Estimating NDs and RFDs

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Goal: Estimate niche differences (NDs) and relative fitness differences (RFDs) for coculture populations of *Eschericia coli* and *Pseudomonas putida* growing at different temperatures.

Contents:


```
## Loading required package: ggplot2
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Methods

Raw data processing

1. **Adjust stationary phase:** Fluorescence keeps increasing even after the bacteria stop growing. To adjust for this, at each temperature, and for monocultures & cocultures, we:
    1. Manually decide on a maximum value for fluorescence at stationary phase based on where the OD flattens out (suggesting that the bacteria have stopped growing).
    2. Identify the time at which the fluorescence reaches the chosen maximum value and make all fluorescence values after that timepoint the chosen maximum value.
2. **Normalize data:** The *E. coli* fluorescence molecule and the *P. putida* fluorescence molecule have very different frequencies, and the frequencies are different at different temperatures. To adjust for this, we use the monoculture ODs and fluorescences:
    1. Find the maximum OD and the maximum fluorescence for the *E. coli* monoculture and for the *P. putida* monoculture. These are denoted as $E_{OD_{max}}$, $E_{f_{max}}$, $PP_{OD_{max}}$, and $PP_{f_{max}}$, respectively.
    2. Normalize all data to 32°C using $E_{OD_{32}}$, $E_{f_{32}}$, and $P_{OD_{32}}$.
    3. Normalize all *E. coli* values to: $(E_{f_{32}}/E_{OD_{32}}) * (E_{OD_{max}}/E_{f_{max}})$
    4. Normalize all *P. putida* values to: $(E_{f_{32}}/E_{OD_{32}}) * (P_{OD_{max}}/P_{f_{max}})$
    5. Divide all normalized values by 10,000 to improve fit.

Curve fitting

Model:

$$\dot{E} = r_E E(1 - \alpha_{EE} * E - \alpha_{EP} P)$$

$$\dot{P} = r_P P(1 - \alpha_{PP} * P - \alpha_{PE} E)$$

- E is the *E. coli* population size.
- P is the *P. putida* population size.
- r_i is the monoculture growth rate.
- $\alpha_{EE} = 1/K_E$ and $\alpha_{PP} = 1/K_P$ are the intra-specific competition coefficients.
- K_i is the monoculture carrying capacity.
- α_{EP} and α_{PE} are the inter-specific competition coefficients.

We estimate the parameters by fitting the model to the data:

1. r_i and K_i are estimated from monoculture data using the the single-species Lotka-Voltera equations (no $\alpha_{EP} P$ and $\alpha_{PE} E$ terms) using a built-in R function (`growthcurver::SummarizeGrowth`).
2. α_{EP} and α_{PE} are estimated using the equations above (two-species equation).
    1. Solve the ode for some initial guess of model parameters (`deSolve::ode` function).
        1. Starting values of α_{EP} and α_{PE} for model fitting were obtained by using the steady-state estimates:

$$\alpha_{EP} = (1 - \alpha_{PP} P_{SS})/E_{SS}$$

$$\alpha_{PE} = (1 - \alpha_{EE} E_{SS})/P_{SS}$$

            1. E_{SS} and P_{SS} are estimated using the single-species Lotka Voltera model.
    2. Evaluate an error function between the model results and the data.
        1. Error function:

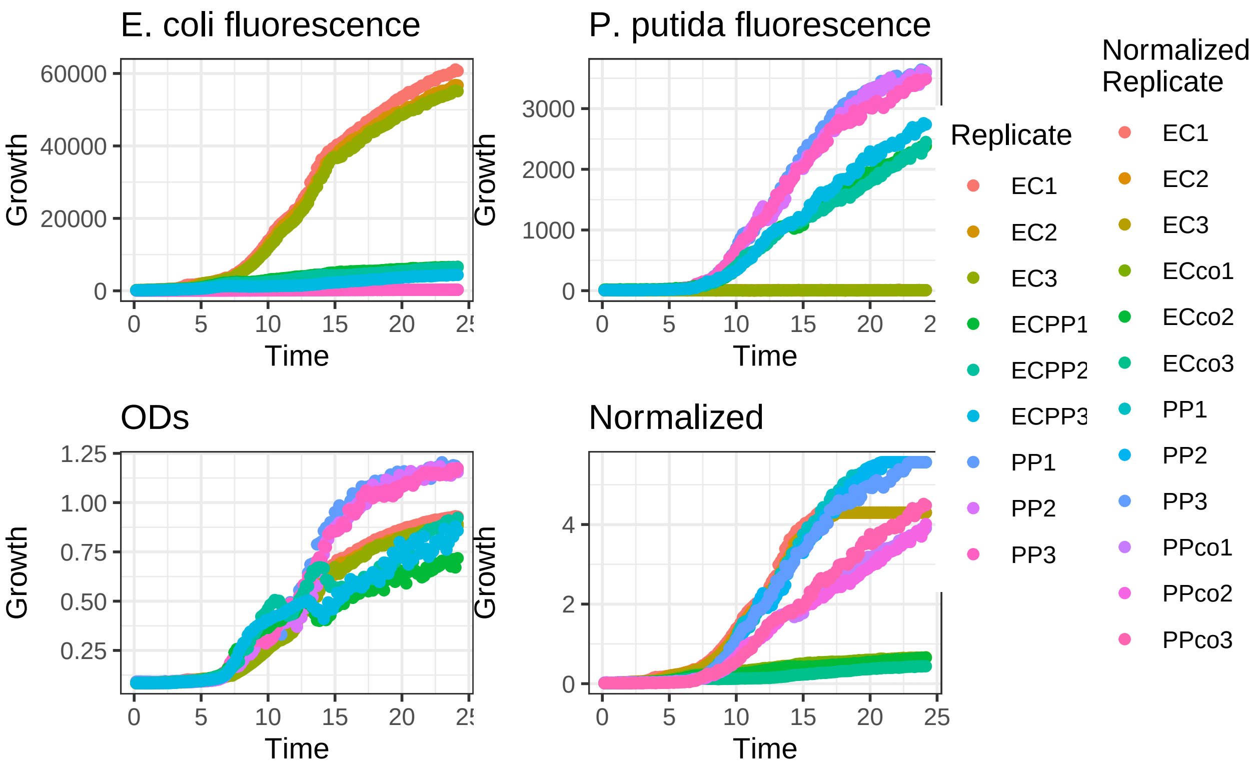
$$error = ((E_{real} - E_{fitted})/E_{real})^2 + ((P_{real} - P_{fitted})/P_{real})^2$$

    3. Employ an optimization scheme (`optim` function) to minimize the error function by choosing the set of model parameters that minimizes the error.

