of the Central Park soil, Moisture data.
Primary bacterial production in the Fram Strait

Current estimates suggest that the ocean microbiome could be responsible for about half of all primary production occurring on Earth [13, 14]. While net primary production is known to be highly influenced by a multitude of environmental drivers, including light, nutrients, and temperature [15], it is not yet established whether amplicon sequencing data alone contain enough information to serve as a stable predictor of (regional) marine primary production.

To investigate this relationship we consider a marine dataset, put forward in [16], that covers the Fram Strait, the main gateway between the North Atlantic and Arctic Oceans. The Fram Strait comprises two distinct oceanic regions, the northward flowing West Spitsbergen Current (WSC), and the East Greenland Current (EGC) flowing southward along the Greenland shelf. Recent ocean simulations, however, suggest substantial horizontal mixing and exchange by eddies between the two regions. We thus trained regression models from amplicon data across both regions and considered the available leucine incorporation (as proxy to bacterial production) as the outcome [16]. We learned separate models for the two different size fractions: \( p = 4530 \) free-living (FL) taxa in the 0.22 \( \mu m \) fraction, and \( p = 3320 \) particle-associated (PA) taxa in 3 \( \mu m \) fraction.

![Figure 4](image)

Figure 4: Predictions by \texttt{trac} \((a = 1)\) of primary production (leucine) from free-living (FL) and particle-associated (PA) taxa. The data points are colored by region in the Fram Strait: West Spitsbergen Current (WSC), and the East Greenland Current (EGC). The correlation between predicted and measured leucine (on the test set of split 1) is 0.57 for FL taxa and 0.90 and PA taxa, respectively. Tables 20 and 23 show the selected taxa for these models.

On the FL dataset, \texttt{trac} \((a = 1)\) identifies a parsimonious model, comprising three aggregated taxonomic groups, strongly associated with bacterial production. The two classes Gammaproteobacteria and Alphaproteobacteria are negatively associated, and the family Flavobacteriaceae is positively associated with bacterial production, leading to a two-factor
log-contrast model. On the PA dataset, standard trac infers a single predictive log-contrast with the Flavobacteriaceae family being positively associated and the entire phylum Proteobacteria negatively associated with primary production. On the test data (split 1), the PA model predictions show a correlation of 0.90 with the measurements. Figure 4 summarizes the scatter plots of leucine measurements vs. trac predictions for the two size fractions, colored by region WSC and EGC, respectively.

We observe that the PA model appears to serve as an implicit region classifier since predicted leucine values of < 17 belong uniquely to samples in the low-productivity EGC region (see top right panel in Figure 4). Our model suggests an important positive association of the heterotrophic Flavobacteriaceae with primary production, independent of size class. Flavobacteriaceae are known to strongly contribute to mineralization of primary-produced organic matter (see [17] and references therein), thus suggesting an indirect relationship between Flavobacteriaceae and primary production. However, previous studies in South polar front and antarctic zone postulated a strong role of Flavobacteriaceae for polar primary production [18].

As highlighted in Tables 3 and 4, weighted trac and log-contrast models lead to sparse models and outperform standard trac in terms of average test error. In the FL data set (data split 1), weighted trac selects both higher order aggregations and two OTUs both of which are also selected by the log-contrast models. For the PA dataset, all models result in single log-ratio models, either on the phylum/family level or OTU level, respectively.

| Base Level | $p$ | trac ($a = 1$) | trac ($a = 1/2$) | Sparse Log-Contrast |
|------------|-----|---------------|------------------|---------------------|
| OTU        | 3320| 1.3e+02 (4)   | 1.2e+02 (5)      | 84 (5)              |
| Genus      | 1796| 1.1e+02 (5)   | 1e+02 (4)        | 81 (4)              |
| Family     | 597 | 1.2e+02 (3)   | 1e+02 (4)        | 99 (6)              |

Table 3: Average out-of-sample test errors (model sparsity in parenthesis) for trac ($a = \{1, 1/2\}$) and sparse log-contrast models, respectively. Each row considers a different base level (OTU, genus, and family). Each number is averaged over ten different training/test splits of the Fram Strait (PA) data.

| Base Level | $p$ | trac ($a = 1$) | trac ($a = 1/2$) | Sparse Log-Contrast |
|------------|-----|---------------|------------------|---------------------|
| OTU        | 4510| 1.9e+02 (2)   | 1.5e+02 (5)      | 1.7e+02 (4)         |
| Genus      | 2930| 1.9e+02 (3)   | 1.5e+02 (4)      | 1.4e+02 (6)         |
| Family     | 1125| 1.8e+02 (4)   | 1.4e+02 (4)      | 1.5e+02 (4)         |

Table 4: Average out-of-sample test errors (model sparsity in parenthesis) for trac ($a = \{1, 1/2\}$) and sparse log-contrast models, respectively. Each row considers a different base level (OTU, genus, and family). Each number is averaged over ten different training/test splits of the Fram Strait (FL) data.
Global predictive model of ocean salinity from Tara data

We complement the Tara data set analysis from the main text with showing the scatter plot of measured vs. predicted salinity for the standard trac model (trained on data split 1) in Figure 5.

