Arbetsrapport

Från Skogforsk nr. 841–2014

OPSEL 1.0: A computer program for optimal selection in forest tree breeding

Opsel 1.0: Dataprogram för optimalt urval i skogsträdsförädlingen

Tim J. Mullin

SKOGFORSK

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The Arbetsrapport series comprises background material, descriptions of methods, results, analyses and conclusions relating to both current and completed research.

Titel:
OPSEL 1.0: a computer program for optimal selection in forest tree breeding.
Opsel 1.0: Dataprogram för optimalt urval i skogsträdsförädlingen.

Bildtext:
"The TreO-T10 Dag Lindgren Seed Orchard established 2013 near Umeå. The orchard has a total of 84 clones represented by varying numbers of ramets, optimized by OPSEL to give maximum genetic value while ensuring adequate genetic diversity"

Fotograf Johan Kroon.

Ämnesord:
Breeding population, Gene diversity, Genetic gain, Group coancestry, Optimal selection, Relatedness, Seed orchard contributions, Selection.

Fröplantage, Förädlingspopulation, Genetisk diversitet, Genetisk vinst, Optimal selektion, Släktskap.

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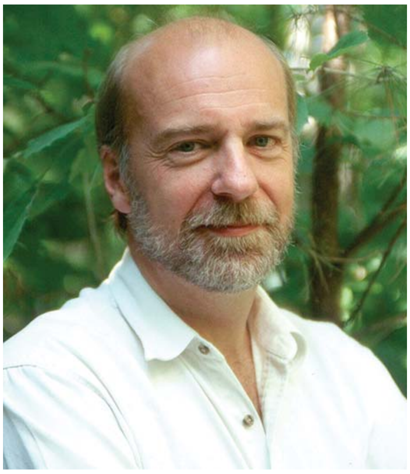
SKOGFORSK

Uppsala Science Park, 751 83 Uppsala
Tel: 018-18 85 00 Fax: 018-18 86 00
skogforsk@skogforsk.se
skogforsk.se



Tim Mullin, is a Canadian forest geneticist with 20 years' experience working closely with tree breeders in Sweden. Since 2008, he has been part-time as Senior Research Scientist at Skogforsk in Sävar.

Abstract

Tree breeders must often consider conservation of genetic diversity, while at the same time maximizing response to selection. Optimal selection will not completely avoid kinship among selected individuals, but rather maximize average gain while imposing a constraint on average relatedness. This report introduces a new, fully-integrated tool called "OPSEL".
The computer software tool uses mathematical programming for optimized selection of both breeding populations and seed orchards. This report is intended as a guide to the installation of the software, preparation of input data, running the optimizations, and interpreting the output. OPSEL and its supporting software tools are freely available from Skogforsk for non-commercial purposes under general public licenses.

Preface

This research has received funding from (1) the European Community's Seventh Framework Programme (FP7/2007–2013) under grant agreement n° 211868 (Project Noveltree), and (2) Föreningen Skogsträdsförädling (The Tree Breeding Association, Sweden).

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Tim J. Mullin

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Sammanfattning

Skogsträdförädlare måste ofta beakta bevarandet av genetisk diversitet och samtidigt maximera selektionsvinsten. Vid urval av kloner till en förädlingspopulation måste förädlaren välja metoder som både stödjer snabba förädlingsframsteg och lämnar utrymme för framtida genetiska förbättringar i kommande generationer. För en köpare av plantagefrö gäller det att maximera värdeproduktionen på odlingslokalen samtidigt som hänsyn måste tas till genetisk diversitet i den etablerade föryngringen.

Vid ett optimalt urval undviks inte släktskap mellan utvalda träd helt och hållet, utan den genetiska vinsten kommer snarare att maximeras givet en fastställd begränsning vad gäller tillåtet genomsnittligt släktskap mellan utvalda träd. I denna rapport presenteras ett nytt hjälpverktyg i förädlingsarbetet ”OPSEL”, som kan användas både vid urval av träd till förädlingspopulationer och till fröplantager. Även om urvalen till förädlingspopulationer och fröplantager verkar likvärdiga, kräver de i realiteten olika angreppssätt vid formulering av funktionen som skall optimeras och hur lösningen skall uppnås. Vid urval till en förädlingspopulation kräver vi att den utvalda populationen skall ha en bestämd storlek, givet antagandet att de utvalda föräldrarna bidrar lika mycket. För fröplantager, är svårigheten att generera en plantage där utvalda föräldrar bidrar till fröskörden så att vinsten maximeras (föräldrarna kan här bidra olika), samtidigt som fröskörden uppfyller fröplantagens diversitetsmål.

