Appendix 4: Results

Inferring species interactions from co-occurrence data with Markov networks

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A: Import packages and data

```
library(dplyr)
library(magrittr)
library(mgcv)
library(ggplot2)
library(tidyr)
library(knitr)
library(lme4)
```

Import the results from Appendix 3:

```
x = read.csv("estimates.csv", stringsAsFactors = FALSE)
x$simulation_type = gsub("[0-9]", "", x$rep_name)
```

Import the results from the *Pairs* software:

```
pairs_txt = readLines("fakedata/matrices/Pairs.txt")
library(stringr)

# Find areas of the data file that correspond
# to species pairs' results
beginnings = grep("Sp1", pairs_txt) + 1
ends = c(
  grep("^[^ ]", pairs_txt)[-1],
  length(pairs_txt) + 1
) - 1

partial_names = sapply(
  strsplit(grep("^>", pairs_txt, value = TRUE), " +"),
  function(x) x[[3]]
)
filename_lines = grep("^>", pairs_txt)

# Sort a vector of alphanumeric strings by the numeric component
```

```
# as if they were integers.  For example, V20 should be larger
# than V12, even though V12 comes first alphabetically
alnum_sort = function(x){
  raw = as.integer(gsub("[[:alpha:]]", "", x))
  x[order(raw)]
}

pairs_results = lapply(
  1:length(filename_lines),
  function(i){

    n_sites = as.integer(strsplit(partial_names[[i]], "-")[[1]][[1]])
    rep_name = strsplit(partial_names[[i]], "-")[[1]][[2]]


    # Find the line where the current data set is mentioned in
    # pairs.txt
    filename_line = filename_lines[i]

    # Which chunk of the data file corresponds to this file?
    chunk = min(which(beginnings > filename_line))

    # Split the chunk on whitespace.
    splitted = strsplit(pairs_txt[beginnings[chunk]:ends[chunk]], " +")

    # Pull out the corresponding chunk of the "x" data frame, based on n_sites
    # and rep_name
    is_correct_sim = x$n_sites == n_sites & x$rep_name == rep_name
    x_subset = x[is_correct_sim & x$method == "correlation", ]

    # Pull out the species numbers and their Z-scores, then join to x_subset
    pairs_results = lapply(
      splitted,
      function(x){
        # in the x data frame, species 1 is always a lower number than species 2
        spp = alnum_sort(x[3:4])
        data.frame(
          sp1 = spp[1],
          sp2 = spp[2],
          z = x[14],
          stringsAsFactors = FALSE
        )
      }
    ) %>%
      bind_rows %>%
      mutate(spp = paste(sp1, sp2, sep = "-"))
```

```
    n_spp = 20

    pairs_results$z = as.numeric(pairs_results$z)

    # Re-order the pairs_results to match the other methods
    m = matrix(NA, n_spp, n_spp)
    new_order = match(
      paste0("V", row(m)[upper.tri(m)], "-V", col(m)[upper.tri(m)]),
      pairs_results$spp
    )
    ordered_pairs_results = pairs_results[na.omit(new_order), ]

    ordered_pairs_results = ordered_pairs_results %>%
      filter(sp1 %in% c(x_subset$sp1) & sp2 %in% x_subset$sp2)

    x_subset$estimate = ordered_pairs_results$z
    x_subset$method = "null"

    x_subset
  }
) %>% bind_rows()

# Manually adjust the Z values less than -1000 so that these outliers
# won't completely dominate the analyses below
pairs_results$estimate[pairs_results$estimate < -1000] = -50

x = rbind(x, pairs_results)
```

B: Compare model estimates

Calculate model performance (R-squared):

