

## The parameters of the proposed method in DREAM4 InSilico Size10

### Network 1

**xgboost parameters:** 'n\_estimators': 398, 'learning\_rate': 0.0133, 'importance\_type': 'weight', 'max\_depth': 5, 'n\_jobs': -1

**alpha:** 0.0214

### Network 2

**xgboost parameters:** 'n\_estimators': 400, 'learning\_rate': 0.0148, 'importance\_type': 'weight', 'max\_depth': 5, 'n\_jobs': -1

**alpha:** 0.0137

### Network 3

**xgboost parameters:** 'n\_estimators': 120, 'learning\_rate': 0.281, 'max\_depth': 5, 'n\_jobs': -1

**alpha:** 0.0123

### Network 4

**xgboost parameters:** 'n\_estimators': 100, 'learning\_rate': 0.1648, 'max\_depth': 5, 'n\_jobs': -1

**alpha:** 0.0123

### Network 5

**xgboost parameters:** 'n\_estimators': 100, 'learning\_rate': 0.1654, 'max\_depth': 5, 'n\_jobs': -1

**alpha:** 0.0122

## The parameters of the proposed method in DREAM4 InSilico Size100

### Network 1

**xgboost parameters:** 'n\_estimators': 500, 'learning\_rate': 0.0122, 'importance\_type': 'weight', 'max\_depth': 4, 'n\_jobs': -1

**alpha:** 0.0142

### Network 2

**xgboost parameters:** 'n\_estimators': 500, 'learning\_rate': 0.0111, 'importance\_type': 'weight', 'max\_depth': 4, 'n\_jobs': -1

**alpha:** 0.0122

### Network 3

**xgboost parameters:** 'n\_estimators': 500, 'learning\_rate': 0.012, 'max\_depth': 4, 'n\_jobs': -1, 'importance\_type': 'weight'

**alpha:** 0.0147

#### Network 4

**xgboost parameters:** 'n\_estimators': 500, 'learning\_rate': 0.0121, 'importance\_type': 'weight', 'max\_depth': 4, 'n\_jobs': -1

**alpha:** 0.012

#### Network 5

**xgboost parameters:** 'n\_estimators': 500, 'learning\_rate': 0.01, 'importance\_type': 'weight', 'max\_depth': 5, 'n\_jobs': -1

**alpha:** 0.0192

### The parameters of the proposed method in yeast

**xgboost parameters:** max\_depth=5, subsample=0.86, n\_jobs=-1, n\_estimators=500, 'learning\_rate': 0.1207

alpha: 0.627

### The parameters of the proposed method in Escherichia coli

#### Cold

**xgboost parameters:** max\_depth=4, subsample=0.86, n\_jobs=-1, n\_estimators=120

#### Heat

**xgboost parameters:** max\_depth=4, subsample=0.86, n\_jobs=-1, n\_estimators=120, learning\_rate=0.008

#### Oxidative

**xgboost parameters:** max\_depth=4, subsample=0.86, n\_jobs=-1, n\_estimators=120, learning\_rate=0.01

#### Lactose

**xgboost parameters:** max\_depth=5, subsample=0.86, n\_jobs=-1, n\_estimators=140, learning\_rate=0.02, reg\_alpha=0.01