OPSEL och dess stödjande program är fritt tillgängliga från Skogforsk för icke-kommersiella ändamål (på villkor fastställda under ”GNU General Public License”). Rapporten är tänkt som en vägledning vid installation av programvaran, preparering av indata samt programstyrning och resultattolkning.

Summary

Tree breeders must often consider conservation of genetic diversity, while at the same time maximizing response to selection. Breeders need to select breeding populations that make rapid progress in terms of genetic gain, while maintaining genetic diversity for future genetic improvement, while buyers of seed-orchard seed want maximum performance, while satisfying a restriction, sometimes legislated, on the diversity deployed to the forest.

Optimal selection will not completely avoid kinship, but rather maximize gain while imposing a constraint on average relatedness. This report introduces a new, integrated tool called “OPSEL”, for optimum selection in tree breeding, both for selection of breeding populations and seed orchards. While the two problems appear similar, they require rather different approaches to formulating the object function to be optimized, and the solvers required to accomplish the task. In the case of breeding populations, we require a selected population of fixed size, on the assumption that the selected parents will contribute equally. For seed orchards, the problem becomes one of generating an orchard where selected parents contribute to the seed crop in such a way that gain is maximized, while satisfying the orchard diversity target.

OPSEL and its supporting software tools are freely available from Skogforsk for non-commercial purposes under general licenses. This report is intended as a guide to the installation of the software, preparation of input data, running the optimizations, and interpreting the output.

Introduction

It is common in tree breeding that selection of populations must consider conservation of genetic diversity, while at the same time attempting to maximize response to selection. It is generally recognized that one cannot to simply select the "best" trees, without also taking into account the degree of relatedness among them. Managing relatedness among selections becomes complicated as early as the first cycle of breeding, when parents, siblings and other close relatives have similar ranks. The optimal solution is not to completely avoid kinship, but rather to find the set of selections that maximizes gain under a relatedness constraint.

The issue of how to truly optimize the balance between gain and relatedness can be approached in several ways. In the context of tree breeding, the problem was formulated by Lindgren and Mullin (1997) who expressed "group merit" of a selected population as a function of average genetic value, penalized by a weight on relatedness among individuals, as expressed by their "group coancestry" (*sensu* Cockerham, 1967). While they provided a way to maximize group merit for a fixed number of selections with equal representation ("Group-Merit Selection": GMS), the constraint on relatedness is applied indirectly, so that achieving a specified level when selecting breeding populations requires a trial-and-error approach, typically with many iterations.

The special case of optimizing deployment of genotypes to a wind-pollinated seed orchard was explored by Lindgren and co-workers (Lindgren et al. 1989; Lindgren and Matheson 1986) who suggested that the optimum relationship between candidate breeding value and their contribution to the population would be linear. The application of "linear deployment" is only possible when the candidates are unrelated, as might be the case when selecting "backward" on progeny tested plus-tree candidates. If the candidate pool includes relatives, Bondesson and Lindgren (1993) suggested that a more complex formulation would be required, perhaps using a Lagrange function. In more recent work, Lindgren's group used the Microsoft Excel add-in tool, "Solver", to maximize gain by Linear Programming under a Lagrange equality constraint on relatedness (Danusevičius and Lindgren 2008; Lindgren et al. 2009).

Other methods to optimize the gain-diversity balance have been proposed. These include the Optimum Contribution (OC) algorithm based on Lagrangian multipliers (LM), originally proposed for selection in dairy cattle (Hinrichs et al. 2006; Meuwissen 1997) and recommended for application to forest trees by Kerr et al. (1998). The application of OC has been demonstrated in the management of breeding (Hallander and Waldmann, 2009a) and in the optimal selection of Scots pine parents for a seed orchard with unequal numbers of ramets (Hallander and Waldmann, 2009b).

There are some serious drawbacks with the LM method. First, by removing candidates or fixing their contributions to zero and re-optimizing with a new subset of candidates, it is possible that the true optimum solution is bypassed in the iterative procedure. Second, there is no restriction on the maximum allowed contribution of any particular candidate. This means that *ad-hoc* manipulations of the final solution may be required to satisfy other operational constraints on its implementation. For example, in forest tree breeding, one major constraint for the establishment of grafted seed orchards is the number of scions that can be collected from a given genotype. Finally, the objective of selection can also be to form a breeding population of fixed size, whose members will contribute equally to a recruitment population; optimal solutions that satisfy such constraints are not possible with the LM approach.