For each combination of `method` and `simulation_type`, fit a linear model. Then, for each combination of `method`, `simulation_type`, and `n_sites`, report the proportion of variance explained by the corresponding linear model.

```
resids = function(data){
  resid(lm(truth ~ estimate + 0, data = data))
}

result_summary = x %>%
  group_by(method, simulation_type) %>%
  do(data.frame(., resids = resids(.))) %>%
  ungroup %>%
  group_by(method, simulation_type, n_sites) %>%
  summarise(r2 = 1 - sum(resids^2) / sum(truth^2))
```

```r
# Set the ordering of the data frame based on R-squared
result_summary$method = reorder(result_summary$method, -result_summary$r2)
result_summary$simulation_type = reorder(
  result_summary$simulation_type,
  -result_summary$r2
)

# Add a column that includes method name and its mean R-squared,
# for plotting purposes below
result_summary = result_summary %>%
  group_by(method) %>%
  summarise(mean_r2 = round(100 * mean(r2))) %>%
  mutate(method_r2 = paste0(method, " (0.", mean_r2, ")")) %>%
  select(method, method_r2) %>%
  inner_join(result_summary, "method")

# Rename the simulation types for clearer graph labels
result_summary$simulation_type_long = plyr::revalue(
  result_summary$simulation_type,
  c(no_env = "constant environment",
    env = "heterogeneous environment",
    abund = "abundance")
)

result_summary$method_r2 = reorder(result_summary$method_r2, -result_summary$r2)
```

Average the R-squared values across methods and simulation types

```r
result_summary %>%
  group_by(method, simulation_type) %>%
  summarise(mean(r2)) %>%
  spread(simulation_type, `mean(r2)`) %>%
  kable(digits = 3)
```

method	no_env	env	abund
Markov network	0.525	0.451	0.384
GLM	0.472	0.405	0.283
partial correlation	0.403	0.322	0.200
partial BayesComm	0.394	0.302	0.166
correlation	0.291	0.183	0.117
null	0.227	0.125	0.075
BayesComm	0.206	0.110	0.060

Save the finer-grained R-squared results as Figure 3

```
legend_name = expression(Method~(mean~R^2))

pdf("manuscript-materials/figures/performance.pdf", width = 8, height = 2.5)
ggplot(result_summary, aes(x = n_sites, y = r2, col = method_r2, shape = method_r2)) +
  facet_grid(~simulation_type_long) +
  geom_line(size = .5) +
  geom_point(size = 2.5, fill = "white") +
  scale_shape_manual(values = c(16, 22, 17, 23, 18, 24, 15), name = legend_name) +
  geom_hline(yintercept = 0, size = 1/2) +
  geom_vline(xintercept = 0, size = 1) +
  coord_cartesian(ylim = c(-.01, 0.76)) +
  ylab(expression(R^2)) +
  xlab("Number of sites (log scale)") +
  scale_x_log10(breaks = unique(x$n_sites), limits = range(x$n_sites)) +
  theme_bw(base_size = 11) +
  theme(panel.margin = grid::unit(1.25, "lines")) +
  theme(panel.border = element_blank(), axis.line = element_blank()) +
  theme(
    panel.grid.minor = element_blank(),
    panel.grid.major.y = element_line(color = "lightgray", size = 1/4),
    panel.grid.major.x = element_blank()
  ) +
  theme(strip.background = element_blank(), legend.key = element_blank()) +
  theme(plot.margin = grid::unit(c(.01, .01, .75, .1), "lines")) +
  theme(
    axis.title.x = element_text(vjust = -0.2, size = 12),
    axis.title.y = element_text(angle = 0, hjust = -.1, size = 12)
  ) +
  scale_color_brewer(palette = "Dark2", name = legend_name)
dev.off()
```

```
## pdf
##   2
```

Estimate uncertainty in mean R-squared:

Fit a linear mixed model describing R-squared as a function of method, landscape size, and simulation type. Note the small standard errors associated with the effect of estimation method.

```
landscape_estimates = x %>%
  group_by(method, simulation_type) %>%
  do(data.frame(., resids = resids(.))) %>%
  ungroup %>%
  group_by(method, simulation_type, rep_name, n_sites) %>%
```

```
  summarise(r2 = 1 - sum(resids^2) / sum(truth^2))


summary(
  lmer(
    r2 ~ method + n_sites + simulation_type + (1|rep_name),
    data = landscape_estimates
  ),
  correlation = FALSE
)
```

```
## Linear mixed model fit by REML ['lmerMod']
## Formula: r2 ~ method + n_sites + simulation_type + (1 | rep_name)
##    Data: landscape_estimates
##
## REML criterion at convergence: -4945.2
##
## Scaled residuals:
##     Min      1Q  Median      3Q     Max
## -7.3997 -0.6350  0.0758  0.6883  2.7104
##
## Random effects:
##  Groups   Name        Variance  Std.Dev.
##  rep_name (Intercept) 0.0008304 0.02882
##  Residual             0.0113238 0.10641
## Number of obs: 3150, groups:  rep_name, 150
##
## Fixed effects:
##                              Estimate Std. Error t value
## (Intercept)                -2.481e-02  7.186e-03   -3.45
## methodcorrelation           6.965e-02  7.094e-03    9.82
## methodGLM                   2.544e-01  7.094e-03   35.85
## methodMarkov network        3.217e-01  7.094e-03   45.35
## methodnull                  1.504e-02  7.094e-03    2.12
## methodpartial BayesComm     1.616e-01  7.094e-03   22.78
## methodpartial correlation   1.796e-01  7.094e-03   25.31
## n_sites                     1.050e-04  2.690e-06   39.04
## simulation_typeenv          8.853e-02  7.402e-03   11.96
## simulation_typeno_env       1.795e-01  7.402e-03   24.25
```

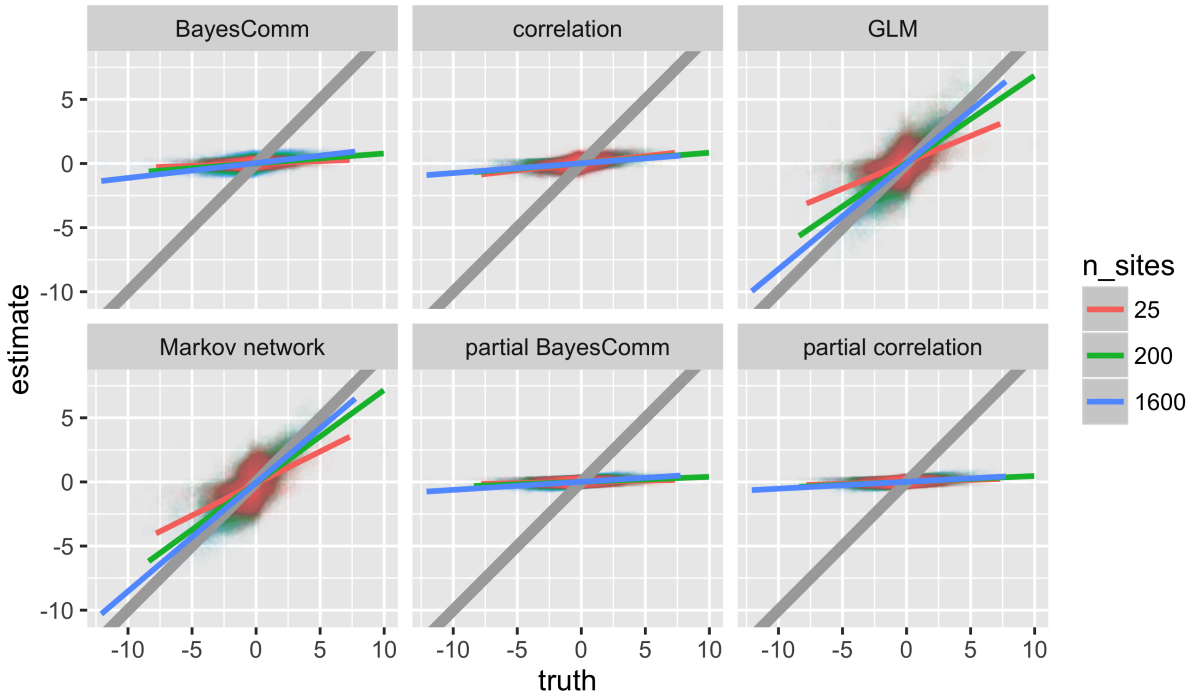
Plot estimates versus "true" values across methods and lanscape sizes

The gray line indicates the 1:1 line, where models recover an unbiased estimate of the "true" β coefficients. The GLM and Markov network methods estimate the coefficients on the original scale, and approach unbiasedness as the number of sites increases. The four methods based on (partial) correlations are constrained to return values between -1 and 1, and do not return values on the

original scale. The covariance and partial covariance (which are not scaled in this way) may avoid this problem in future analyses (Loh and Wainwright 2013; see main text for full citation).

