Appendix 4: Results

Inferring species interactions from co-occurrence data with Markov networks

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

Import the results from Appendix 4:

```
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 is 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
    x_subset = x[x$n_sites == n_sites & x$rep_name == rep_name & 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)
```

Calculate model performance:

```
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))

result_summary$method = reorder(result_summary$method, -result_summary$r2)

result_summary$simulation_type = reorder(result_summary$simulation_type, -result_summary$r2)


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")

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)
```

Model performance with no environmental variation:

```
result_summary %>%
  filter(simulation_type == "no_env") %>%
  group_by(method) %>%
  summarise(mean(r2)) %>%
  kable(digits = 3)
```

method	mean(r2)
Markov network	0.525
GLM	0.472
partial correlation	0.403
partial BayesComm	0.394
correlation	0.291
null	0.227
BayesComm	0.206

Model performance with environmental heterogeneity:

```
result_summary %>%
  filter(simulation_type == "env") %>%
  group_by(method) %>%
  summarise(mean(r2)) %>%
  kable(digits = 3)
```

method	mean(r2)
Markov network	0.451
GLM	0.405
partial correlation	0.322
partial BayesComm	0.302
correlation	0.183
null	0.125

method	mean(r2)
BayesComm	0.110

Model performance with per-capita species interactions:

```
result_summary %>%
  filter(simulation_type == "abund") %>%
  group_by(method) %>%
  summarise(mean(r2)) %>%
  kable(digits = 3)
```

method	mean(r2)
Markov network	0.384
GLM	0.283
partial correlation	0.200
partial BayesComm	0.166
correlation	0.117
null	0.075
BayesComm	0.060

Plot the R-squared results (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) +
  #scale_shape_manual(values = c(21, 25, 15, 18)) +
  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 R-squared uncertainty:

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
  )
)
```

```
## 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
##
## Correlation of Fixed Effects:
##             (Intr) mthdcr mthGLM mthdMn mthdnl mtBysC mthdpc n_sits smltn_
## methdcrrltn -0.494
## methodGLM   -0.494  0.500
## mthdMrkvntw -0.494  0.500  0.500
## methodnull  -0.494  0.500  0.500  0.500
## mthdprtBysC -0.494  0.500  0.500  0.500  0.500
## mthdprtlcrr -0.494  0.500  0.500  0.500  0.500  0.500
## n_sites     -0.228  0.000  0.000  0.000  0.000  0.000  0.000
## smltn_typnv -0.515  0.000  0.000  0.000  0.000  0.000  0.000  0.000
## smltn_typn_ -0.515  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.500
```

Summarize the inferential results of the Markov network and the null model:

```
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 positive interactions == negative estimates
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
```

Create Figure 4:

```
# Function for smoothing the error rates with a generalized additive model
# and plotting the results
my_geom_smooth = function(data, color, ...){
  geom_smooth(
    data = data,
    aes(
      x = truth,
      y = as.integer((sig_neg & truth > 0) | (sig_pos & truth < 0)),
      color = color
    ),
    method = gam,
    family = binomial,
    formula = y ~ s(x),
    se = FALSE,
    n = 1024,
    ...
  )
}


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

plotfun = function(..., add){
  if(add){
    lines(...)
  }else{
    plot(...)
  }
}


error_smoother = function(data){
  predict(
    gam(
      I((sig_neg & truth > 0) | (sig_pos & truth < 0)) ~ s(truth),
      data = data,
      family = binomial
    ),
    data.frame(truth = truth_seq),
    type = "response"
  )
}

y_pairs = error_smoother(pairs_summary)
y_markov = error_smoother(markov_summary)
```

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

# 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))

plotfun(
  truth_seq,
  y_pairs,
  type = "l",
  xlab = "\"True\" interaction strength",
  ylab = "P(confidently predict wrong sign)",
  bty = "l",
  yaxs = "i",
  col = 2,
  add = FALSE,
  ylim = c(0, .4),
  lwd = 2
)
mtext("C. Error rate vs.\ninteraction strength", side = 3, adj = 0,
      font = 2, line = 1.2, cex = .9)
plotfun(truth_seq, y_markov, add = TRUE, 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)
with(markov_summary, mean((sig_neg & truth > 0) | (sig_pos & truth < 0)))
```

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

```r
# P(Pairs rejects null)
with(pairs_summary,  mean(sig_neg | sig_pos))
```

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

```r
# P(Markov network rejects null)
with(markov_summary,  mean(sig_neg | sig_pos))
```