Figure 5: Measured salinity (y-axis) vs. standard trac \((a = 1)\) model prediction (x-axis) on the Tara data (model training performed on data split 1). Each sample is colored by one of the four Longhurst Biome definitions. Outliers to the model are located in Coastal and Westerlies Biomes.
Table 5: Coefficients selected by trac \((a = 1)\) for Gut (HIV): sCD14

| Kingdom | Phylum      | Class     | Order      | Family            | Genus   | Species | OTU          | \(\alpha\) |
|---------|-------------|-----------|------------|-------------------|---------|---------|--------------|-----------|
| Bacteria| Firmicutes  | Clostridia| Clostridiales| Ruminococcaceae  |         |         |              | 2221.75   |
| Bacteria| Firmicutes  | Clostridia| Clostridiales| Lachnospiraceae  |         |         |              | -1644.86  |
| Bacteria| Actinobacteria|        |            |                   |         |         |              | -501.43   |
| Bacteria|             |           |            |                   |         |         |              | -362.27   |
| Bacteria| Bacteroidetes| Bacteroidia| Bacteroidales| Bacteroidaceae | Bacteroides | |              | 286.80    |

Table 6: Coefficients selected by trac \((a = 1/2)\) for Gut (HIV): sCD14

| Kingdom | Phylum      | Class     | Order      | Family            | Genus   | Species | OTU          | \(\alpha\) |
|---------|-------------|-----------|------------|-------------------|---------|---------|--------------|-----------|
| Bacteria| Firmicutes  | Clostridia| Clostridiales| Ruminococcaceae  |         |         |              | 629.10    |
| Bacteria| Actinobacteria|        |            |                   |         |         |              | -570.60   |
| Bacteria| Firmicutes  | Negativicutes| Selenomonadales| Veillonellaceae | Mitsuokella |       | Otu000070  | -126.83   |
| Bacteria| Firmicutes  | Clostridia| Clostridiales| Lachnospiraceae  | Lachnospira|        |              | -124.49   |
| Bacteria| Firmicutes  | Clostridia| Clostridiales| Ruminococcaceae  | Subdoligranulum|        |              | 121.80    |
| Bacteria| Bacteroidetes| Bacteroidia| Bacteroidales| Bacteroidaceae  | Bacteroides |       |              | 82.62     |
| Bacteria| Bacteroidetes| Bacteroidia| Bacteroidales| Bacteroidaceae  | Bacteroides | Otu000014 | 51.81        |
| Bacteria| Firmicutes  | Clostridia| Clostridiales| Lachnospiraceae  | Lachnospira| Otu000038 | -49.69       |
| Bacteria| Bacteroidetes| Bacteroidia| Bacteroidales| Prevotellaceae  | Alloprevotella| Otu000011 | -41.31       |
| Bacteria| Firmicutes  | Clostridia| Clostridiales| Ruminococcaceae  | Incertae_Sedis | Otu000073 | -39.42       |
| Bacteria| Actinobacteria| Actinobacteria| Bifidobacteriales| Bifidobacteriaceae | Bifidobacterium | Otu000098 | -12.61       |

D  Additional Selected Coefficient Tables

Table 7: Coefficients selected by the sparse log-contrast method for Gut (HIV): sCD14

| Kingdom   | Phylum      | Class     | Order      | Family            | Genus   | Species | OTU          | \(\beta\) |
|-----------|-------------|-----------|------------|-------------------|---------|---------|--------------|-----------|
| Bacteria  | Bacteroidetes| Bacteroidia| Bacteroidales| Bacteroidaceae  | Bacteroides | Otu000014 | 123.92       |
| Bacteria  | Firmicutes  | Negativicutes| Selenomonadales| Veillonellaceae | Mitsuokella | Otu000070 | -105.59      |
| Bacteria  | Firmicutes  | Clostridia| Clostridiales| Ruminococcaceae  |         |         |              | 83.15     |
| Bacteria  | Actinobacteria| Coriobacteriia| Coriobacteriales| Coriobacteriaceae | Collinsella | Otu000020 | -71.72       |
| Bacteria  | Actinobacteria| Bacteroidetes| Bacteroidiales| Prevotellaceae  | Alloprevotella| Otu000011 | 59.25        |
| Bacteria  | Firmicutes  | Clostridia| Clostridiales| Lachnospiraceae  | Lachnospira| Otu000038 | -79.26       |
| Bacteria  | Proteobacteria| Deltaproteobacteria| Desulfovibrionales| Desulfovibrionaceae | Desulfovibrio | Otu000143 | 16.21        |
Table 8: Coefficients selected by trac on family level (a = 1) for Gut (HIV): sCD14

