Supplement material for Variational Inference of Sparse Network from Count Data (ICML 2019)

S1 Proof of Proposition 1

We first prove the concavity of $J(\mathbf{B}, \mathbf{M}, \mathbf{S})$. For fixed $\mathbf{\Omega}$, the quadratic form associated to the Hessian of J is

$$f : \boldsymbol{\theta} = \mathrm{vec}(\Delta\mathbf{B}, \Delta\mathbf{M}, \Delta\mathbf{S}) \mapsto f(\boldsymbol{\theta}) = \boldsymbol{\theta}^\intercal \, \nabla^2_{\mathbf{B},\mathbf{M},\mathbf{S}} J(\mathbf{B}, \mathbf{M}, \mathbf{S}, \mathbf{\Omega}) \, \boldsymbol{\theta}.$$

Let $\sqrt{\mathbf{A}}$ be the element-wise square-root of matrix $\mathbf{A}$ and $\mathbf{S}^{\oslash}$ the element-wise inverse of matrix $\mathbf{S}$. The quadratic form simplifies to

$$\begin{aligned} f(\boldsymbol{\theta}) = & - \mathrm{tr}([\sqrt{\mathbf{A}} \odot \mathbf{X}\Delta\mathbf{B}]^\intercal [\sqrt{\mathbf{A}} \odot \mathbf{X}\Delta\mathbf{B}]) - 2\,\mathrm{tr}([\sqrt{\mathbf{A}} \odot \mathbf{X}\Delta\mathbf{B}]^\intercal [\sqrt{\mathbf{A}} \odot \Delta\mathbf{M}]) \\ & - \mathrm{tr}([\sqrt{\mathbf{A}} \odot \mathbf{X}\Delta\mathbf{B}]^\intercal [\sqrt{\mathbf{A}} \odot \Delta\mathbf{S}]) - \mathrm{tr}([\sqrt{\mathbf{A}} \odot \Delta\mathbf{M}]^\intercal [\sqrt{\mathbf{A}} \odot \Delta\mathbf{M}]) \\ & - \mathrm{tr}([\sqrt{\mathbf{A}} \odot \Delta\mathbf{M}]^\intercal [\sqrt{\mathbf{A}} \odot \Delta\mathbf{S}]) - \mathrm{tr}([\sqrt{\mathbf{A}} \odot \Delta\mathbf{S}]^\intercal [\sqrt{\mathbf{A}} \odot \Delta\mathbf{S}])/4 \\ & - \mathrm{tr}(\Delta\mathbf{M}\mathbf{\Omega}\Delta\mathbf{M}^\intercal) - \mathrm{tr}([\mathbf{S}^{\oslash} \odot \Delta\mathbf{S}]^\intercal [\mathbf{S}^{\oslash} \odot \Delta\mathbf{S}])/2 \\ & = -\|\sqrt{\mathbf{A}} \odot [\mathbf{X}\Delta\mathbf{B} + \Delta\mathbf{M} + \Delta\mathbf{S}/2]\|_F^2 - \|\Delta\mathbf{M}\mathbf{\Omega}^{1/2}\|_F^2 - \|\mathbf{S}^{\oslash} \odot \Delta\mathbf{S}\|_F^2/2 \\ & \leq 0, \end{aligned}$$

hence the Hessian matrix is negative semi-definite, which proves the concavity of $J(\mathbf{B}, \mathbf{M}, \mathbf{S})$. For strictness, consider a triplet $(\Delta\mathbf{B}, \Delta\mathbf{M}, \Delta\mathbf{S})$ such that $f(\boldsymbol{\theta}) = 0$. By definition of $\mathbf{S}^{\oslash}$ and the positive definiteness of $\mathbf{\Omega}$, $\Delta\mathbf{S} = \Delta\mathbf{M} = 0$. Finally, since all entries in $\mathbf{A}$ are positive, it leads to $\mathbf{X}\Delta\mathbf{B} = 0$ which implies $\Delta\mathbf{B} = 0$ as soon as $\mathbf{X}$ has full rank. The lower bound $J(\mathbf{B}, \mathbf{M}, \mathbf{S})$ is thus strictly concave with this assumption.

