Multiple Objectives

MOLP: opt $\{c^1x, c^2x, \ldots, c^qx\}$: $Ax = b$, $x \geq 0$

> ➢ **maximize metabolite production**
> ➢ **minimize by-product production**
> ➢ **minimize substrate requirements**
> ➢ **maximize growth flux**
> ➢ **minimize mass nutrient uptake**
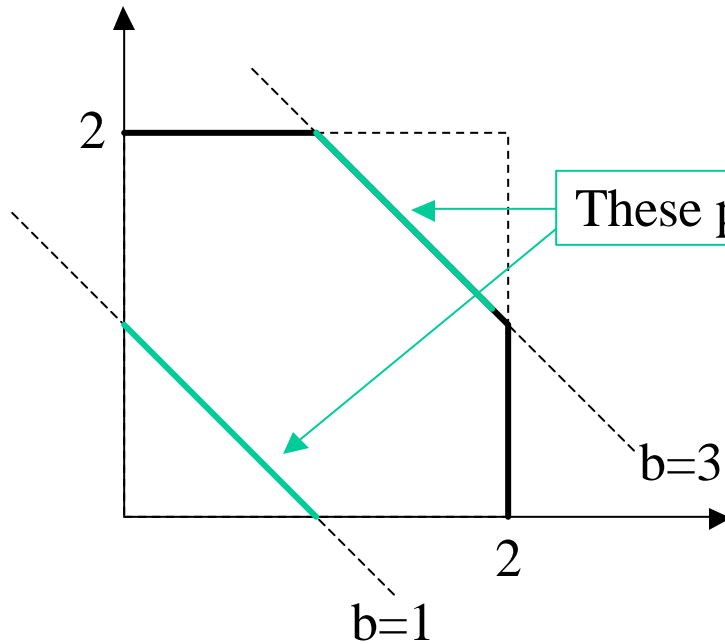
– Palsson , Schilling, Schuster et al., 1992 – 2002

◆ In general, these objectives *conflict* – there does not exist x*
for which each c^kx is optimized simultaneously

Life was simple before World War II. After that we had systems.
– Grace Hopper

Example

max {x(1), x(2)}: $0 \leq x(1), x(2) \leq 2, \ x(1) + x(2) \leq b$

These points seem like best compromise - why?

max x(1) = 2; max x(2)=2
infeasible to have x = (2, 2)

b=3

upper bounds redundant

b=1

What is best for x(1) is worst possible for x(2);
what is best for x(2) is worst possible for x(1)

How do we resolve conflicting objectives?

Extending Usual Definition of Maximum

➢ Definition 1: x* maximizes f on X if

   1. $x^* \in X$

   2. $f(x^*) \geq f(x)$ for all $x \in X$

➢ Definition 2: x* maximizes f on X if

   1. $x^* \in X$

   2. does not exist $x \in X$ such that $[f(x^*) \geq f(x)$ and $f(x^*) \neq f(x)]$

Efficient points

A feasible point x* is *efficient* if there does not exist another feasible point for which each each objective is at least as good and one is strictly better.

In MOLP let opt = max for all objectives and consider feasible points, u, v:
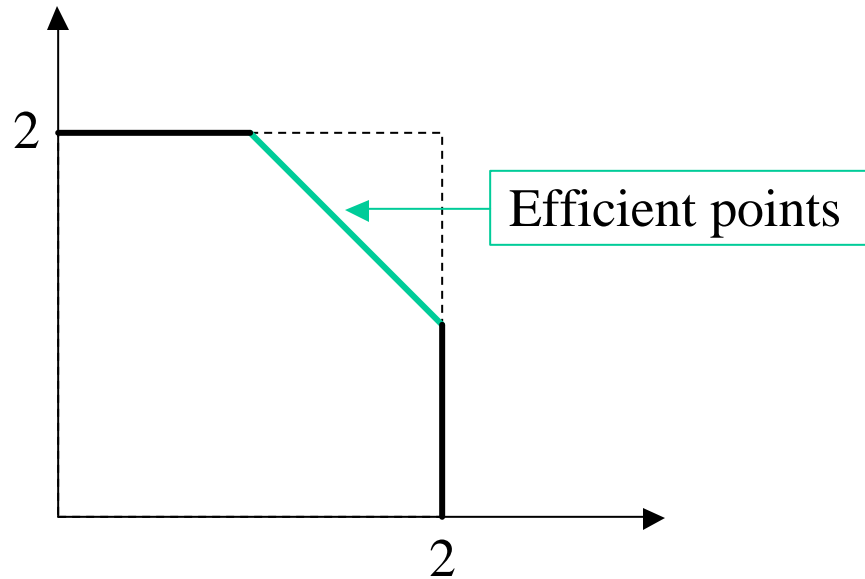
$$Au = Av = b, \quad u, v \geq 0$$