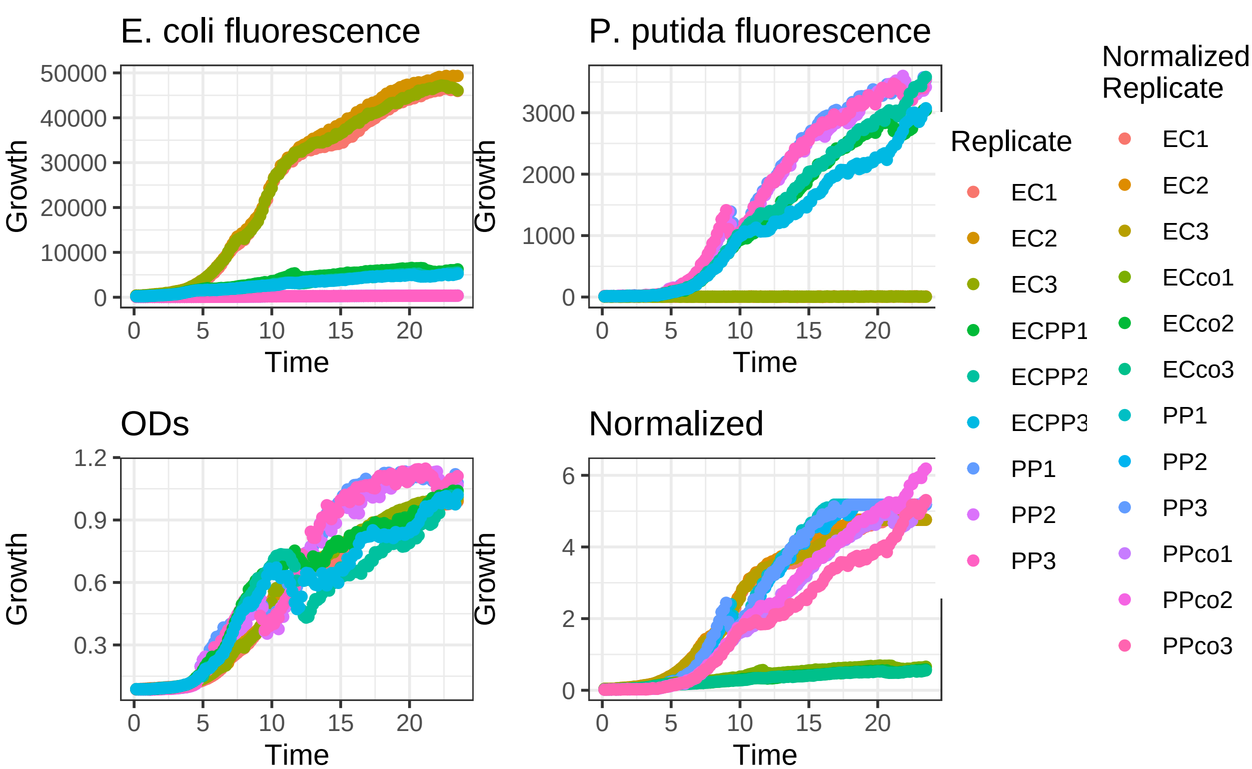
Results

Raw & normalized data

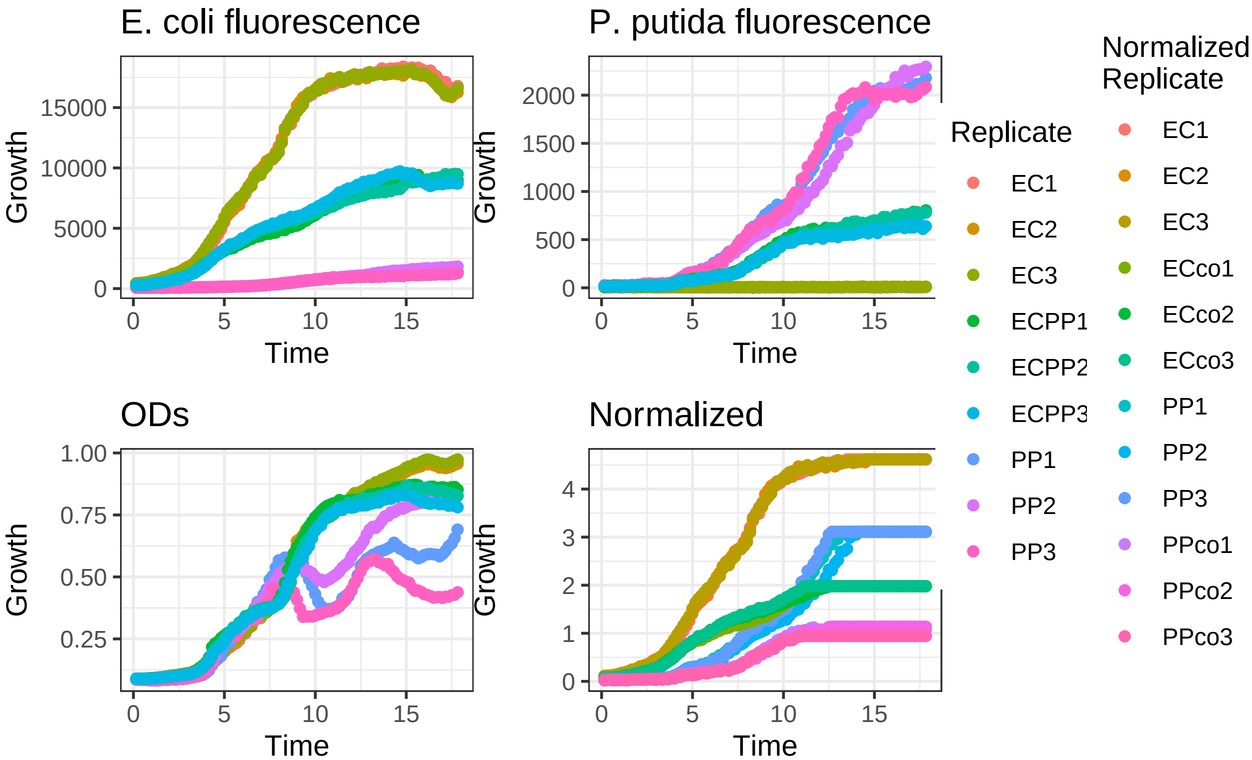
32C



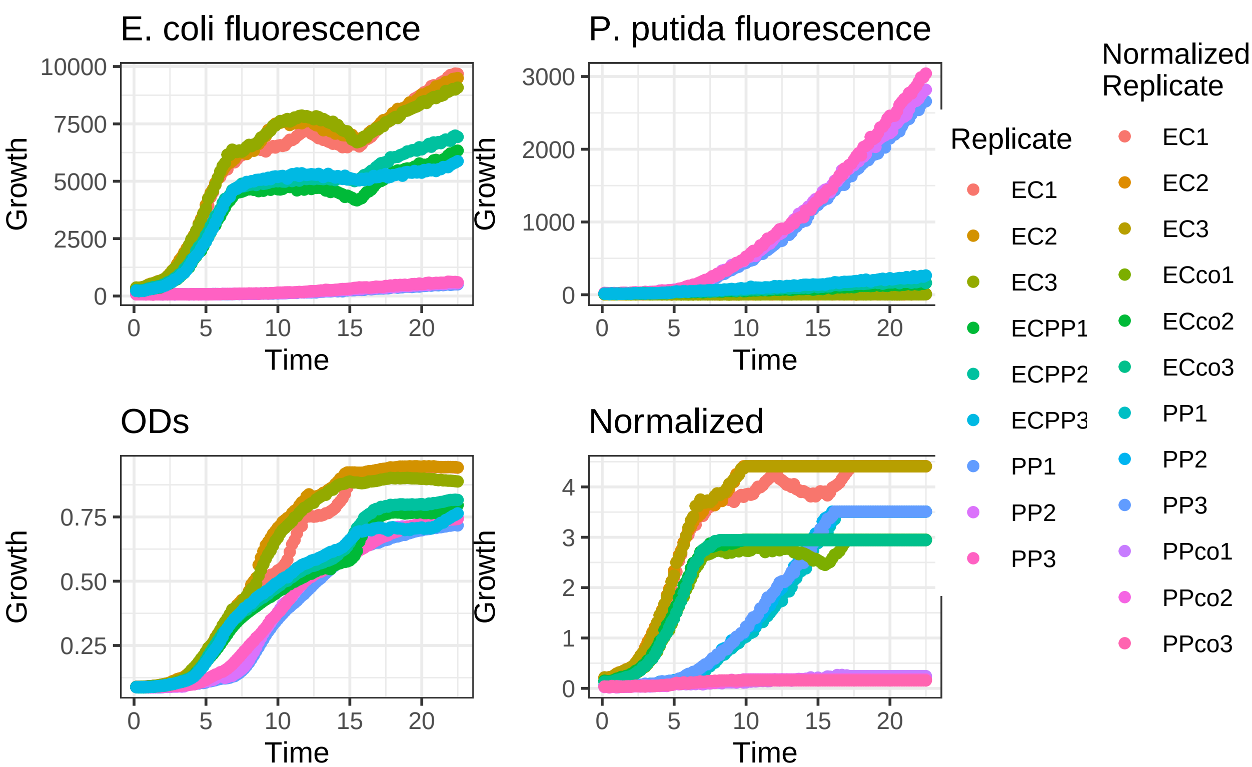
34C



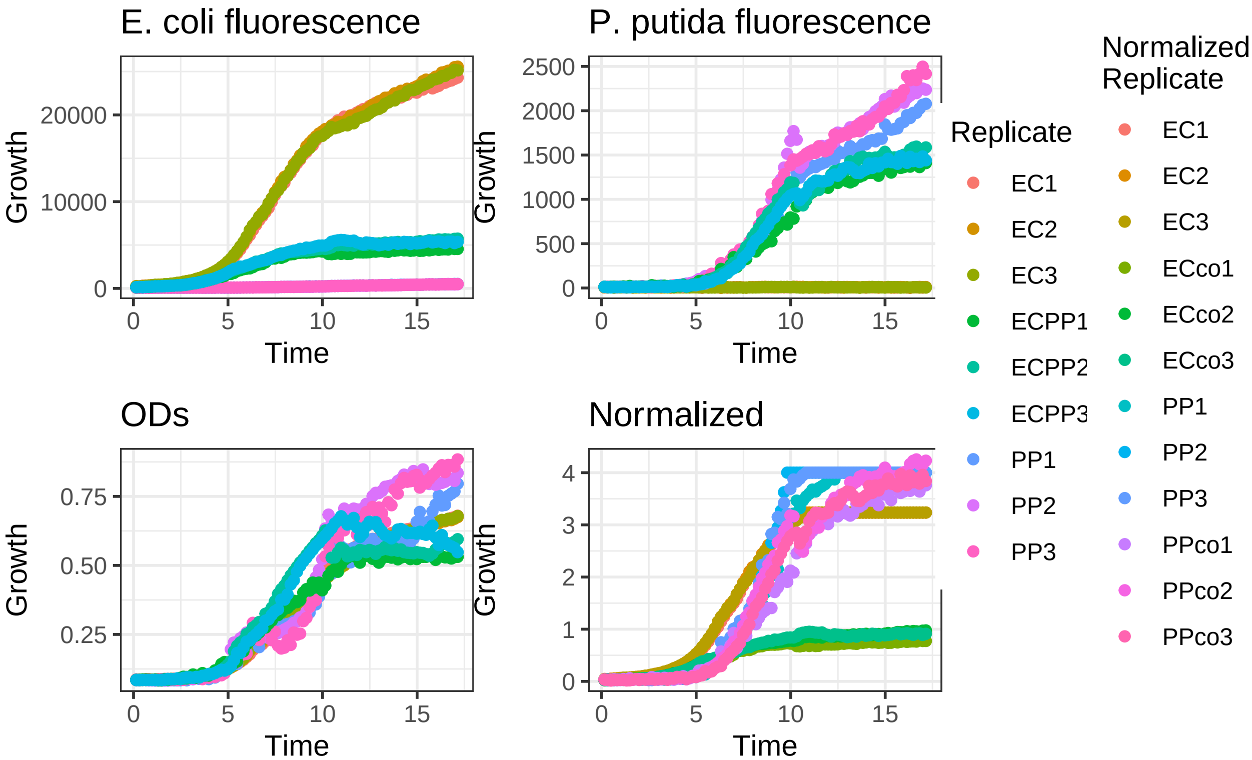
38C


E. coli fluorescence
P. putida fluorescence
ODs
Normalized
Growth
Time