We now prove the concavity of $J(\mathbf{\Omega})$. The Hessian for fixed $(\mathbf{B}, \mathbf{M}, \mathbf{S})$ is

$$-\frac{n}{2}\mathbf{\Omega}^{-1} \otimes \mathbf{\Omega}^{-1},$$

where $\otimes$ denotes the Kronecker product. Since $\mathbf{\Omega}^{-1}$ is positive definite, so is $\mathbf{\Omega}^{-1} \otimes \mathbf{\Omega}^{-1}$ and therefore J is strictly concave in $\mathbf{\Omega}$. .

S2 Simulation scheme

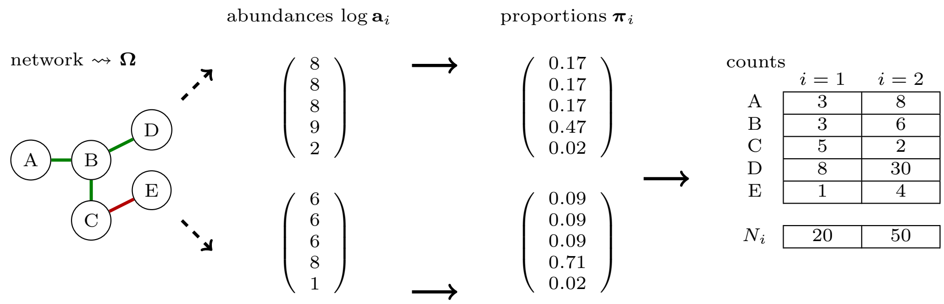

Figure 1: Compositional model used for data generation

S3 Simulation study: accounting for covariates

		area under the ROC			area under the PR		
covar.	**method**	**n = p/2**	**n = p**	**n = 2p**	**n = p/2**	**n = p**	**n = 2p**
		scale-free network					
small	PLNnetwork	.66 (0.05)	**.78** (0.05)	**.91** (0.03)	**.11** (0.04)	**.25** (0.07)	**.49** (0.08)
	sparCC	.66 (0.05)	.73 (0.05)	.79 (0.05)	.09 (0.03)	.16 (0.05)	.24 (0.07)
	SPiEC-Easi	**.67** (0.04)	.77 (0.05)	.85 (0.04)	.10 (0.03)	.17 (0.05)	.27 (0.07)
medium	PLNnetwork	**.62** (0.05)	**.73** (0.05)	**.85** (0.05)	**.09** (0.03)	**.18** (0.06)	**.34** (0.08)
	sparCC	.55 (0.05)	.57 (0.05)	.58 (0.05)	.05 (0.01)	.05 (0.01)	.06 (0.01)
	SPiEC-Easi	.61 (0.04)	.66 (0.04)	.71 (0.03)	.06 (0.01)	.06 (0.01)	.07 (0.01)
large	PLNnetwork	**.58** (0.05)	**.67** (0.05)	**.78** (0.05)	**.07** (0.03)	**.12** (0.04)	**.23** (0.07)
	sparCC	.52 (0.04)	.53 (0.04)	.53 (0.05)	.04 (0.01)	.04 (0.01)	.04 (0.01)
	SPiEC-Easi	.57 (0.04)	.60 (0.03)	.65 (0.03)	.05 (0.01)	.05 (0.01)	.05 (0.01)
		random network					
small	PLNnetwork	.77 (0.07)	**.90** (0.04)	**.96** (0.01)	**.14** (0.07)	**.36** (0.11)	**.64** (0.09)
	sparCC	.76 (0.06)	.83 (0.06)	.89 (0.04)	.11 (0.05)	.23 (0.09)	.36 (0.11)
	SPiEC-Easi	**.78** (0.05)	.87 (0.04)	.92 (0.03)	.11 (0.05)	.23 (0.09)	.36 (0.11)
medium	PLNnetwork	**.72** (0.06)	**.85** (0.05)	**.94** (0.02)	**.09** (0.04)	**.24** (0.09)	**.49** (0.10)
	sparCC	.59 (0.06)	.61 (0.07)	.62 (0.06)	.03 (0.01)	.04 (0.02)	.04 (0.02)
	SPiEC-Easi	.67 (0.05)	.74 (0.05)	.77 (0.03)	.04 (0.01)	.05 (0.02)	.05 (0.01)
large	PLNnetwork	**.64** (0.07)	**.78** (0.06)	**.88** (0.04)	**.06** (0.03)	**.14** (0.07)	**.29** (0.09)
	sparCC	.54 (0.05)	.53 (0.06)	.54 (0.06)	.02 (0.01)	.02 (0.01)	.03 (0.01)
	SPiEC-Easi	.61 (0.05)	.65 (0.04)	.68 (0.03)	.03 (0.00)	.03 (0.00)	.03 (0.01)
		community network					
small	PLNnetwork	.60 (0.04)	.69 (0.04)	**.78** (0.05)	**.17** (0.03)	**.26** (0.04)	**.38** (0.05)
	sparCC	**.62** (0.04)	.66 (0.04)	.70 (0.04)	.16 (0.02)	.21 (0.04)	.26 (0.04)
	SPiEC-Easi	**.62** (0.04)	**.70** (0.04)	.77 (0.04)	**.17** (0.02)	.24 (0.04)	.31 (0.04)
medium	PLNnetwork	.57 (0.03)	**.65** (0.04)	**.73** (0.05)	**.15** (0.02)	**.22** (0.03)	**.31** (0.05)
	sparCC	.55 (0.03)	.56 (0.04)	.56 (0.03)	.11 (0.02)	.12 (0.02)	.12 (0.02)
	SPiEC-Easi	**.58** (0.03)	.63 (0.03)	.67 (0.03)	.13 (0.02)	.14 (0.02)	.15 (0.02)
large	PLNnetwork	**.55** (0.03)	**.60** (0.04)	**.67** (0.04)	**.13** (0.02)	**.17** (0.03)	**.24** (0.04)
	sparCC	.52 (0.03)	.52 (0.03)	.52 (0.03)	.10 (0.02)	.10 (0.02)	.10 (0.02)
	SPiEC-Easi	**.55** (0.03)	.58 (0.03)	.62 (0.03)	.11 (0.01)	.11 (0.02)	.12 (0.01)