| Kingdom | Phylum    | Class      | Order         | Family     | Genus    | Species | OTU | α   |
|---------|-----------|------------|---------------|------------|----------|---------|-----|-----|
| Bacteria| Actinobacteria | -440.80   |               |            |          |         |     |     |
| Bacteria|            |            |               |            |          |         |     | 303.19 |
| Bacteria| Cyanobacteria | Melainabacteria | Gastranaerophilales | 137.61 |          |         |     |     |

Table 9: Coefficients selected by trac on family level (a = 1/2) for Gut (HIV): sCD14

| Kingdom | Phylum    | Class      | Order         | Family     | Genus    | Species | OTU | α   |
|---------|-----------|------------|---------------|------------|----------|---------|-----|-----|
| Bacteria| Actinobacteria | -419.10   |               |            |          |         |     |     |
| Bacteria|            |            |               |            |          |         |     | 301.98 |
| Bacteria| Proteobacteria | Gammaproteobacteria | Enterobacteriales | Enterobacteriaceae | 112.87 |          |     |     |
| Bacteria| Bacteroidetes | Bacteroidia | Bacteroidales | Bacteroidiaceae | 9.42     |          |     |     |
| Bacteria| Proteobacteria | Gammaproteobacteria | Aeromonadales | Succinivibrionaceae | -5.18   |          |     |     |

Table 10: Coefficients selected by the sparse log-contrast method on family level for Gut (HIV): sCD14

| Kingdom | Phylum    | Class      | Order         | Family     | Genus    | Species | OTU | β   |
|---------|-----------|------------|---------------|------------|----------|---------|-----|-----|
| Life    | Bacteria  | Actinobacteria | Coriobacteriia | Coriobacteriales | Coriobacteriaceae | -317.40 |   |
| Life    | Bacteria  | Proteobacteria | Gammaproteobacteria | Enterobacteriales | Enterobacteriaceae | 177.47 |   |
| Life    | Bacteria  | Cyanobacteria | Melainabacteria | Gastranaerophilales | [Unclassified] | 138.24 |   |
| Life    | Bacteria  | Firmicutes  | Clostridia    | Clostridiales | Lachnospiraceae | -68.26 |   |
| Life    | Bacteria  | Firmicutes  | Clostridia    | Clostridiales | Delfluvitalaceae | 44.07  |   |
| Life    | Bacteria  | Firmicutes  | Clostridia    | Clostridiales | [Unclassified] | 25.88  |   |

Table 11: Top 15 coefficients selected by trac (a = 1) for Gut (AGP): BMI

| Kingdom | Phylum    | Class      | Order         | Family     | Genus    | Species | OTU | α   |
|---------|-----------|------------|---------------|------------|----------|---------|-----|-----|
| Bacteria| Firmicutes | Clostridia | Clostridiales | Ruminococcaceae | 2.86 |          |     |     |
| Bacteria| Firmicutes | Clostridia | Clostridiales | Lachnospiraceae | 2.23 |          |     |     |
| Bacteria| Bacteroidetes |            |               |            |          |         |     | 1.45 |
| Bacteria| Firmicutes | Clostridia | Clostridiales | Veillonellaceae | 1.18 |          |     |     |
| Bacteria| Firmicutes | Erysipelotrichi | Erysipelotrichaelaceae | 0.90 |          |     |     |
| Bacteria| Firmicutes | Clostridia | Clostridiales | Lachnospiraceae | Blautia | 0.73  |   |
| Bacteria| Firmicutes | Bacilli    | Lactobacillales |          | 0.72  |          |     |     |
| Bacteria| Firmicutes | Clostridia | Clostridiales | Veillonellaceae | 0.71  |          |     |     |
| Bacteria| Firmicutes | Clostridia | Clostridiales | Lachnospiraceae | Dorea | 0.51  |   |
| Bacteria| Firmicutes | Clostridia | Clostridiales | Ruminococcaceae | Ruminococcus | 0.49  |   |
| Bacteria| Firmicutes | Clostridia | Clostridiales | [Mogibacteriaceae] | -0.36 |          |     |     |
| Bacteria| Bacteroidetes | Bacteroidia | Bacteroidiales | [Barnesiellaceae] | 0.32  |          |     |     |
| Bacteria| Firmicutes | Clostridia | Clostridiales | Ruminococcaceae | - | - | 4356062 | 0.30 |
Table 12: Top 15 coefficients selected by trac \((a = 1/2)\) for Gut (AGP): BMI