Note that the null model (Pairs) is not included in these graphs, as its test statistic depends strongly on the size of the landscape and fills a range that would not fit on these graphs.

```
ggplot(filter(x, simulation_type == "no_env", method != "null"),
       aes(x = truth, y = estimate, color = factor(n_sites))) +
  facet_wrap(~method) +
  geom_point(alpha = 0.01) +
  geom_abline(intercept = 0, slope = 1, size = 2, col = "darkgray") +
  geom_smooth(method = "lm", fullrange = FALSE) +
  coord_equal() +
  scale_color_discrete(name = "n_sites")
```



C: Inferential statistics

Identify statistical significance for the Markov network and Pairs

For Pairs, compare the Z-scores with Gaussian quantiles for 95% coverage; for the Markov network, use the approximate confidence intervals estimated in Appendix 3.

```
pairs_summary = x[x$method == "null" & !grepl("pop", x$rep_name), ]
markov_summary = x[x$method == "Markov network" & !grepl("pop", x$rep_name), ]


# Pairs's Z score is based on C-scores, which are positive when species are
# disaggregated.  So significantly negative scores imply positive interactions
# and vice versa
pairs_summary$sig_pos = pairs_summary$estimate < qnorm(.025)
pairs_summary$sig_neg = pairs_summary$estimate > qnorm(.975)

# Markov network is significant when lower bound is above zero or lower bound is
# below zero
markov_summary$sig_pos = markov_summary$lower > 0
markov_summary$sig_neg = markov_summary$upper < 0
```

The `error_smoother` is a function that fits a generalized additive model to estimate the probability that a model estimate will match some criterion (e.g. statistical significance) for some parameter as a function of that parameter's "true" value. This function is used in Figure 4C and in calculating Type I error rates below.

```
truth_seq = seq(min(markov_summary$truth), max(markov_summary$truth), length = 1000)

error_smoother = function(data, f, values = truth_seq){
  predict(
    gam(
      f(data) ~ s(truth),
      data = data,
      family = binomial
    ),
    data.frame(truth = values),
    type = "response"
  )
}
```

Create Figure 4

Panels A and B plot the point estimates or test statistics for different models against one another.