u *dominates* v if $c^k u \geq c^k v$ for all k and $c^k u > c^k v$ for some k

An efficient point is a feasible point that is not dominated.

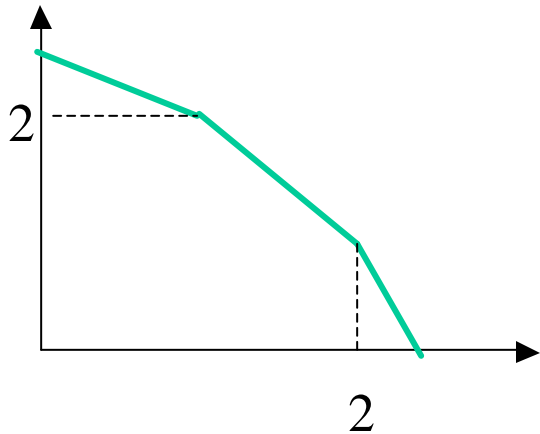The set of efficient points is called the *efficient frontier*

Example

Cannot improve one objective without worsening the other

The reasonable man adapts himself to the world. The unreasonable one persists in trying to adapt the world to himself. Therefore, all progress depends upon the unreasonable man.

– George Bernard Shaw

Properties of Efficient Points

➢ If feasible set is bounded, the set of efficient points, X*, is not empty and every x in X* is in convh{Ext(X*)}

  (caution: X* need not be a convex set)

  – X* is the union of faces of the feasible set

The set of **non-efficient** points is convex.

➢ Let x and x' be feasible solutions with the same number of active constraints. Then, x is efficient iff x' is efficient.

Constraints, Objectives, and Goals

➤ *Constraint* - some relation that must be satisfied (like mass balance equations)

➤ *Objective* - some function that represents preference (we'd like to minimize or maximize its value)

➤ *Goal* - some relation that is desirable to achieve, but could be violated at some penalty to overall value of solution

$$\max f(x) - P(g(x)): \ x \in X$$

$$\text{goal: } g(x) \le 0 \Rightarrow P(v) \begin{cases} = 0 \ \text{ if } g(x) \le 0 \\ > 0 \ \text{ otherwise} \end{cases}$$

+ Targets

➢ ***Constraint*** - some relation that must be satisfied (like mass balance equations)

➢ ***Objective*** - some function that represents preference (we'd like to minimize or maximize its value)

➢ ***Goal*** - some relation that is desirable to achieve, but could be violated at some penalty to overall value of solution ("soft constraint")

➢ ***Target*** - constraints on objectives

x* is a *target-optimal solution* if it solves

$$\max c^k x: \ Ax = b, \ x \geq 0, \ c^i x \geq c^i x^* \text{ for all } i \neq k$$