This report introduces a new, integrated tool called "OPSEL", for optimum selection in tree breeding, both for selection of seed orchard and breeding populations. While this documentation is intended to be complete, we have assumed that the user is familiar with the terminology and procedures commonly used in genetic evaluation, selection, and measures of relatedness. Some users, particularly those without formal training in quantitative genetics, may find it useful to review concepts in an introductory textbook on forest tree breeding or crop improvement (e.g., White et al. 2007). Similarly, the guide assumes a general familiarity with basic procedures and configuration of PC-compatible personal computers. Details on these procedures can be found in the original hardware and operating system documentation and in a host of other references available in any computer store or library.

Background theory

In OPSEL, the two variations on the optimal selection problem are solved by means of mathematical programming techniques, but the approaches are quite different. What follows is a brief description of each approach; for detailed theoretical development, the reader is referred to Mullin and Belotti (2014) and Ahlinder et al. (2014)

BRANCH-AND-BOUND OPTIMIZATION OF FIXED-SIZE BREEDING POPULATIONS

When selecting a fixed-size breeding population, we are searching for a cohort of exactly N individual genotypes from a complex pedigree containing totally Z members that are to contribute their genes as breeding parents in equal proportions. The object is to maximize the expected genetic merit of contributions from the selected cohort, given by $\mathbf{c}^T\mathbf{g}$ where the estimated breeding values (EBV) for all pedigree members are found in vector $\mathbf{g}$, of size $Z \times 1$; the contribution of genes as a proportion is denoted $\mathbf{c}$, of size $(Z \times 1)$, where $\mathrm{c}_i \in \{0, 1/N\}$ so that each individual in the selected cohort contributes exactly $1/N$ to the future gene pool, and if not selected contributes zero; and the sum of all contributions must equal unity ($\sum_1^Z \mathrm{c}_i = 1$).

To control relatedness in the breeding population, we wish to impose a constraint on the group coancestry, $\boldsymbol{\theta}$, of the selected cohort of trees, such that $\theta \geq \mathbf{c}^T\mathbf{Ac}/2$, where the additive or numerator relationship matrix of the pedigree is denoted $\mathbf{A}$, of size $Z \times Z$.

For the variable $\boldsymbol{c} \in \mathbb{R}^Z$, the problem can be expressed in a form that uses binary variables, i.e., variables that can take only values 0 or 1. This formulation is suited to a particular class of solution algorithms called *branch-and-bound*, which are very well known in the optimization literature (Land and Doig 1960). A new variable $\boldsymbol{y}$ is defined such that $\boldsymbol{y} = N\mathbf{c}$ and the problem respecified to minimize the objective function:

$$\text{Minimize:} \qquad -\boldsymbol{y}^T\mathbf{g} \tag{1a}$$

$$\text{Subject to:} \qquad \boldsymbol{y}^T\mathbf{A}\boldsymbol{y} \leq 2\theta N^2 \tag{1b}$$

$$\boldsymbol{y}^T\mathbf{1} = N \tag{1c}$$

$$y_i \in \{0,1\} \quad (i = 1, \ldots, Z) \tag{1d}$$

The advantage in using binary variables lies in the availability of mixed-integer linear programming (MILP) software packages, such as CBC[1] (COIN-OR branch and cut) that accept models with optimization variables that are discrete in nature and take on integer values. The solver used by OPSEL to optimize selection of fixed-size breeding populations, dsOpt, was custom written by Dr. Pietro Belotti using the open-source MILP routines available in CBC.

OPSEL accepts input regarding the total number of genotypes to select for the breeding population, the constraint on relatedness (as group coancestry or Status Number), and the name of a text file containing the EBVs of all candidate genotypes, as well as the complete pedigree including ancestors. These data are used to prepare the input file for solving by dsOpt. If the solver completes successfully, OPSEL will read the solution output and generate a file with the original data, as submitted in the pedigree file, and with an additional columns specifying the N selected genotypes with “1” and the remainder as “0”.