Replicate
EC1
EC2
EC3
ECPP1
ECPP2
ECPP3
PP1
PP2
PP3
Normalized Replicate
EC1
EC2
EC3
ECco1
ECco2
ECco3
PP1
PP2
PP3
PPco1
PPco2
PPco3

40C

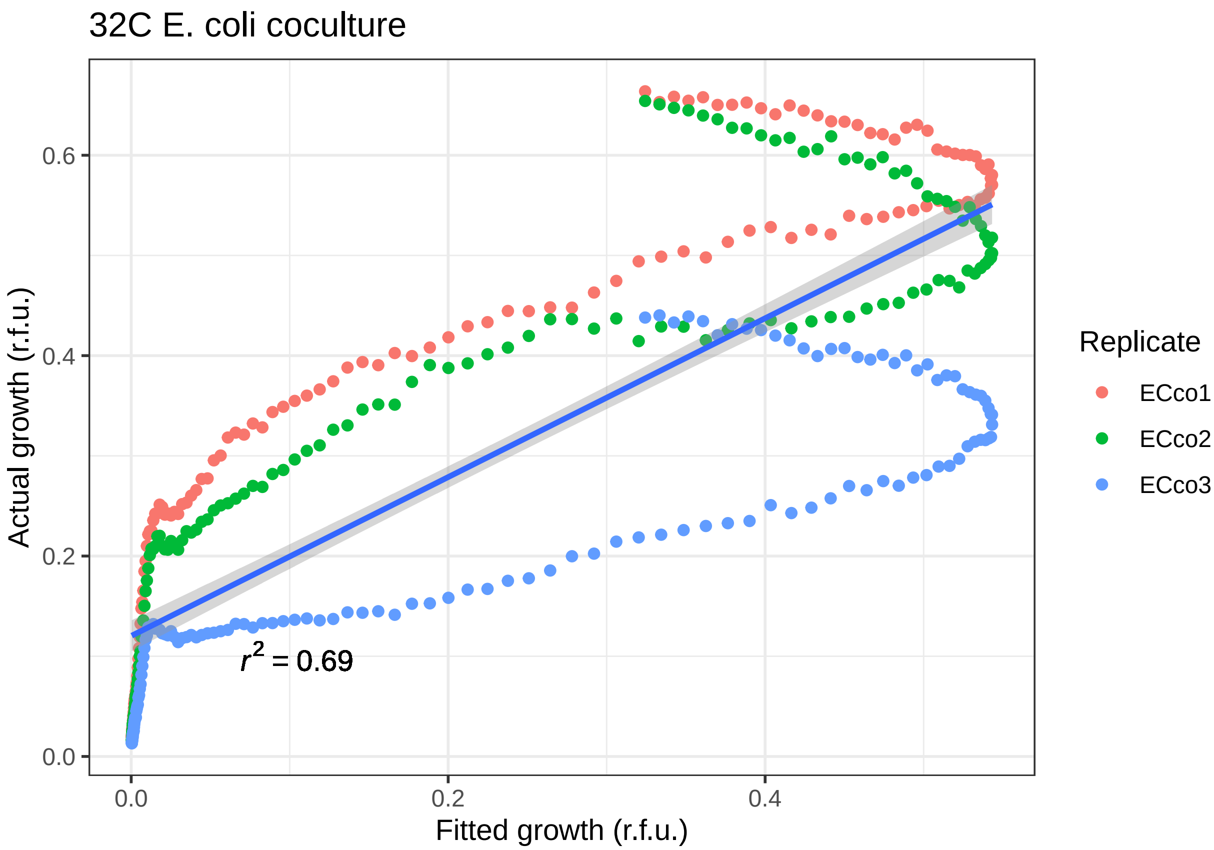

E. coli fluorescence
P. putida fluorescence
ODs
Normalized
Growth
Time
Replicate
EC1
EC2
EC3
ECPP1
ECPP2