for all k=1, …, q

Example
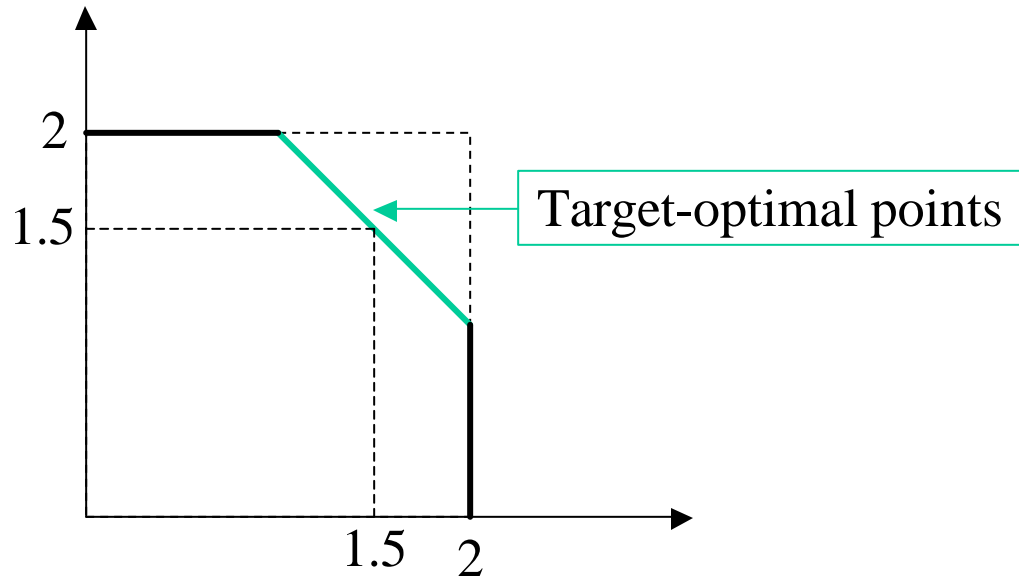
x* = (1.5, 1.5) is target-optimal because

$$1.5 = \max\{x(2): 0 \le x(1),\ x(2) \le 2,\ x(1) + x(2) \le 3,\ x(1) \ge 1.5$$
$$1.5 = \max\{x(1): 0 \le x(1),\ x(2) \le 2,\ x(1) + x(2) \le 3,\ x(2) \ge 1.5$$

A theory has only the alternative of being right or wrong. A model has a third possibility – it may be right but irrelevant.

– Manfred Eigen

Lexico-optimal

Order objectives, making the value of $c^i x$ "more important" than the value of $c^{i+1} x$ (*ordinal ranking*)

$$z^1 = \text{opt}\{c^1 x: \ Ax = b, x \geq 0\}$$

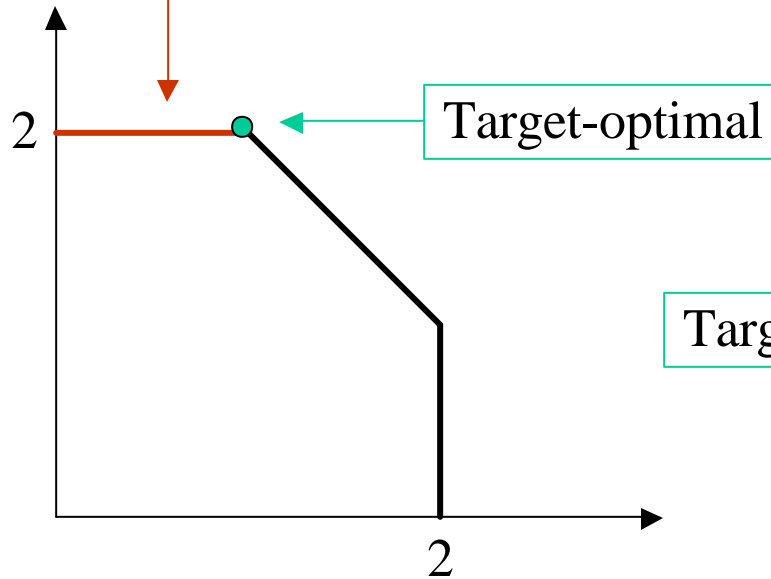$$z^2 = \text{opt}\{c^2 x: \ Ax = b, x \geq 0, c^1 x = z^1 \}$$

$\vdots$

$$z^k = \text{opt}\{c^k x: \ Ax = b, x \geq 0, c^i x = z^i \text{ for all } i < k\}$$

Last optimality region is target-optimal
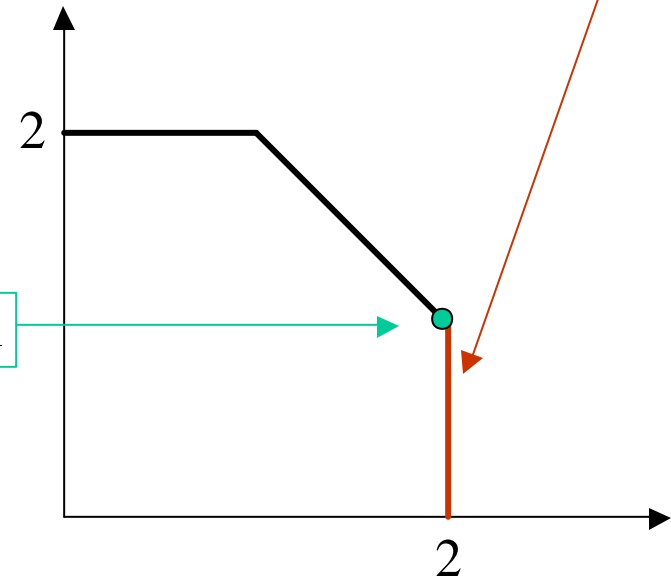(meaningful only if there are alternative optima at each step)