[1] The CBC libraries are written in C++ and are available as open-source code at http://coin-or.org/

SEMIDEFINITE PROGRAMMING FOR OPTIMUM SELECTION OF SEED ORCHARDS

Semidefinite programming (SDP) is an optimization method to minimize a linear objective function, subject to the constraint that a linear combination of symmetric matrices is positive semidefinite (Vandenberghe and Boyd 1996). The constraint is convex, meaning that if two points satisfy the constraint, then any point on the segment between the two points also satisfies the constraint. It is the convex nature of constraints that allows SDPs to be solved efficiently. The objective to find a minimum for a linear function over a linear matrix inequality can be described by the general form:

$$\text{Minimize:} \sum_{i=1}^{Z} f_i x_i \quad \text{Subject to:} \mathbf{Y_0} - \sum_{i=1}^{Z} \mathbf{Y}_i x_i \geq \mathbf{0}$$

The input data are $f_1, f_2, \ldots, f_Z \in R$ and $\mathbf{Y}_0, \mathbf{Y}_1, \ldots, \mathbf{Y}_Z$ being matrices of the same dimension, while the decision variable is $\mathbf{x} \in R^Z$. The notation $\mathbf{Y} \geq \mathbf{0}$ indicates that matrix $\mathbf{Y}$ is positive semidefinite, i.e., all the eigenvalues of $\mathbf{Y}$ are non-negative. SDP can be considered as an extension of Linear Programming to the space of matrices.

To formulate the selection of genotypes with unequal numbers of ramets to a grafted seed orchard as an SDP, we first consider selecting a cohort from a complex pedigree, containing totally Z genotypes that are to contribute their genes in optimal proportions. The object is to maximize the expected genetic merit of contributions from the selected cohort, given by $\mathbf{c}^T\mathbf{g}$ where: the estimated breeding values (EBV) for all pedigree members are found in vector $\mathbf{g}$, of size $Z \times 1$; and the contribution of genes as a proportion is denoted $\mathbf{c}$, also of size $Z \times 1$. In our problem, the decision variable is $\mathbf{c}$, where $1 \geq \mathrm{c}_i \geq 0$, and the sum of all contributions from the selected cohort equals unity ($\sum_1^Z \mathrm{c}_i = 1$).

There are a number of constraints required to fully formulate the selection problem. First, we wish to impose a quadratic restriction on the relatedness or group coancestry, θ, of the selected cohort, specified as $\theta \geq \mathbf{c}^T\mathbf{A}\mathbf{c}/2$, where the additive or numerator relationship matrix of the pedigree is denoted $\mathbf{A}$, of size $Z \times Z$. The maximum and minimum contributions that a particular individual can make are denoted $\mathbf{m}$ and $\mathbf{u}$, respectively, with both vectors of size $Z \times 1$. Here, if pedigree member i is not itself a candidate for selection (e.g., not physically available for use), the corresponding maximum contribution is set to zero (i.e., $m_i = 0$). Similarly, while the minimum number of contributions for a genotype might normally be zero, there may be times when prior investments or operational requirements might motivate setting u_i to a specific value greater than zero, provided that $m_i \geq u_i$.

In order to find the optimal gene contributions, we wish to:

$$\text{Maximize:} \quad \mathbf{c}^{T}\mathbf{g} \tag{2a}$$

$$\text{Subject to:} \quad \mathbf{c}^{T}\mathbf{A}\mathbf{c}/2 \leq \theta \tag{2b}$$

$$\mathbf{c}^{T}\mathbf{1} = 1 \tag{2c}$$

$$\mathbf{c} \geq \mathbf{u} \tag{2d}$$

$$\mathbf{c} \leq \mathbf{m} \tag{2e}$$

where $\mathbf{1}$ is a vector of size $Z \times 1$ containing 1's.

When reformulating as an SDP problem, the quadratic constraint (2b) is expressed in linear form using its *Shur complement* and the equality constraint (2c) replaced by two inequality constraints, so that the selection problem is reformulated:

$$\text{Minimize:} \quad -\mathbf{c}^{T}\mathbf{g} \tag{3a}$$

$$\text{Subject to:} \quad \begin{bmatrix} \mathbf{A}^{-1} & \mathbf{c} \\ \mathbf{c}^{T} & 2\theta \end{bmatrix} \geq \mathbf{0} \tag{3b}$$