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

```r
# P(reject null | small interaction) for Makrov network
# (approximate Type I error rates)
markov_summary %>%
  group_by(simulation_type) %>%
  filter(abs(truth) < .1) %>%
  summarize(Type_1_error_rate = mean(sig_neg | sig_pos)) %>%
  kable(digits = 3)
```

simulation_type	Type_1_error_rate
abund	0.220
env	0.136
no_env	0.019

```r
# P(reject null | small interaction) for Pairs
# (approximate Type I error rates)
pairs_summary %>%
  group_by(simulation_type) %>%
  filter(abs(truth) < .1) %>%
  summarize(Type_1_error_rate = mean(sig_neg | sig_pos)) %>%
  kable(digits = 3)
```

simulation_type	Type_1_error_rate
abund	0.575
env	0.501
no_env	0.297

```r
# Confidence interval coverage across all values
# What's the probability that any "true" value falls inside the 95% CI?
markov_summary %>%
  group_by(simulation_type) %>%
  summarize(mean(truth > lower & truth < upper)) %>%
```

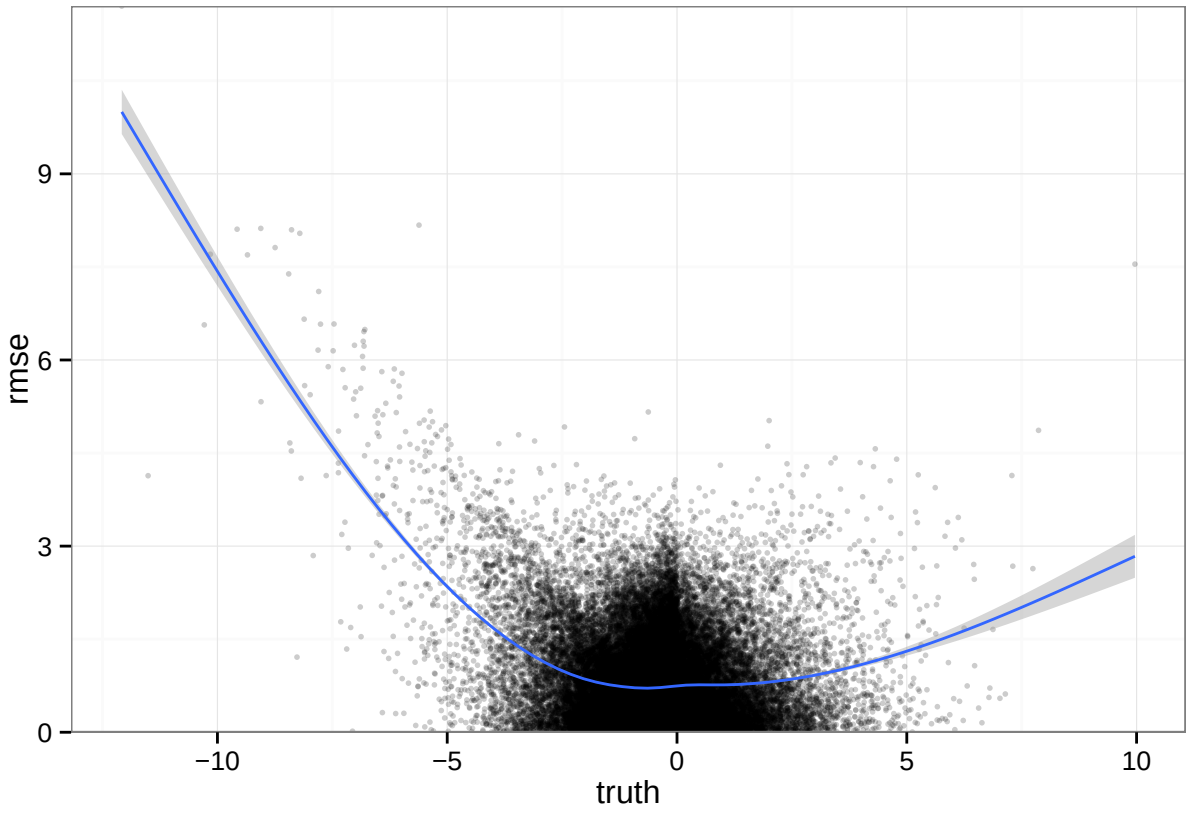
```
  kable(digits = 3)
```

simulation_type	mean(truth > lower & truth < upper)
abund	0.868
env	0.857
no_env	0.975