ECPP3
PP1
PP2
PP3
Normalized Replicate
EC1
EC2
EC3
ECco1
ECco2
ECco3
PP1
PP2
PP3
PPco1
PPco2
PPco3

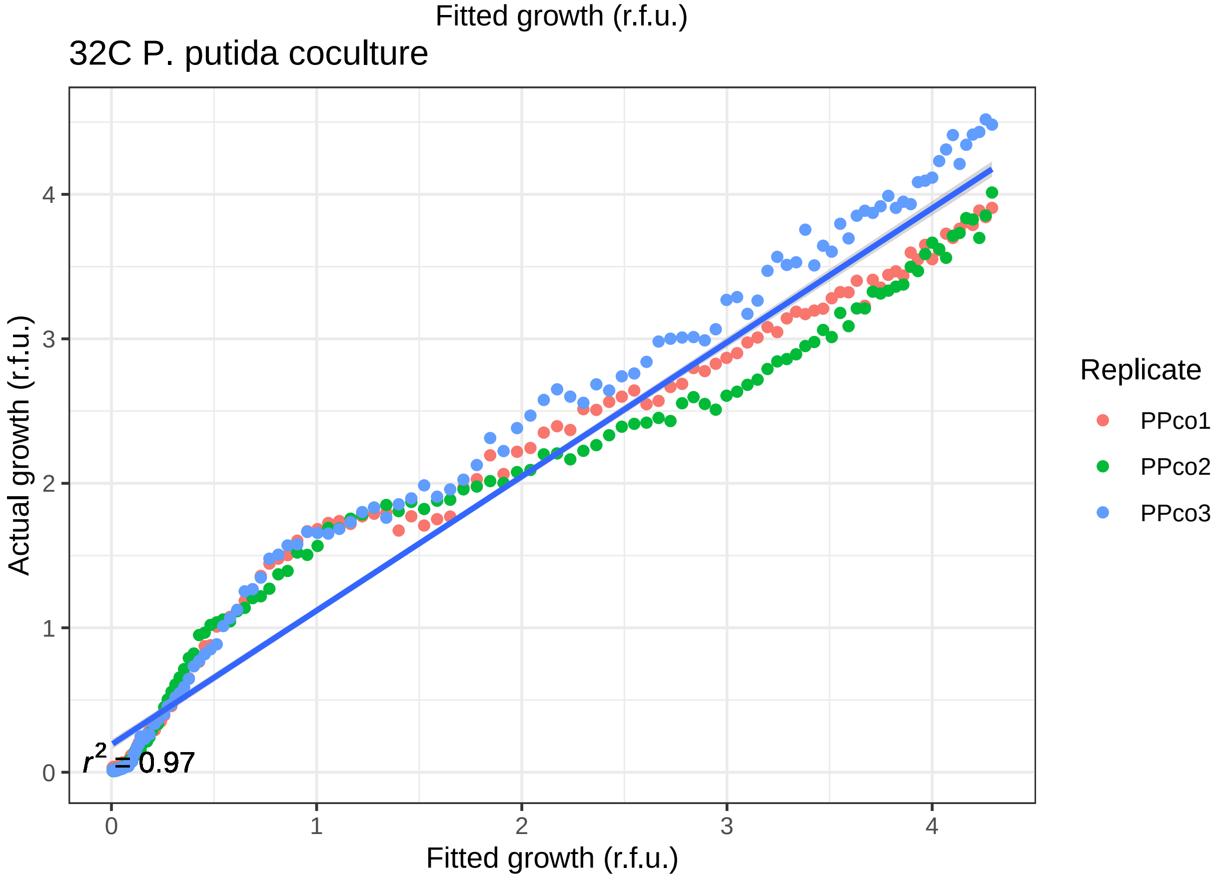
36C

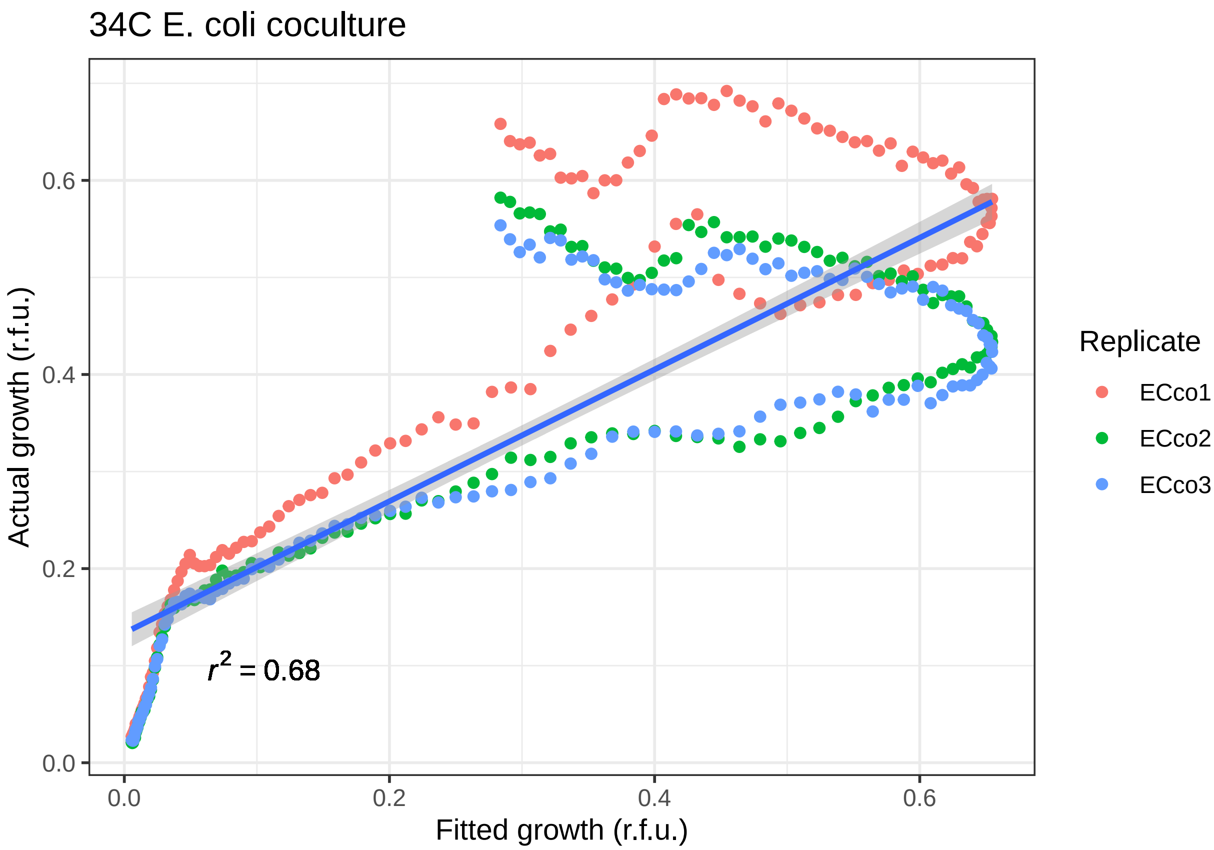


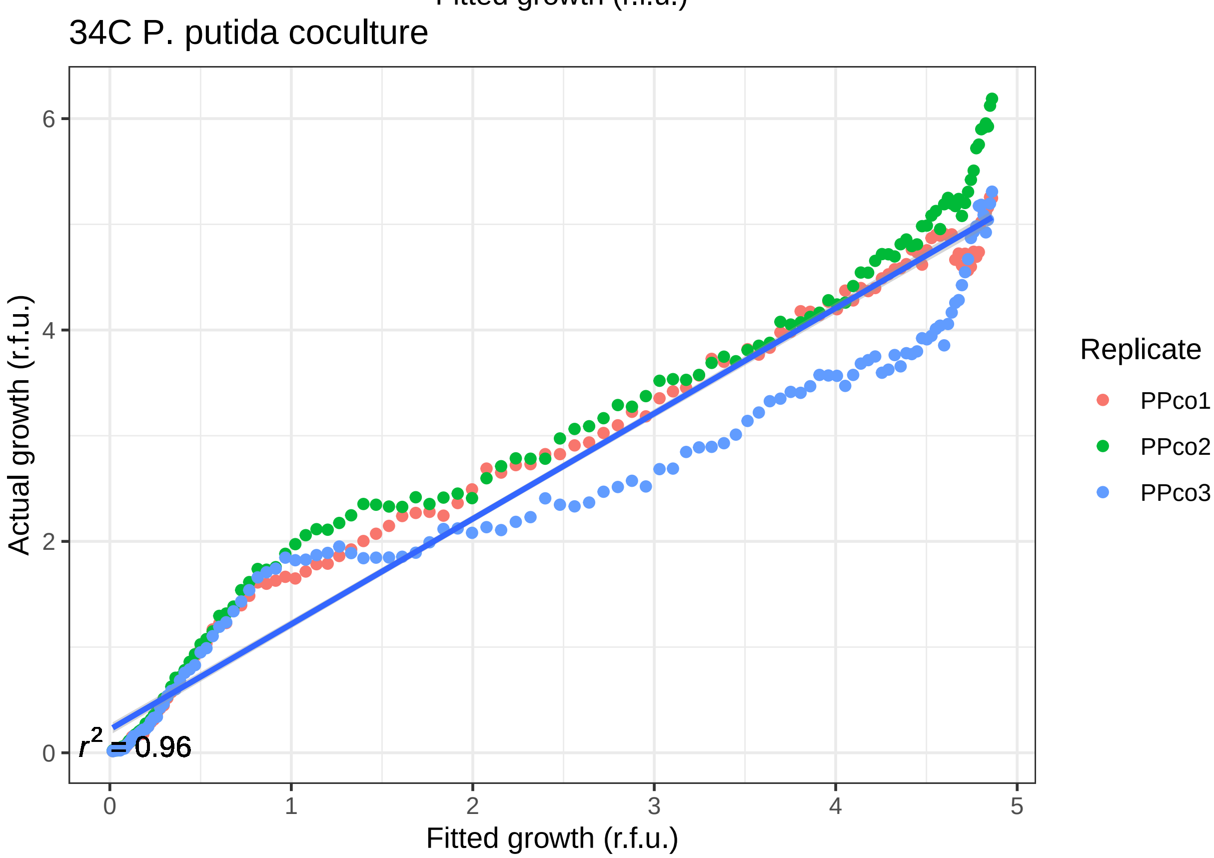
E. coli fluorescence
P. putida fluorescence
ODs
Normalized