| Kingdom   | Phylum      | Class          | Order         | Family            | Genus       | Species | OTU         | \(\alpha\) |
|-----------|-------------|----------------|---------------|-------------------|-------------|---------|-------------|------------|
| Bacteria  | Firmicutes  | Erysipelotrichi| Erysipelotrichales | Erysipelotrichaceae | -          | -       | 4356062     | -0.30      |
| Bacteria  | Firmicutes  | Clostridia     | Clostridiales  | Ruminococcaceae   | -           | -       | 4361859     | 0.29       |
| Bacteria  | Gammaproteobacteria | Enterobacteriales | Enterobacteriaceae | -               | -           | -       | -           | -0.24      |
| Bacteria  | Firmicutes  | Bacilli        | Lactobacillales| -                 | -           | -       | 0.23        |            |
| Bacteria  | Gammaproteobacteria | Pasteurellales | Pasteurellaceae | Haemophilus       | parainfluenza | 4477696 | -0.21       |            |
| Bacteria  | Firmicutes  | Clostridia     | Clostridiales  | Lachnospiraceae   | Blautia     | -       | 181871      | 0.19       |
| Bacteria  | Firmicutes  | Clostridia     | Clostridiales  | Lachnospiraceae   | Blautia     | -       | 4361859     | 0.19       |
| Bacteria  | Firmicutes  | Clostridia     | Clostridiales  | [Tissierellaceae] | Finegoldha  | -       | 1096610     | 0.17       |
| Bacteria  | Firmicutes  | Erysipelotrichi| Erysipelotrichales | Erysipelotrichaceae | -          | -       | 4480861     | 0.16       |
| Bacteria  | Firmicutes  | Erysipelotrichi| Erysipelotrichales | Erysipelotrichaceae | -          | -       | 145801      | -0.15      |
| Bacteria  | Firmicutes  | Clostridia     | Clostridiales  | -                 | -           | -       | 195004      | 0.14       |
| Bacteria  | Firmicutes  | Erysipelotrichi| Erysipelotrichales | Erysipelotrichaceae | -          | -       | -           | -0.14      |
| Bacteria  | Firmicutes  | Erysipelotrichi| Erysipelotrichales | Erysipelotrichaceae | -          | -       | 181871      | 0.15       |
| Bacteria  | Firmicutes  | Clostridia     | Clostridiales  | -                 | -           | -       | 4356062     | 0.29       |
| Bacteria  | Firmicutes  | Clostridia     | Clostridiales  | Lachnospiraceae   | Blautia     | -       | 4361859     | 0.16       |
| Bacteria  | Firmicutes  | Clostridia     | Clostridiales  | Lachnospiraceae   | Dorea       | -       | 181871      | 0.15       |
| Bacteria  | Firmicutes  | Clostridia     | Clostridiales  | -                 | -           | -       | 340876      | -0.10      |
| Actinobacteria | Firmicutes | Erysipelotrichi| Erysipelotrichales | Erysipelotrichaceae | -          | -       | 4480861     | 0.14       |
| Bacteria  | Firmicutes  | Erysipelotrichi| Erysipelotrichales | Erysipelotrichaceae | -          | -       | 4393532     | -0.12      |

Table 13: Top 15 coefficients selected by the sparse log-contrast method for Gut (AGP): BMI