$$\mathbf{c}^{T}\mathbf{1} - 1 \geq 0 \tag{3c}$$

$$-\mathbf{c}^{T}\mathbf{1} + 1 \geq 0 \tag{3d}$$

$$\mathbf{c} - \mathbf{u} \geq 0 \tag{3e}$$

$$\mathbf{m} - \mathbf{c} \geq \mathbf{0} \tag{3f}$$

OPSEL uses an open-source solver to optimize the SDP, known as SDPA (Fujisawa et al. 2008; Yamashita et al. 2003; Yamashita et al. 2010). While SDPA is very flexible, with flexibility comes complexity and room for error in setting up the SDP properly and interpreting the output. OPSEL simplifies the task, receiving input regarding the total number of ramets to be established in the orchard, the constraint on relatedness (as group coancestry or Status Number), whether a minimum is to be imposed on individual genotype contributions (i.e., $\mathbf{u} \neq \mathbf{0}$), and the name of a file containing the EBVs of all candidate genotypes, their maximum (and optionally minimum) frequency in the selected group, as well as the complete pedigree including ancestors. These data are used to prepare the SDP for solving by SDPA. Once SDPA has completed its work, OPSEL then reads the SDPA output and generates a file with the original data, as submitted in the pedigree file, and with additional columns specifying the optimum contribution as a proportion and as an integer number of ramets for each genotype.

Hardware/software requirements for OPSEL

OPSEL is written as a 64-bit program for PC-compatible computers, but will run on any computer under the Microsoft Windows Operating System from version "XP" to present, provided a 64-bit version is installed. OPSEL will also require access to *dsOpt.exe* and/or *SDPA.exe*, depending on the type of selection required. A text editor is required to prepare input files and interpret some files created by OPSEL. While not absolutely necessary, most users will also find it helpful to have access to an Excel-compatible spreadsheet program for editing of pedigree and breeding value data, converting these to text or comma-separated files for input to OPSEL, and manipulation of files created when OPSEL is run.

Becoming a registered user of OPSEL

OPSEL and its supporting tools are available from Skogforsk. Registered users will receive the package components in a zip file emailed directly to them. While distribution OPSEL is not restricted, registration is strongly encouraged. Periodic updates, bug fixes and lists of known issues will be circulated to all registered users as they are released.

A note on copyright, licensing and warranty

While copyright for OPSEL is held by Skogforsk, distribution is without fee for research and non-commercial use under GNU General Public License Version 2.0. A copy of the GPLv2 license must accompany distribution of OPSEL and work derived from it. In addition, there is ABSOLUTELY NO WARRANTY expressed or implied, and the user bears all the risk when using OPSEL. Users should be aware that OPSEL uses open-source software to perform some of its functions, including SDPA, CBC and dsOpt – copies of licenses for these products are distributed with the OPSEL package. In accepting the conditions of use on the opening screen, the user also agrees to the conditions of use for these components – please read these!

Distribution of OPSEL

OPSEL, its supporting solvers and up-to-date documentation can be found at www.skogforsk.se/opsel. The following files are provided in the package:

- *opsel.exe* – the executable binary for running OPSEL.
- *sdpa.exe* – the solver for semi-definite programs, used by OPSEL.
- *dsOpt.exe* – the branch-and-bound solver for MILP, used by OPSEL.
- *GNUv2_license.txt* – GNU General Public License, Version 2, applies to OPSEL and SDPA.
- *Eclipse_license.txt* – Eclipse General Public License, Version 1, applies to CBC and dsOpt.
- *Example1.csv* and *Example2.csv* – the example datasets discussed in this document, formatted as comma-separated values.
- *Example1.cntl* and *Example2.cntl* – control parameter files for running examples through the command line in Command Prompt window
- *OPSEL_Userguide_v1.pdf* – this document.

Installing OPSEL

The following procedure is recommended for installing the program, although file locations could be changed, once successful operation of the program has been verified.

1. Extract the zip file to a convenient folder on your machine, such as *C:\OPSEL\. The "OPSEL.exe", "dsOpt.exe",* and *"SDPA.exe"* files may have had the *".exe"* extensions stripped, to enable the sending of the zip file through institution firewalls; if so, you will need to restore the names by adding "*.exe*" to distributed file names. We recommend that all files in the package be placed in the folder where optimization is to occur, i.e., the same file as the user-prepared input files.

2. Test your installation by working through the optimization of example data sets provided with the package and detailed in the next sections.

Running the examples provided with OPSEL

THE CANDIDATE FILE

OPSEL is distributed with example candidate files, formatted as *.csv* files for selection of a breeding population and a seed orchard, and distributed with the package as *Example1.csv* and *Example2.csv*, respectively. The files describe the pedigree of the selection candidates and their ancestors, using the Me-Mum-Dad standard that will be familiar to most users of pedigree analysis tools and databases, and appends extra fields to describe the genetic values and frequency constraints in the selected population. Open this file in a text editor or in Excel and note the following structure:

1. The first line of the file will be skipped, so can contain column headers to document the file.

2. Each of the subsequent lines describes an each individual with its ID, those of its Female and Male parents, its genetic value, and finally the maximum (and optionally for seed orchard selection the minimum) number of times that the individual can occur in the selected population.

