Determining MinSpan vectors of COBRA model

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wrmonucznow

If this station, we then three to calculate Medigan vectors (I) the a COSEA model. COSEA A model are presummany aduled under restay-insect condition. The hand specific after the state of long inverses. If they are condition, the state is a region inverse state or long inverses. When the present been stated are desired as the state of the and space as the latest increasing the biological model and thereopyrenic commitment of the COSEA model (Figure 1). The States has deleneated up to a quie the set in a model of a member of membershale as in the a vector of the state of the set in the set



Figure 1 (Overview of the Mindignal algorithms, (A) A metabolic network is mathematically represented as a sociationnesis matrix (B). Pleadon fluxes (v) are determined assuming casely state. All potential flux states (iii in the nut largour (B), (B) the Mindigna algorithm determines the shortest, independent pathways of the metabolic network by decomposity in a nut (special of the adsistrationnesis chassis to be not the squarest behavior.) (C) is stated to the control of the companies of the TSA by (see

is presented with 14 metabolites, 16 macrions, and a 4-dimensional rule space. Revenible reactions are shown, (b) The box pathways calculat by Mindgan for the simplified model are presented, not of which reaching projects and the TOA spoke, while the other two represent other possible metabolic pathways. The flux directions of a pathway though revenible reactions are shown as invenedible reactions.

MATERIALS Equipment Setup

Running the Minligan algorithm requires the installation of a mixed-integer linear programming (MLP) solver. We have used Guroti vishttp://www.guroti.com/down/sads/download-center) which is freely available for academic use. This tutorial and the algorithm has been rigorously tested and

ittp://www.gurobi.com/down/cads/down/cad-center) which is freely available for ac upport Gurobi v5=..desXis.tgws.will not work with GLPK; other solvers are unter

Implementation
For Minispa vectors to be calculated, the model must (1) consist of only reactions that are able to carry flux under that particular condition, (5) allow for the trivial
solution (in = (6) be featible, and (5) have the biomass function removed de-existing-an will automatically dreck and complete the first two modifications, but the

The algorithm is an iterative pruning of null space basis vectors to the spannest possible matrix. The problem is NS-hand, meaning that an optimal adultion is not guaranteed for large COSRA models; an approximate solution is found by setting a time limit on the MLP calculation.

In this example, we will calculate the MinSpan vectors for the £ coil core network.

Ensure that the Gurobi MILP and LP solvers are working:

tett1 = ChangeCobrakelver('qurchi', 'MILP'); tett2 = ChangeCobrakelver('qurchi', 'DP'); tett3 = ChangeCobrakelver('qurchi', 'QP'); if tett1 == 0 || tett2 == 0 || tett3 == 0

cod the core mod

global CHTDOR sodelfiletime = 'ecoli_core_model.mat';

monifications o "colligion monimati" incondificación; poligion monimati poligion de la constitución de la colligion de la c The MinSpan algorithm takes the model as input and retu culated Minlipan vectors (Table 1)

Table 1 I Inputs and outputs of the desitivatives function Punning the algorithm on the modified £, coll core model returns the calculated MinSpans for the network

The biomass function is then removed from the model using the COSPA function reservetures behave - ("Rismoss_Scoli_core_w_SHOT"); model = removeRxns(model, bmEane);

minfoan/vctors = detMinfoan(model);

minutes over it a matrix that consists of 23 linearly independent vectors. A further description of these vectors is provided and their companison to Extreme Pathways (2) is provided in the Supplementary Material of Bondbar et al 2014 (1) (Section 1 and Figure S2) Numerical properties of the stoichiometric matrix

[nMet,nMun]=size(madel.5)

Independent dimensions of the right nullspace of the stoichiometric matrix

farietf("Newson', "Musber of right sullsage basis vectors espected; "LeMon-rank(full(model,5))) Numerical properties of the mirripan basis:

Rank of the minSpanVectors

fprintf('newgyo','Rank of minipassectors matrix:',rank(full(minipassectors)))

Check the minipan is really a basis for the nullspace

fprintf('scage', 'Should be zero: ',ears(model,5*miniganVectors)) Investigate the spansity pattern of the minSpan basis:

11 Bordon A. Naparajan H. Levis NE, Latif H. Ebshim A. Federovicz S. Schellenberger J. Palsson RO. "Minimal metabolic pathway structure is consistent associated biomolecular interactions? Mol Syst Biol 10:737 (2014). DI Schilling CH. Lettscher D. Paleson RD. "Theory for the systemic definition of metabolic pathways and their use in interpreting metabolic function from a pathwaygriented perspective. J Theor Biol 202 (209-048 (2000).

fprintf("scape", "Should be zero (?): ',norm(nkun-rank(full(model.S))-rank(full(minipanmectors)))) fprintf("weegon", "Sparsity ratio of minipassectors: ",eng(minipassectors)/(nbunk-eminipassectors))