Example

argmax{x(1): $0 \leq x(1), x(2) \leq 2,$
$x(1) + x(2) \leq 3$}

argmax{x(2): $0 \leq x(1), x(2) \leq 2,$
$x(1) + x(2) \leq 3$}

Target-optimal

Target-optimal

2

2

2

2

$c^1x :> c^2x$

$c^2x :> c^1x$

$:>$ more important than

Nearly lexico-optimal

Give some slack, allowing objective values to be less than max

$$z^1 = \max\{c^1 x: \ Ax = b, x \geq 0\}$$

$$z^2 = \max\{c^2 x: \ Ax = b, x \geq 0, c^1 x \geq r^1 z^1 - t^1\}$$

$$\vdots$$

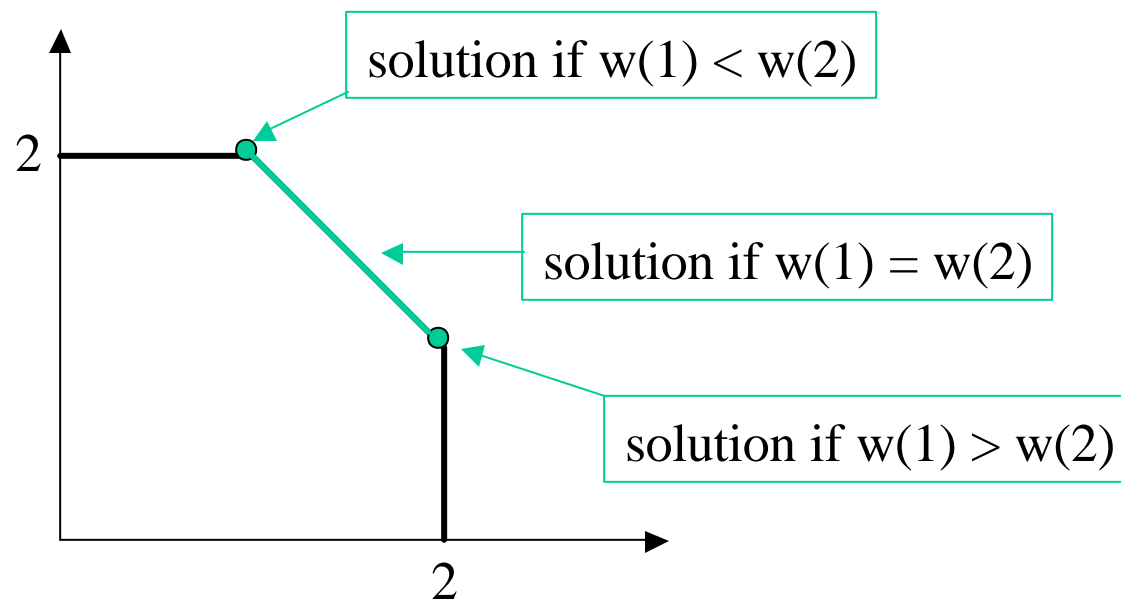$$z^k = \mathrm{opt}\{c^k x: \ Ax = b, x \geq 0, c^i x \geq r^i z^i - t^i \text{ for all } i < k\}$$

If alternative optima exist in last set, tighten tolerances in some order until exact lexico-optimal solution is achieved or solution is unique. Then, last optimality region is target-optimal

Weights

$$\max w(1)c^1x + w(2)c^2x + \ldots + w(q)c^qx: \; Ax = b, \; x \geq 0$$

$$\text{for some } w > 0.$$

Example:
$$\max w(1)x(1) + w(2)x(2)\}: 0 \leq x(1), x(2) \leq 2, \; x(1) + x(2) \leq 3$$