| Kingdom   | Phylum      | Class          | Order         | Family            | Genus       | Species | OTU         | \(\beta\) |
|-----------|-------------|----------------|---------------|-------------------|-------------|---------|-------------|-----------|
| Bacteria  | Firmicutes  | Clostridia     | Clostridiales  | Ruminococcaceae   | -           | -       | 4356062     | 0.29      |
| Bacteria  | Proteobacteria | Gammaproteobacteria | Pasteurellales | Pasteurellaceae | Haemophilus | parainfluenza | 4477696 | -0.19     |
| Bacteria  | Firmicutes  | Erysipelotrichi| Erysipelotrichales | Erysipelotrichaceae | -          | -       | 145801      | -0.16     |
| Bacteria  | Firmicutes  | Clostridia     | Clostridiales  | Lachnospiraceae   | Blautia     | -       | 4361859     | 0.16      |
| Bacteria  | Firmicutes  | Clostridia     | Clostridiales  | Lachnospiraceae   | Dorea       | -       | 181871      | 0.15      |
| Bacteria  | Firmicutes  | Erysipelotrichi| Erysipelotrichales | Erysipelotrichaceae | -          | -       | 4480861     | 0.14      |
| Bacteria  | Firmicutes  | Clostridia     | Clostridiales  | -                 | -           | -       | 1096610     | 0.13      |
| Bacteria  | Firmicutes  | Bacilli        | Bacillales     | Staphylococcaceae | Staphylococcus | aureus | 4446058     | -0.13     |
| Bacteria  | Firmicutes  | Clostridia     | Clostridiales  | Lachnospiraceae   | -           | -       | 4457438     | 0.11      |
| Bacteria  | Firmicutes  | Clostridia     | Clostridiales  | Ruminococcaceae   | -           | -       | 2018038     | 0.13      |
| Actinobacteria | Firmicutes | Erysipelotrichi| Erysipelotrichales | Erysipelotrichaceae | -          | -       | 4393532     | -0.10     |
| Actinobacteria | Firmicutes | Clostridia     | Clostridiales  | Lachnospiraceae   | -           | -       | 4379449     | -0.10     |
| Bacteria  | Firmicutes  | Clostridia     | Clostridiales  | -                 | -           | -       | 340876      | -0.10     |
| Bacteria  | Firmicutes  | Clostridia     | Clostridiales  | -                 | -           | -       | 2018038     | 0.13      |
| Bacteria  | Firmicutes  | Clostridia     | Clostridiales  | -                 | -           | -       | 173876      | -0.09     |
| Bacteria  | Proteobacteria | Betaproteobacteria | Burkholderiales | Oxalobacteraceae | Oxalobacter | formigenes | 7366       | -0.09     |

Table 14: Coefficients selected by trac \((a = 1)\) for Central Park Soil: pH

| Kingdom   | Phylum      | Class          | Order         | Family            | Genus       | Species | OTU         | \(\alpha\) |
|-----------|-------------|----------------|---------------|-------------------|-------------|---------|-------------|------------|
| Bacteria  | Acidobacteria | Acidobacteria-6 | -            | -                 | -           | -       | -           | -0.74      |
| Bacteria  | Bacteroidetes | -            | -            | -                 | -           | -       | -           | 0.58       |
| Bacteria  | Proteobacteria | Gammaproteobacteria | -        | -                 | -           | -       | -           | 0.45       |
| Bacteria  | Acidobacteria | Acidobacteriia | Acidobacteriales | -           | -           | -       | -           | -0.19      |
| Bacteria  | Verrucomicrobia | -        | -            | -                 | -           | -       | -           | -0.13      |
| Bacteria  | -            | -            | -            | -                 | -           | -       | -           | 0.03       |
Table 15: Top 15 coefficients selected by $\text{trac (a = 1/2)}$ for Central Park Soil: pH

| Kingdom | Phylum | Class | Order | Family | Genus | Species | OTU | $\alpha$ |
|---------|--------|-------|-------|--------|-------|---------|-----|---------|
| Bacteria | Acidobacteria | Acidobacteria-6 | | | | | | 0.38 |
| Bacteria | Proteobacteria | Gammaproteobacteria | Xanthomonadales | Xanthomonadaceae | | | | -0.23 |
| Bacteria | WPS-2 | | | | | | | -0.19 |
| Bacteria | Gemmatimonadales | Gemm-1 | | | | | | -0.11 |
| Bacteria | Bacteroidetes | Cytophagia | Cytophagales | Cytophagaceae | | | | 0.09 |
| Bacteria | Proteobacteria | Gammaproteobacteria | Xanthomonadales | Xanthomonadaceae | Rhodanobacter | | | -0.05 |
| Bacteria | Bacteroidetes | | | | | | | 0.05 |
| Bacteria | Acidobacteria | Acidobacteria-6 | iiil-15 | RB40 | - | - | OTU_444 | 0.05 |
| Bacteria | Proteobacteria | Alphaproteobacteria | Ellin329 | | | | | -0.04 |
| Bacteria | Acidobacteria | DA052 | Ellin6513 | | | | | -0.04 |
| Bacteria | Bacteroidetes | [Saprospirae] | [Saprospirales] | Chitinophagaceae | | | | OTU_114 | -0.06 |
| Bacteria | Bacteroidetes | Cytophagia | Cytophagales | Cytophagaceae | | | | OTU_176 | -0.04 |
| Bacteria | Proteobacteria | Gammaproteobacteria | Alteromonadales | OM60 | | | | 0.02 |
| Bacteria | Chloroflexi | Ktedonobacteria | Ktedonobacterales | Ktedonobacteraceae | | | | 0.02 |