Growth
Time
Replicate
EC1
EC2
EC3
ECPP1
ECPP2
ECPP3
PP1
PP2
PP3
Normalized Replicate
EC1
EC2
EC3
ECco1
ECco2
ECco3
PP1
PP2
PP3
PPco1
PPco2
PPco3

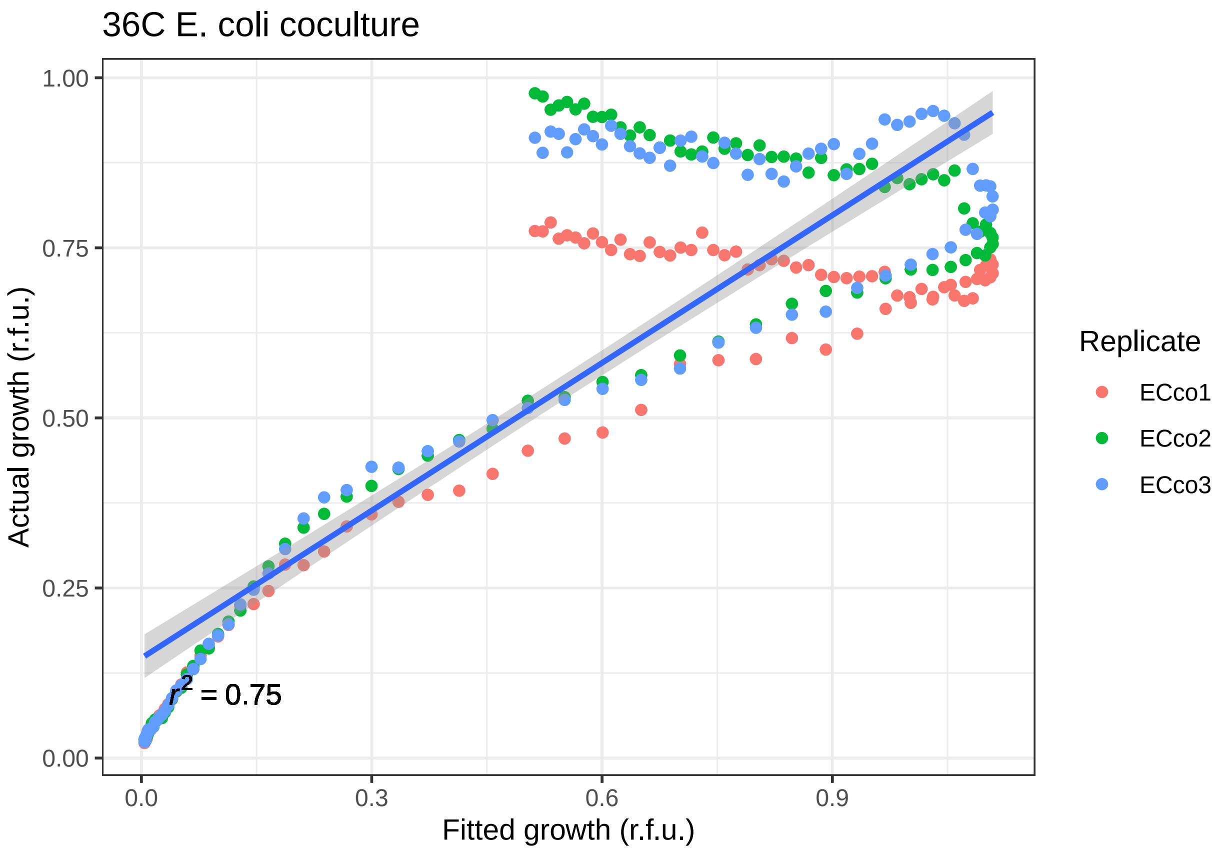
Fitted data

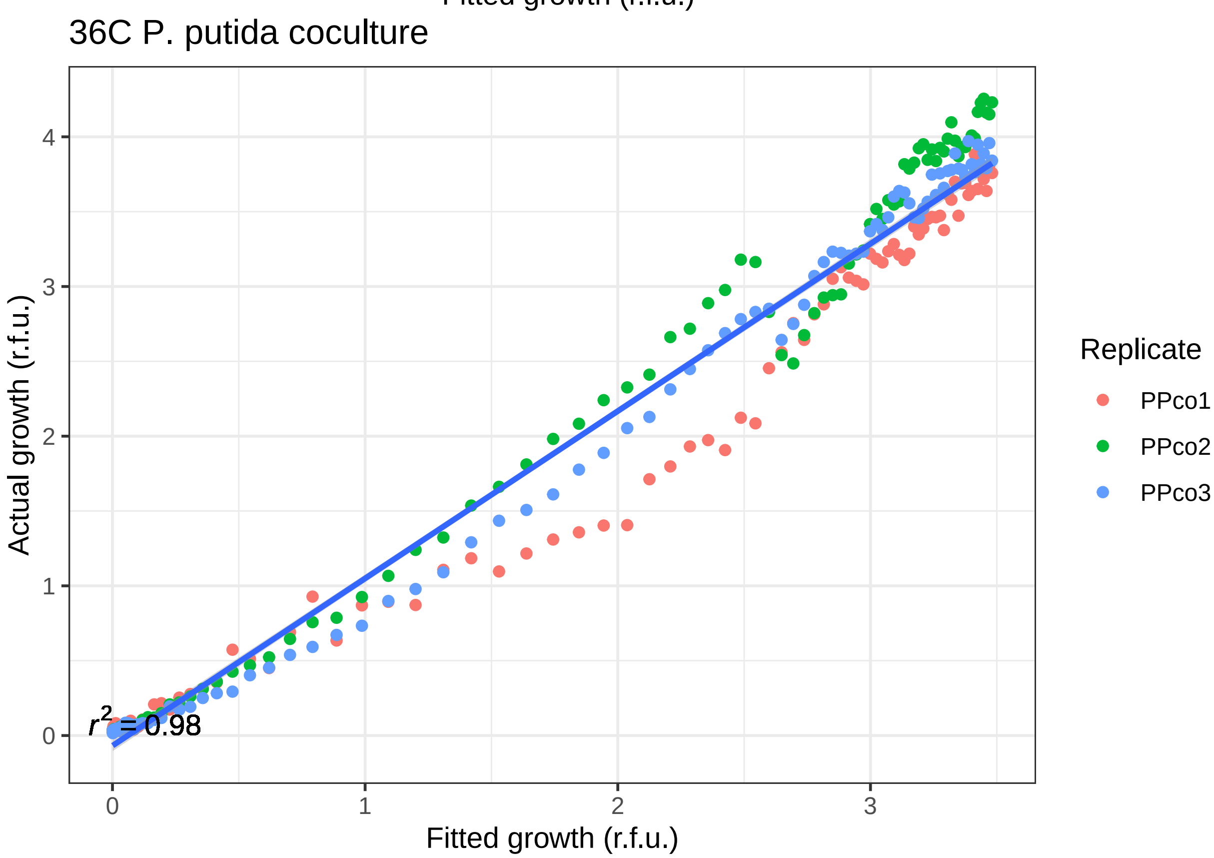

32C E. coli coculture
Actual growth (r.f.u.)