Combine coefficients

Given $w > 0$, compute $C = w(1)c^1 + w(2)c^2 + \ldots + w(q)c^q$

So, $w(1)c^1x + w(2)c^2x + \ldots + w(q)c^qx = Cx$

w-weighted LP is max Cx: $Ax = b$, $x \geq 0$

x^* is w-*optimal* if it solves this LP
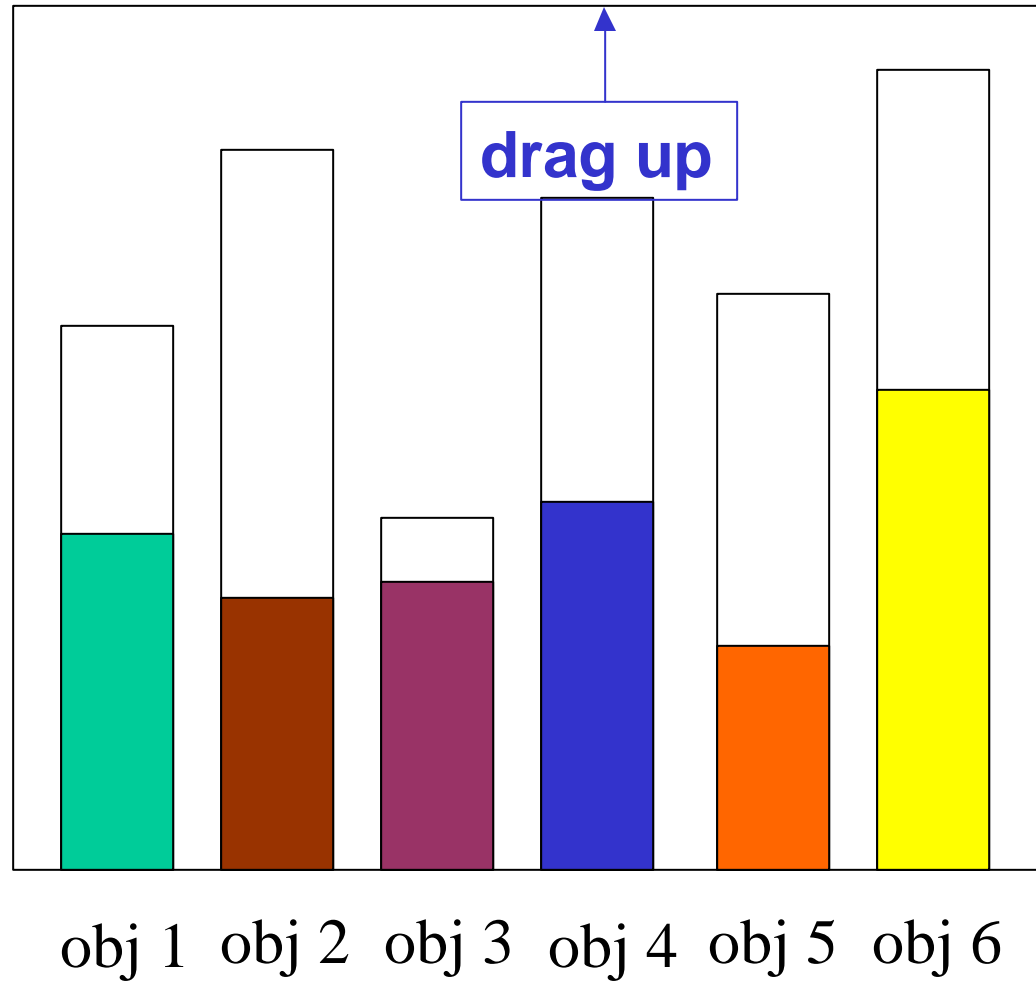
Good questions outrank easy answers.
– Paul A. Samuelson