Table 16: Top 15 coefficients selected by the sparse log-contrast method for Central Park Soil: pH

| Kingdom | Phylum | Class | Order | Family | Genus | Species | OTU | $\beta$ |
|---------|--------|-------|-------|--------|-------|---------|-----|---------|
| Bacteria | Bacteroidetes | [Saprospirae] | [Saprospirales] | Chitinophagaceae | | | | OTU_7 | -0.04 |
| Bacteria | Acidobacteria | Solibacteres | Solibacterales | Solibacteraceae | Candidatus Solibacter | | | OTU_114 | -0.06 |
| Bacteria | Acidobacteria | Acidobacteria-6 | iiil-15 | RB40 | - | - | OTU_444 | 0.05 |
| Bacteria | Acidobacteria | [Chloracidobacteria] | | | | | | OTU_129299 | 0.04 |
| Bacteria | Bacteroidetes | [Saprospirae] | [Saprospirales] | Chitinophagaceae | | | | OTU_124173 | -0.04 |
| Bacteria | Actinobacteria | Actinobacteria | | | | | | OTU_4 | -0.04 |
| Bacteria | Verrucomicrobia | [Spartobacteria] | [Chthoniobacterales] | [Chthoniobacteraceae] | | | | OTU_435 | 0.03 |
| Bacteria | Acidobacteria | Solibacteres | Solibacterales | Solibacteraceae | | | | OTU_178 | -0.02 |
| Bacteria | Acidobacteria | DA052 | Ellin6513 | | | | | OTU_432 | -0.02 |
| Bacteria | Bacteroidetes | [Saprospirae] | [Saprospirales] | Saprospiraceae | | | | OTU_77 | 0.02 |
| Bacteria | Proteobacteria | Deltaproteobacteria | Syntrophobacterales | Syntrophobacteraceae | | | | OTU_407 | -0.01 |
| Bacteria | Proteobacteria | Gammaproteobacteria | Enterobacterales | Enterobacteriaceae | Klebsiella | | | OTU_62 | -0.01 |
| Bacteria | Planctomycetes | Planctomycetacia | Pirellulales | Pirellulaceae | | | | OTU_12778 | -0.01 |
| Bacteria | Proteobacteria | Alphaproteobacteria | Ellin329 | | | | | OTU_90 | -0.01 |
| Bacteria | Bacteroidetes | [Saprospirae] | [Saprospirales] | Chitinophagaceae | | | | OTU_190 | -0.01 |

Table 17: Top 15 coefficients selected by $\text{trac (a = 1)}$ for Central Park Soil: Mois

| Kingdom | Phylum | Class | Order | Family | Genus | Species | OTU | $\alpha$ |
|---------|--------|-------|-------|--------|-------|---------|-----|---------|
| Bacteria | Proteobacteria | | | | | | | 26.58 |
| Bacteria | Bacteroidetes | Proteobacteria | | | | | | 13.68 |
| Bacteria | Bacteroidetes | Deltaproteobacteria | | | | | | 9.71 |
| Bacteria | Bacteroidetes | Alphaproteobacteria | | | | | | 6.77 |
| Bacteria | Bacteroidetes | | | | | | | 4.89 |
| Bacteria | Acidobacteria | | | | | | | 4.68 |
| Bacteria | Bacteroidetes | Sphingobacterales | Sphingobacteriales | | | | | 3.25 |
| Bacteria | Actinobacteria | Thermoleophilia | Gaellales | | | | | 3.01 |
| Bacteria | Verrucomicrobia | | | | | | | 2.66 |
| Bacteria | Proteobacteria | Alphaproteobacteria | Sphingomonadales | Sphingomonadaceae | | | | 2.40 |
| Bacteria | Actinobacteria | | | | | | | 2.38 |
| Bacteria | Proteobacteria | Betaproteobacteria | | | | | | 2.16 |
| Bacteria | Acidobacteria | Acidobacteriales | | | | | | 1.99 |
| Bacteria | Verrucomicrobia | [Pedosphaerae] | [Pedosphaerales] | | | | | 1.37 |
| Bacteria | Actinobacteria | Thermoleophilia | Solirubrobacterales | | | | | 1.24 |
Table 18: Top 15 coefficients selected by trac \((a = 1/2)\) for Central Park Soil: Mois

| Kingdom | Phylum | Class | Order | Family | Genus | Species | OTU | \(\alpha\) |
|---------|--------|-------|-------|--------|-------|---------|-----|---------|
| Bacteria | Proteobacteria | | | | | | 6.07 | |
| Bacteria | Verrucomicrobia | | | | | | -3.44 | |
| Bacteria | Proteobacteria | | | | | | 1.83 | |
| Bacteria | Actinobacteria | | | | | | -1.51 | |
| Bacteria | Actinobacteria | | | | | | -0.71 | |
| Bacteria | Acidobacteria | | | | | | -0.57 | |
| Archaean | Crenarchaeota | | | | | | -0.47 | |
| Bacteria | Proteobacteria | | | | | | -0.17 | |
| Bacteria | Proteobacteria | | | | | | 0.24 | |
| Bacteria | Actinobacteria | | | | | | -0.47 | |