0.0
0.2
0.4
0.6
0.0
0.2
0.4
Fitted growth (r.f.u.)
$r^2 = 0.69$
Replicate
ECco1
ECco2
ECco3

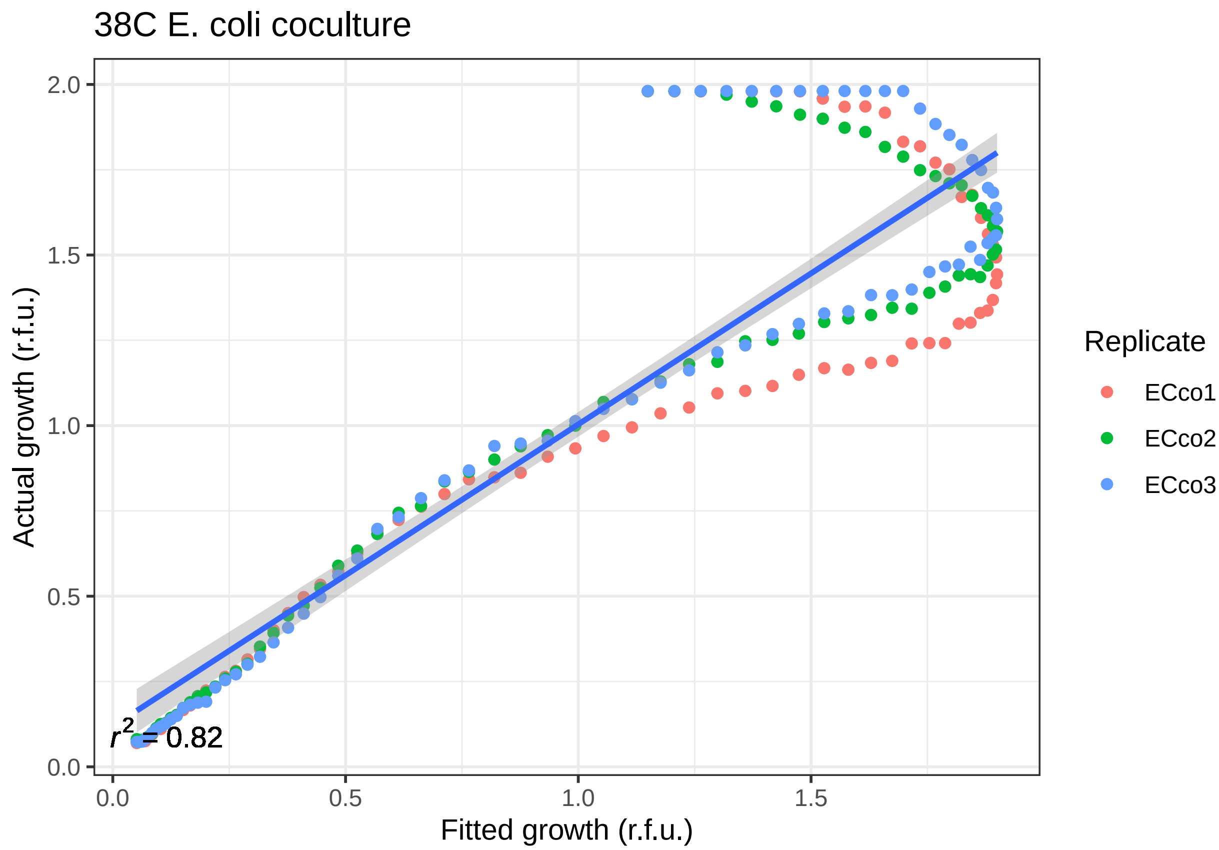

32C P. putida coculture
Actual growth (r.f.u.)
0
1
2
3
4
0
1
2
3
4
Fitted growth (r.f.u.)
$r^2 = 0.97$
Replicate
PPco1
PPco2
PPco3


34C E. coli coculture
Actual growth (r.f.u.)
0.0
0.2
0.4
0.6
0.0
0.2
0.4
0.6
Fitted growth (r.f.u.)
$r^2 = 0.68$
Replicate
ECco1
ECco2
ECco3

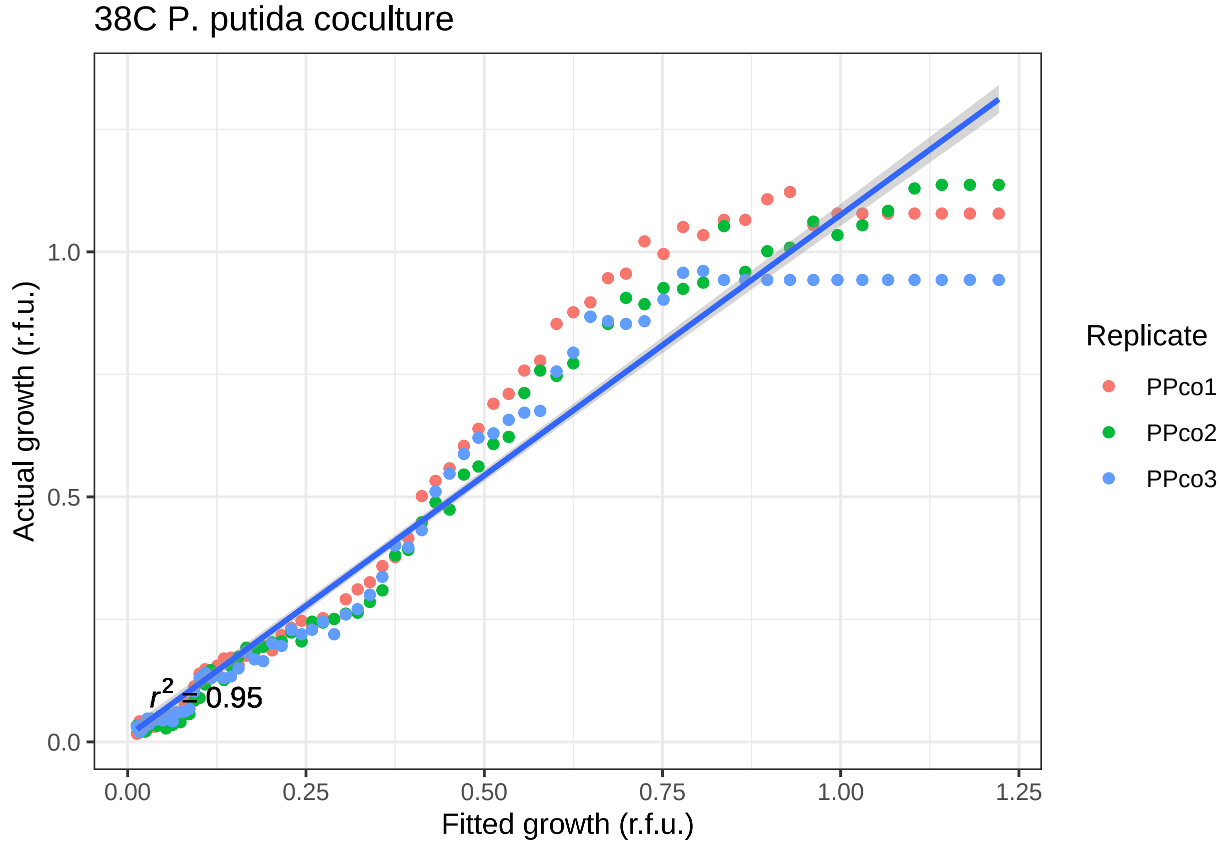

34C P. putida coculture
Actual growth (r.f.u.)
0
2
4
6
0
1
2
3
4
5
Fitted growth (r.f.u.)
$r^2 = 0.96$
Replicate
PPco1
PPco2
PPco3


36C E. coli coculture
1.00
0.75
0.50
0.25
0.00
Actual growth (r.f.u.)