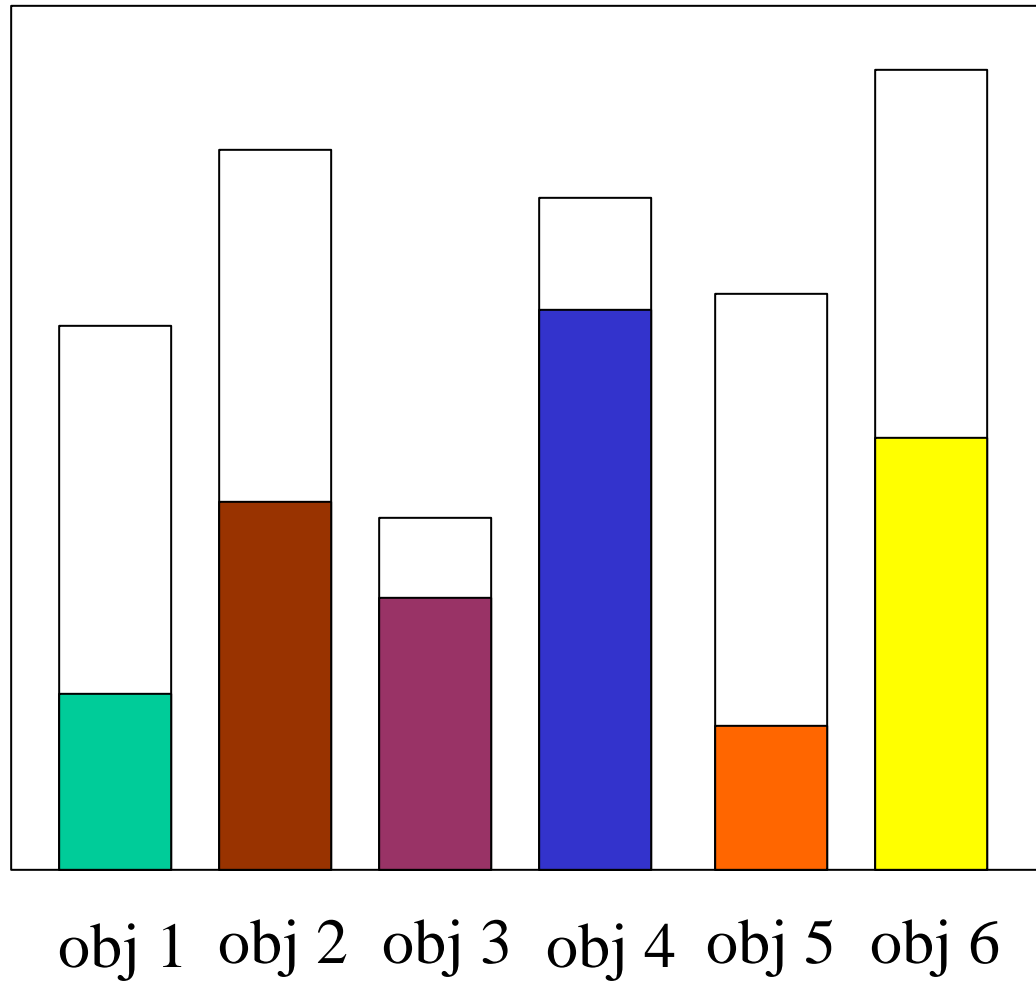# Solution Equivalence

The following are equivalent statements
1. x* is an efficient point
2. x* is target-optimal
3. x* is w-optimal for some w > 0

For 2 objectives, the efficiency frontier can be computed by
parametric programming

Visualizing solutions

Visualizing solutions

Enumerating Efficient Extreme Points

➢ Maybe analysis of Extreme pathways of the flux cone can be "reduced" to analysis of *extreme points* in the efficiency frontier – e.g., how are extreme pathways distributed for particular weighted objective?

The pure and simple truth is rarely pure and never simple.
– Oscar Wilde

Software

➤ ADBASE (Steuer, '72) - should arrive here

➤ NIMBUS (http://nimbus.mit.jyu.fi/)

➤ PROTASS (R. Cytrycki & A. Dzik)

References

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J. Vera, P. De Atuari, M. Cascante and N.V. Torres, Multicriteria Optimization of Biochemical Systems by Linear Programming. Application to the Ethanol Production by *Saccharomyces cerevisiae*, Technical Report, Department de Bioquimica y Biologia Molecular, Universidad de La Laguna, Spain, 2003.

Y. Mamamoto, *Optimization over the Efficient Set: Overview*, Technical Report, Institute of Policy and Planning Sciences, University of Tsukuba, Japan, 2001.