Table 1: Areas under the ROC curve and Areas under the Precision-Recall curve of the compositional methods (`PLNnetwork`, `sparCC` and `SPiEC-Easi`) in various settings, averaged over 100 simulations, with standard errors.

S4 Table of OTU

Type	OTU	Family	Genus	Species
Fungi	f1	Dermateaceae	Naevala	Naevala minutissima
	f3	–	–	–
	f4	Erysiphaceae	Erysiphe	Erysiphe hypophylla
	f8	Hyaloscyphaceae	Catenulifera	Catenulifera brevicollaris
	f10	–	–	–
	f12	Amphisphaeriaceae	Monochaetia	Monochaetia kansensis
	f17	Herpotrichiellaceae	Cyphellophora	Cyphellophora hylomeconis
	f19	–	–	–
	f25	unidentified	Cryptococcus	Cryptococcus magnus
	f27	unidentified	Strelitziana	Strelitziana mali
	f29	Mycosphaerellaceae	Xenosonderhenia	Xenosonderhenia syzygii
	f32	–	–	–
	f39	–	–	–
	f1085	Mycosphaerellaceae	Mycosphaerella	Mycosphaerella marksii
	f1090	Herpotrichiellaceae	Cyphellophora	Cyphellophora hylomeconis
	f1278	Mycosphaerellaceae	Mycosphaerella	Mycosphaerella punctiformis
	Ea	Erysiphaceae	Erysiphe	Erysiphe alphitoides
Bacteria	b13	Oxalobacteraceae	–	–
	b153	Oxalobacteraceae	–	–
	b21	Pseudomonadaceae	Pseudomonas	–
	b25	Enterobacteriaceae	–	–
	b26	Oxalobacteraceae	–	–
	b33	Microbacteriaceae	Rathayibacter	–
	b364	Oxalobacteraceae	–	–
	b37	Beijerinckiaceae	Beijerinckia	–
	b44	–	–	–
	b60	–	–	–

Table 2: Type of microorganism (bacteria or fungi) and higher level taxonomic assignments (family, genus and species) of the 27 operational taxonomic units (OTUs) interacting in the inferred microbial networks. Unknown assignments at a given rank are reported as '–'.