0.0
0.3
0.6
0.9
Fitted growth (r.f.u.)
$r^2 = 0.75$
Replicate
ECco1
ECco2
ECco3

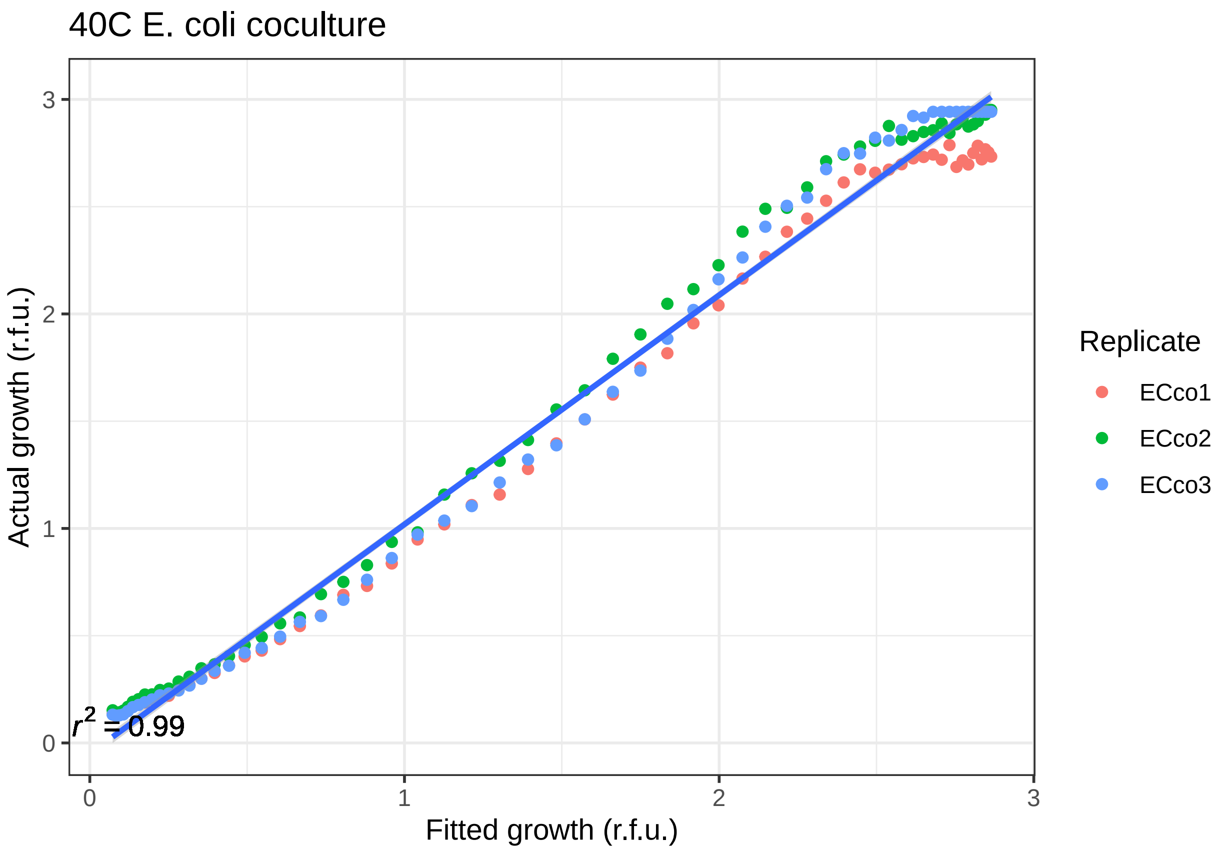

36C P. putida coculture
4
3
2
1
0
Actual growth (r.f.u.)
0
1
2
3
Fitted growth (r.f.u.)
$r^2 = 0.98$
Replicate
PPco1
PPco2
PPco3

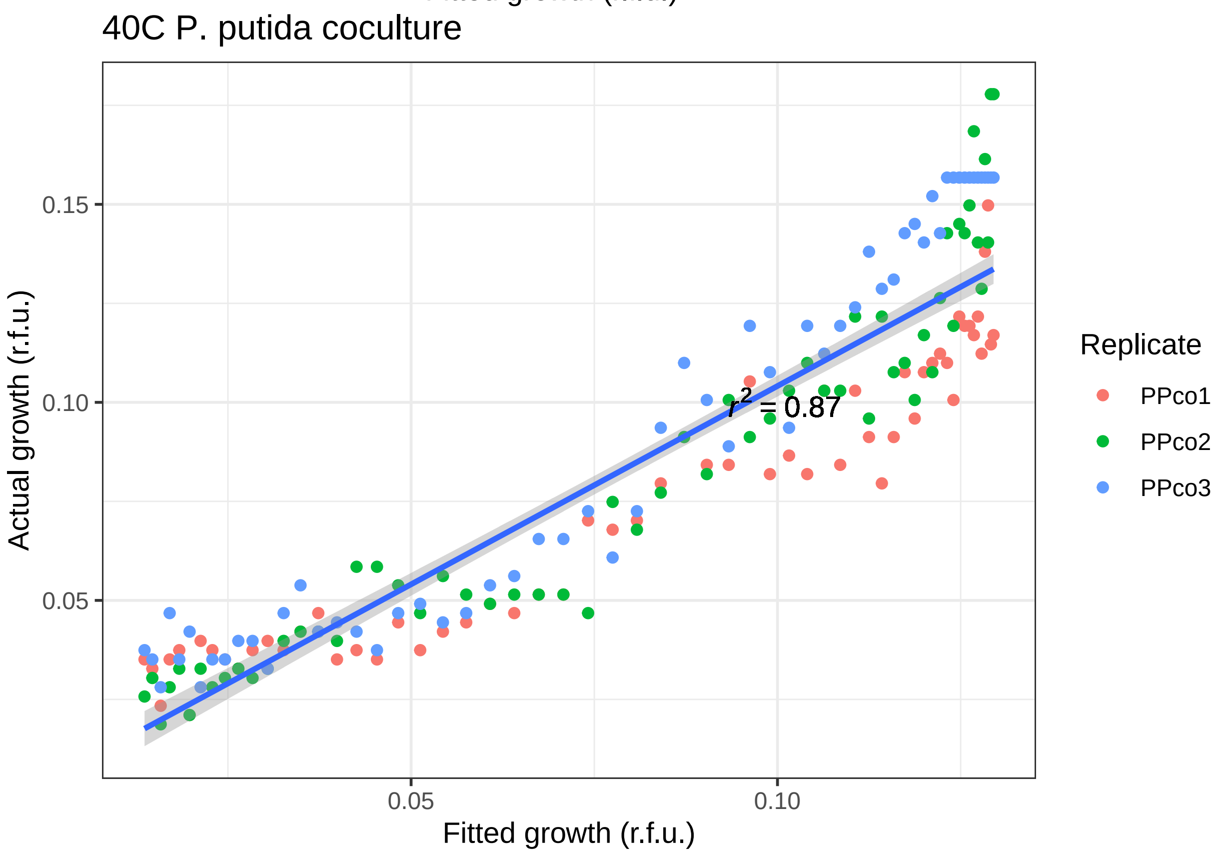


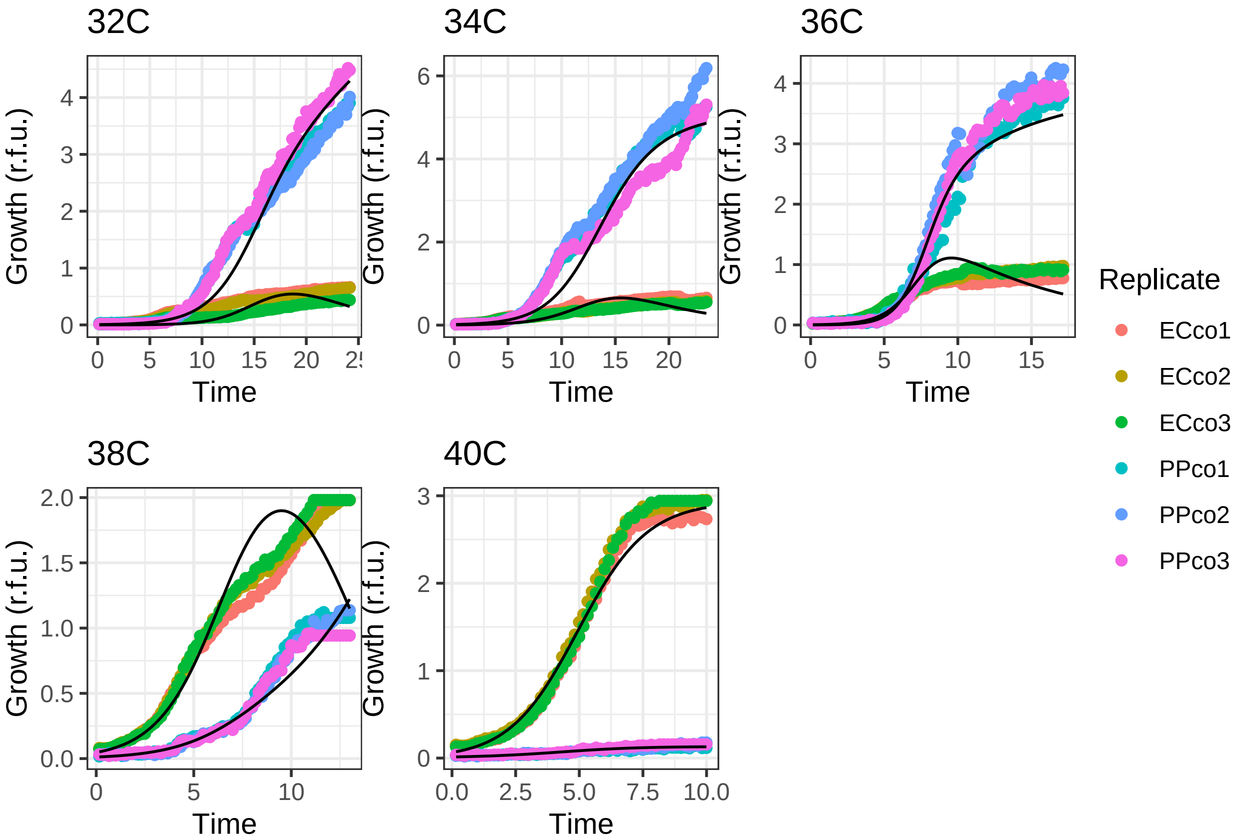
38C E. coli coculture
Actual growth (r.f.u.)
Fitted growth (r.f.u.)
$r^2 = 0.82$
Replicate
ECco1
ECco2
ECco3



38C P. putida coculture
Actual growth (r.f.u.)
Fitted growth (r.f.u.)
$r^2 = 0.95$
Replicate
PPco1
PPco2
PPco3

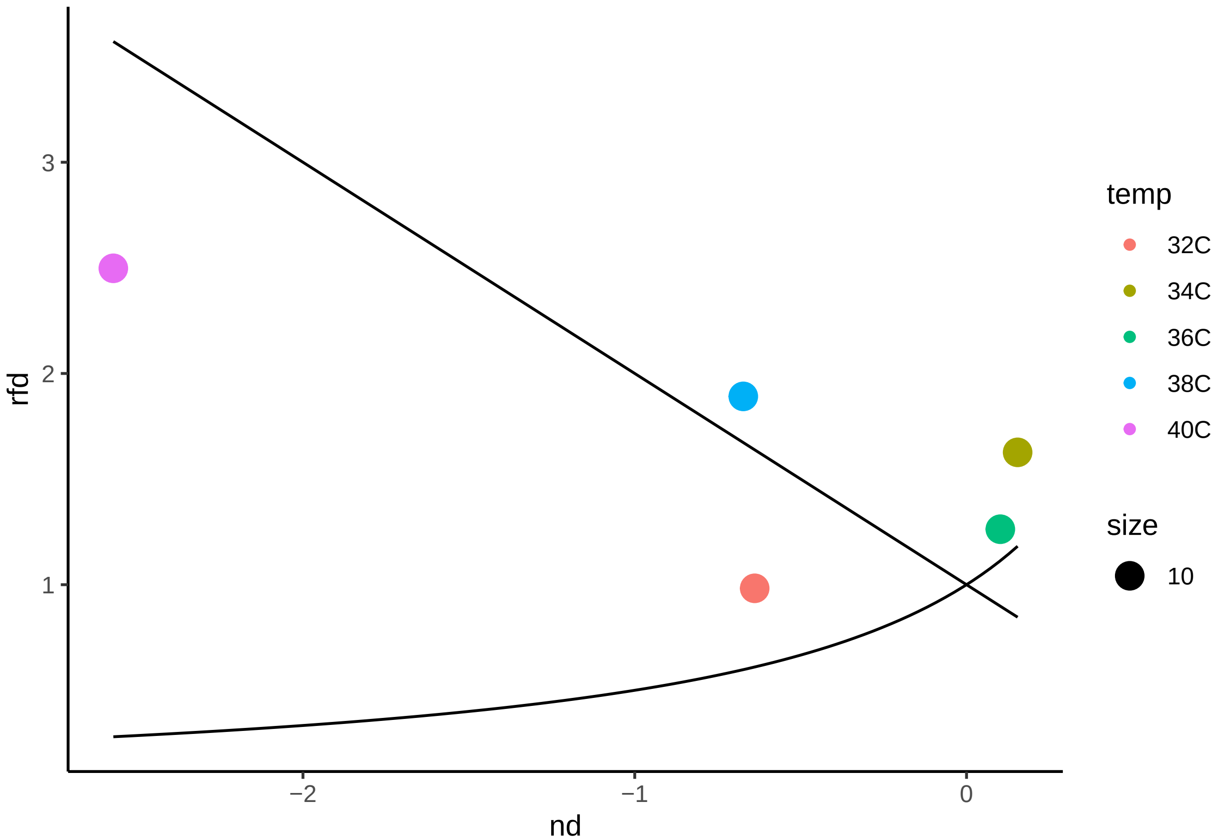

40C E. coli coculture
Actual growth (r.f.u.)
Fitted growth (r.f.u.)
$r^2 = 0.99$
0
1
2
3
Replicate
ECco1
ECco2
ECco3


40C P. putida coculture
Actual growth (r.f.u.)
Fitted growth (r.f.u.)
$r^2 = 0.87$
0.05
0.10
0.15
Replicate
PPco1
PPco2
PPco3



NDs & RFDs

```
##   temp               ec_r               pp_r             ec_k             pp_k
## 1  32C 0.528147399434647 0.415003407814728              4.3 5.56629670736219
## 2  34C 0.428501290924326 0.430024506056806 4.76133925268221 5.18131705512394
## 3  36C 