Panel C shows the probability of rejecting the null hypothesis (of no interaction between two species) in the opposite direction of the true value (see main text).

```
pdf("manuscript-materials/figures/error_rates.pdf", height = 8.5, width = 8.5/3)
par(mfrow = c(3, 1))

# Calculate p(confidently wrong) for each model as a function of
# the true values
confidently_wrong = function(data){
```

```
  (data$sig_pos & data$truth < 0) | (data$sig_neg & data$truth > 0)
}
y_markov = error_smoother(markov_summary, confidently_wrong)
y_pairs = error_smoother(pairs_summary, confidently_wrong)

# Compare estimates
spread_estimates = x %>%
  dplyr::select(-lower, -upper, -X) %>%
  spread(method, estimate) %>%
  na.omit()

# R-squared for null versus correlation
round(
  summary(lm(null ~ I(correlation*sqrt(n_sites)), data = spread_estimates))$r.squared,
  2
)
```

```
## [1] 0.95
```

```
# R-squared for glm markov network versus glm
round(summary(lm(`Markov network` ~ GLM, data = spread_estimates))$r.squared, 2)
```

```
## [1] 0.94
```

```
with(
  spread_estimates,
  plot(
    `Markov network`,
    GLM,
    pch = ".",
    col = "#00000020",
    ylab = "Markov network estimate",
    xlab = "GLM estimate",
    bty = "l"
  )
)
mtext("A. Markov network estimates\nvs. GLM estimates", adj = 0, side = 3,
      font = 2, line = 1.2, cex = .9)
abline(lm(`Markov network` ~ GLM, data = spread_estimates))
text(0, 5, expression(R^2==0.94))

with(
  spread_estimates,
  plot(
    correlation * sqrt(n_sites),
    null,
```

```
    pch = ".",
    col = "#00000020",
    ylab = "Z-score",
    xlab = expression("correlation" %*% sqrt(number~~of~~sites)),
    bty = "l"
  )
)
mtext("B. Null model estimates vs.\nscaled correlation coefficients",
      adj = 0, side = 3, font = 2, line = 1.2, cex = .9)
abline(lm(null ~ I(correlation*sqrt(n_sites)), data = spread_estimates))
text(10, 12, expression(R^2==0.95))

plot(
  truth_seq,
  y_pairs,
  type = "l",
  xlab = "\"True\" interaction strength",
  ylab = "P(confidently predict wrong sign)",
  bty = "l",
  yaxs = "i",
  col = 2,
  ylim = c(0, .4),
  lwd = 2
)
mtext("C. Error rate vs.\ninteraction strength", side = 3, adj = 0,
      font = 2, line = 1.2, cex = .9)
lines(truth_seq, y_markov, lwd = 2)
legend("topleft", lwd = 2, legend = c("Null model", "Markov network"),
       col = c(2, 1), bty = "n")
dev.off()
```

```
## pdf
##   2
```

Summarize inferential statistics:

P(Pairs confidently wrong):

```
with(pairs_summary,  mean((sig_neg & truth > 0) | (sig_pos & truth < 0)))
```

```
## [1] 0.1533758
```

P(Markov network confidently wrong)

```r
with(markov_summary, mean((sig_neg & truth > 0) | (sig_pos & truth < 0)))
```

```
## [1] 0.02861541
```

P(Pairs rejects null)

```r
with(pairs_summary,  mean(sig_neg | sig_pos))
```

```
## [1] 0.4520535
```

P(Markov network rejects null)

```r
with(markov_summary,  mean(sig_neg | sig_pos))
```

```
## [1] 0.2116561
```

Type I error rates:

Type I error rates (probability of rejecting the null hypothesis given a "true" interaction strength of zero, according to the spline model defined by `error_smoother` above). The smoother focuses on the 64% of the data points whose "true" values fall between -1 and 1, because its estimates near 0 are more accurate when they aren't affected by distant data points.

Markov network Type I error rates

```r
markov_summary %>%
  filter(abs(truth) < 1) %>%
  group_by(simulation_type) %>%
  do(data.frame(
    `Type I error rate` =
      error_smoother(., function(x){x$sig_pos | x$sig_neg}, values = 0)
  )) %>%
  kable(digits = 3)
```

simulation_type	Type.I.error.rate
abund	0.258
env	0.142
no_env	0.024

Null model Type I error rates

```
pairs_summary %>%
  filter(abs(truth) < 1) %>%
  group_by(simulation_type) %>%
  do(data.frame(
    `Type I error rate` =
      error_smoother(., function(x){x$sig_pos | x$sig_neg}, values = 0)
  )) %>%
  kable(digits = 3)
```