Plot root mean square error versus "true" beta

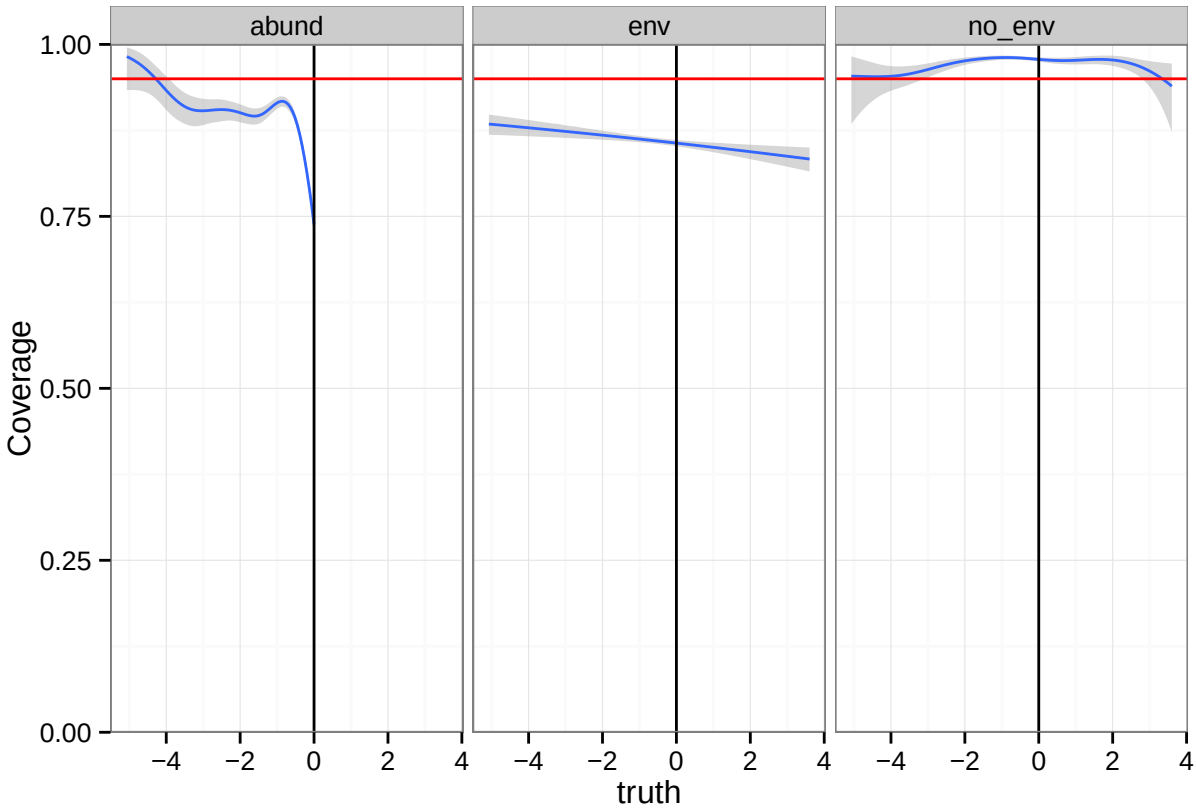
```
# Exclude the "abundance" simulations because the interpretation of $\beta$
# is different
rmses = markov_summary %>%
  filter(simulation_type != "abund") %>%
  mutate(rmse = sqrt((truth - estimate)^2))

ggplot(rmses, aes(x = truth, y = rmse)) +
  geom_point(alpha = .2, size = 1) +
  geom_smooth() +
  theme_bw() +
  coord_cartesian(ylim = c(0, max(rmses$rmse)))
```

```
## geom_smooth: method="auto" and size of largest group is >=1000, so using gam with formula: y
```



Plot confidence interval coverage versus true β value

```
# Coverage versus true beta value.  The top and bottom 0.5%
# of the distribution have been omitted to prevent bad behavior
# by the smoother in the tails.
markov_summary %>%
  filter(percent_rank(truth) > .005 & percent_rank(truth) < .995) %>%
  mutate(covered = truth > lower & truth < upper) %>%
  ggplot(aes(x = truth, y = as.integer(covered))) +
  facet_grid(~simulation_type) +
  geom_smooth(method = gam, formula = y ~ s(x), family = binomial) +
  theme_bw() +
  coord_cartesian(ylim = c(0, 1)) +
  geom_vline(xintercept = 0) +
  geom_hline(yintercept = 0.95, color = "red") +
  ylab("Coverage")
```


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