0.811339483827165  1.06068165520433 3.23573806881243 4.00092489826119
## 4  38C  0.61228666645508  0.52136074491322 4.61657417684055 3.11165371809101
## 5  40C 0.812286917314655 0.464662948321378 4.40976692563818 3.50935997040326
##                 a_ii              a_jj       a_ij_start              a_ij
## 1 0.232558139534884 0.179652658234579 0.210995983221711 0.289306053838501
## 2 0.210024941918741   0.1930011210202 0.164944032595464  0.26559901246809
## 3 0.309048501063319 0.249942207221786 0.196505102733138 0.283444372124406
## 4 0.216610837754235 0.321372521044372 0.550575071410256  1.01687358719446
## 5 0.226769354676331  0.28495224440743  2.13915506582591  2.54214196451577
##            a_ji_start               a_ji         nd       rfd
## 1   0.450204491598223 0.387712041265015 -0.6385165 0.9828179
## 2 -0.0564333486068892 0.109244386212218  0.1539473 1.6265566
## 3  0.0647353161386145 0.219841829634261  0.1018353 1.2626189
## 4   0.341652356391173 0.191571659735335 -0.6728410 1.8914879
## 5   0.341288746324016 0.324236762149857 -2.5715177 2.4978992
```



temp
32C
34C
36C
38C
40C
size
10
rfd
nd
3
2
1
−2
−1
0