Table 19: Coefficients selected by the sparse log-contrast method for Central Park Soil: Mois

| Kingdom | Phylum | Class | Order | Family | Genus | Species | OTU | \(\beta\) |
|---------|--------|-------|-------|--------|-------|---------|-----|---------|
| Bacteria | Acidobacteria | | | | | | -0.77 | |
| Bacteria | Bacteroidetes | | | | | | 0.46 | |
| Bacteria | Bacteroidetes | | | | | | 0.33 | |
| Bacteria | Proteobacteria | | | | | | 0.27 | |
| Bacteria | Actinobacteria | | | | | | -0.20 | |
| Bacteria | Proteobacteria | | | | | | 0.20 | |
| Bacteria | Planctomyxetes | | | | | | -0.16 | |
| Bacteria | Proteobacteria | | | | | | 0.13 | |
| Bacteria | Bacteroidetes | | | | | | -0.12 | |
| Bacteria | Actinobacteria | | | | | | -0.11 | |
| Bacteria | Proteobacteria | | | | | | 0.03 | |
| Bacteria | Verrucomicrobia | | | | | | 0.03 | |
| Archaean | Crenarchaeota | | | | | | 0.01 | |

Table 20: Coefficients selected by trac \((a = 1)\) for Fram Strait (FL): Leucine

| Kingdom | Phylum | Class | Order | Family | Genus | Species | OTU | \(\alpha\) |
|---------|--------|-------|-------|--------|-------|---------|-----|---------|
| Bacteria | Bacteroidetes | Flavobacteria | Flavobacteriales | Flavobacteriaceae | | | 27.90 | |
| Bacteria | Proteobacteria | Alphaproteobacteria | | | | | -23.40 | |
| Bacteria | Proteobacteria | Gammaproteobacteria | | | | | -4.49 | |

Table 21: Coefficients selected by trac \((a = 1/2)\) for Fram Strait (FL): Leucine

| Kingdom | Phylum | Class | Order | Family | Genus | Species | OTU | \(\alpha\) |
|---------|--------|-------|-------|--------|-------|---------|-----|---------|
| Bacteria | Bacteroidetes | Flavobacteria | Flavobacteriales | Flavobacteriaceae | | | 14.30 | |
| Bacteria | Proteobacteria | Alphaproteobacteria | | | | | -8.99 | |
| Bacteria | Proteobacteria | Gammaproteobacteria | | | | | -4.30 | |
| Bacteria | Proteobacteria | Alphaproteobacteria | | | | | 0.79 | |
| Bacteria | Proteobacteria | Gammaproteobacteria | | | | | -0.22 | |

Table 22: Coefficients selected by the sparse log-contrast method for Fram Strait (FL): Leucine

| Kingdom | Phylum | Class | Order | Family | Genus | Species | OTU | \(\beta\) |
|---------|--------|-------|-------|--------|-------|---------|-----|---------|
| Bacteria | Bacteroidetes | Flavobacteria | Flavobacteriales | Flavobacteriaceae | | | -0.79 | |
| Bacteria | Bacteroidetes | Flavobacteria | Flavobacteriales | NS9 marine group | | | 1.44 | |
| Bacteria | Proteobacteria | Alphaproteobacteria | | | | | -0.83 | |
| Bacteria | Proteobacteria | Gammaproteobacteria | | | | | -0.61 | |
Table 23: Coefficients selected by trac \((a = 1)\) for Fram Strait (PA): Leucine

| Kingdom | Phylum      | Class           | Order                | Family            | Genus     | Species | OTU | \(\alpha\) |
|---------|-------------|-----------------|----------------------|-------------------|-----------|---------|-----|------------|
| Bacteria| Proteobacteria |                |                      |                   |           |         |     | -13.93     |
| Bacteria| Bacteroidetes| Flavobacteriia  | Flavobacteriales      | Flavobacteriaceae |           |         |     | 13.93      |

Table 24: Coefficients selected by trac \((a = 1/2)\) for Fram Strait (PA): Leucine

| Kingdom | Phylum      | Class           | Order                | Family            | Genus     | Species | OTU | \(\alpha\) |
|---------|-------------|-----------------|----------------------|-------------------|-----------|---------|-----|------------|
| Bacteria| Planctomycetes |                |                      |                   |           |         |     | -6.79      |
| Bacteria| Proteobacteria | Alphaproteobacteria | Rhodobacterales    | Rhodobacteriaceae |           |         |     | 6.79       |