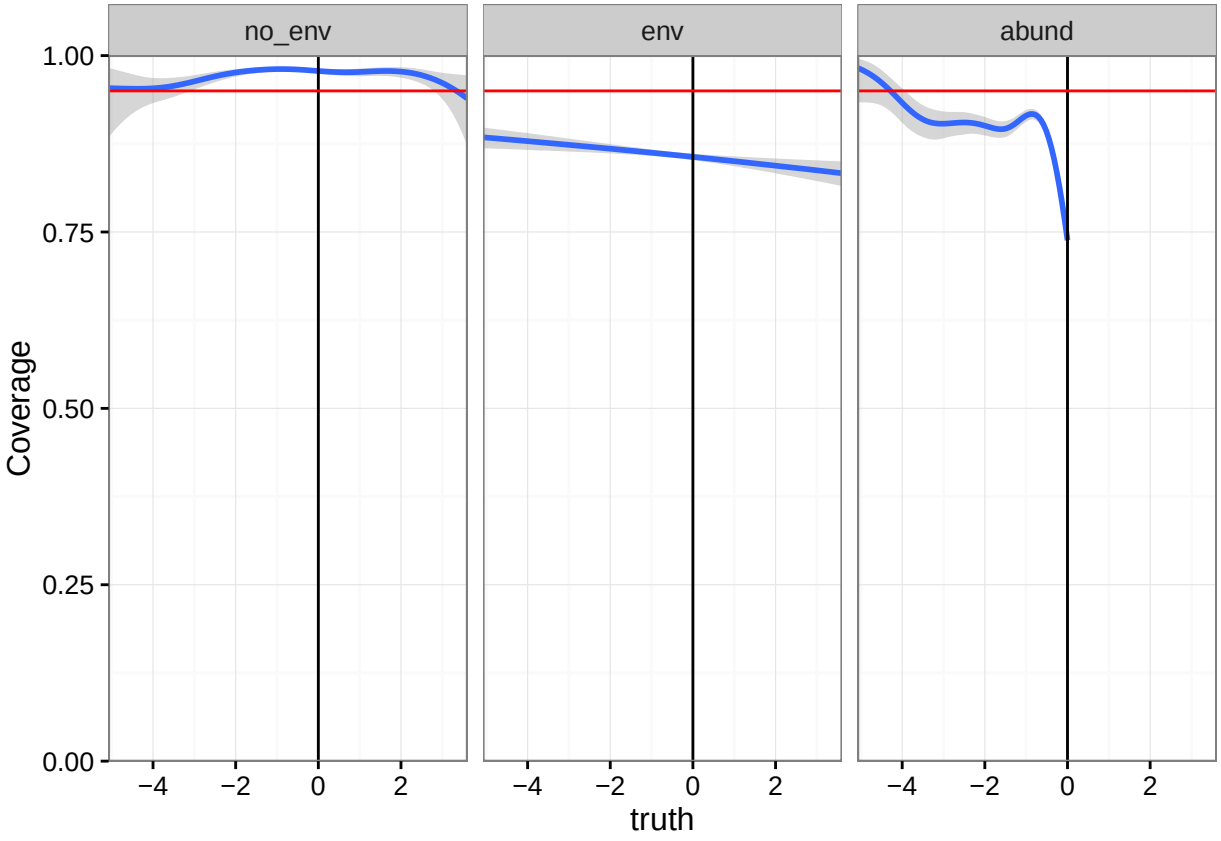
simulation_type	Type.I.error.rate
abund	0.597
env	0.530
no_env	0.308

Plot Markov network confidence interval coverage versus true β value

The top and bottom 0.5% of the distribution have been omitted to prevent bad behavior by the smoother in the tails. The horizontal red line shows the nominal 95% coverage rate and the black vertical line marks where the "true" value of β was zero. The Type I error rates calculated above for the Markov network closely match (one minus) the values of these curves at zero.

```
coverage_data = markov_summary %>%
  filter(percent_rank(truth) > .005 & percent_rank(truth) < .995) %>%
  mutate(covered = truth > lower & truth < upper) %>%
  mutate(simulation_type = factor(simulation_type, c("no_env", "env", "abund")))

ggplot(coverage_data, aes(x = truth, y = as.integer(covered))) +
  facet_grid(~simulation_type) +
  geom_smooth(method = gam, formula = y ~ s(x), method.args = list(family = binomial)) +
  theme_bw() +
  coord_cartesian(ylim = c(0, 1), expand = FALSE) +
  geom_vline(xintercept = 0) +
  geom_hline(yintercept = 0.95, color = "red") +
  ylab("Coverage")
```


no_env
env
abund
1.00
0.75
0.50
0.25
0.00
Coverage
−4
−2
0
2
truth