Table 25: Coefficients selected by the sparse log-contrast method for Fram Strait (PA): Leucine

| Kingdom | Phylum      | Class           | Order                | Family            | Genus     | Species | OTU | \(\beta\) |
|---------|-------------|-----------------|----------------------|-------------------|-----------|---------|-----|----------|
| Bacteria| Proteobacteria | Alphaproteobacteria | Rhodobacterales    | Sulfitobacter     |           |         |     | 1.41     |
| Bacteria| Proteobacteria | Deltaproteobacteria | Bdellovibrionales  | OM27 clade        |           |         |     | -1.41    |

Table 26: Coefficients selected by trac \((a = 1)\) for Ocean (TARA): Salinity

| Kingdom | Phylum      | Class           | Order                | Family            | Genus     | Species | OTU | \(\alpha\) |
|---------|-------------|-----------------|----------------------|-------------------|-----------|---------|-----|------------|
| Bacteria| Proteobacteria | Alphaproteobacteria |                |                   |           |         |     | 4.00      |
| Bacteria| Bacteroidetes |                |                      |                   |           |         |     | -2.92     |
| Bacteria| Bacteroidetes |                |                      |                   |           |         |     | -1.38     |
| Bacteria| Proteobacteria | Gammaproteobacteria |                |                   |           |         |     | 0.30      |

Table 27: Coefficients selected by trac \((a = 1/2)\) for Ocean (TARA): Salinity

| Kingdom | Phylum      | Class           | Order                | Family            | Genus     | Species | OTU | \(\alpha\) |
|---------|-------------|-----------------|----------------------|-------------------|-----------|---------|-----|------------|
| Bacteria| Bacteroidetes | Flavobacteriia  | Flavobacteriales      | NS9marinegroup    |           |         |     | -0.96     |
| Bacteria| Proteobacteria | Alphaproteobacteria | SAR1 clade         |                   |           |         |     | 0.55      |
| Bacteria| Proteobacteria | Alphaproteobacteria |                   |                   |           |         |     | 0.38      |
| Bacteria| Proteobacteria | Gammaproteobacteria | Oceanospirillales   | Halomonadaceae    |           |         |     | -0.37     |
| Bacteria| Cyanobacteria |                |                      |                   |           |         |     | 0.25      |
| Bacteria| Cyanobacteria | Cyanobacteriia  | Subsection1          | Family            | Synochococcus |     | 0.12 |
| Bacteria| Proteobacteria | Gammaproteobacteria | E01-9C-26 marine group |                |           |         |     | 0.09      |
| Bacteria| Proteobacteria | Gammaproteobacteria | Alteromonadaceae    | SAR86 clade       |           |         |     | -0.07     |
| Bacteria| Cyanobacteria | Cyanobacteriia  |                        |                   |           |         |     | 0.02      |
| Bacteria| Bacteroidetes |                |                      |                   |           |         |     | -0.02     |

Table 28: Coefficients selected by the sparse log-contrast method for Ocean (TARA): Salinity

| Kingdom | Phylum      | Class           | Order                | Family            | Genus     | Species | OTU | \(\beta\) |
|---------|-------------|-----------------|----------------------|-------------------|-----------|---------|-----|----------|
| Bacteria| Proteobacteria | Gammaproteobacteria | E01-9C-26 marine group | |           |         |     | 0.25  |
| Bacteria| Proteobacteria | Gammaproteobacteria | Oceanospirillales | SAR86 clade |           |         |     | -0.11  |
| Bacteria| Verrucomicrobia | Verrucomicrobia | Verrucomicrobiaceae | Roseibacillus     |           |         |     | -0.05  |
| Bacteria| Proteobacteria | Gammaproteobacteria | Alteromonadaceae    | Meltkea           |           |         |     | 0.05  |
| Bacteria| Verrucomicrobia | Verrucomicrobia | Verrucomicrobiaceae | Salimphycaceae    |           |         |     | 0.04  |
| Bacteria| Bacteroidetes | Flavobacteriia  | Flavobacteriales      | NS9 marine group  |           |         |     | -0.04  |
| Bacteria| Proteobacteria | Gammaproteobacteria | Alteromonadaceae    | Idiomarinaceae    |           |         |     | -0.02  |
| Bacteria| Actinobacteria | Acidimicrobiia  | Acidimicrobiaceae    | OC3 marine group  |           |         |     | 0.02  |
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