The pedigree must respect the usual rule that parents precede their progeny in the file sequence, and that all ancestors must be listed. Unknown Female and Male IDs are indicated with a 0 (zero). All other pedigree IDs are alphanumeric labels up to 256 characters in length. As spaces, commas and tab characters are used to delimit fields, these characters are not permitted in any field. Small examples of candidate files for breeding populations and seed orchard selection are illustrated in Figures 1 and 2, respectively.

The 4th field of each line contains the genetic value of the individual as a real number. If the individual is not regarded as a selection candidate (an ancestor or other relative). While we suggest setting this value to 0 (zero) or some other "undesirable" value if the individual is not a valid candidate, this column does NOT constrain the use of an individual in selection. Rather, the maximum number of times the individual can be used in the selected population, is specified in column 5, as an integer. When selecting a breeding population, this value should be 0 or 1 (see *Example1.csv*); an orchard problem would specify the maximum number of ramets that could be generated for establishment in the orchard (see *Example2.csv*). If the individual is not regarded as a selection candidate (an ancestor or other relative), the value in the Max field should always be 0 (zero). Note, in *Example2.csv*, we have specified a maximum of 2 800 when the candidate is a founder (a large older individual in an archive, capable of providing many scions for orchard grafting), whereas the F1 candidates are constrained to a maximum of 50 (as these individuals are much younger with smaller crowns).

When preparing the input file, the user will normally use a spreadsheet program to organize and create the various fields. Simple save the spreadsheet as a comma-separated value (*csv*) or tab-delimited txt file before submitting to OPSEL. When submitted to OPSEL, any additional columns will be ignored and not transferred to the output file.

INTERACTIVE DIALOGUE OR COMMAND LINE

OPSEL is a Windows program. It can be started by double-clicking on the program icon (*opsel.exe*), which will take the user through an online dialogue to define the constraints, declare the path to the candidate file and initiate the optimization. Alternatively, the user can run the program from the command-line in the Command Prompt window, declaring a control file as a parameter that defines the constraints and declares the location of the candidate file. The following sections describe the running of each example through both the online dialogue and via the command line.

Table 1.
Small example of a candidate file for optimum selection of a fixed-size breeding population. The *Max* column will always contain either the value *1*, indicating that the individual is a candidate, or 0, indicating that the individual is not a candidate, but is included as an ancestor to another individual (e.g., individual 2).

Indiv.	Female	Male	EBV	Max
1	0	0	90.4	1
2	0	0	0.0	0
3	0	0	75.5	1
4	1	2	100.4	1
5	1	3	130.5	1
6	2	4	150.3	1
.	.	.	.	.
.	.	.	.	.
.	.	.	.	.

Table 2.
Small example of a candidate file for optimum selection of a seed orchard. The Max column will always contain a value >= 1 (indicating that the individual is a candidate up to the specified maximum frequency) or = 0, indicating that the individual is not a candidate, but is included as an ancestor to another individual (e.g., individual B). The last column is optional if a minimum frequency is to be specified; in this case individual C will be included in the solution up to 5 times.

Indiv.	Female	Male	EBV	Max	Min
A	0	0	200.4	25	0
B	0	0	0.0	0	0
C	0	0	180.4	25	5
D	A	B	223.5	10	0
E	A	C	165.3	10	0
F	B	C	225.7	10	0
G	A	F	300.2	15	0
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.

SELECTING A FIXED-SIZE BREEDING POPULATION – *EXAMPLE1.CSV*

Prepare the candidate list

In this example, we wish to select a breeding population of exactly 50 parents from a candidate list. OPSEL will submit the constraint data and candidate list to dsOpt.exe and interpret the output. The time required for the optimization is difficult to predict, but it is recommended to truncate the candidate list in a sensible way, to reduce the size of the problem and decrease the time required to find a solution. This can be done through a combination of techniques such as:

1. Limiting the number of full-sibs so that the candidate list contains only the best sibs in each family; and/or
2. Apply a breeding value threshold, below which candidates are dropped from the list.

The candidate file must conform to the format and sort order described earlier, and must contain the following 5 columns (other columns in this file are ignored):

Indiv *Female* *Male* *EBV* *Max*

The estimated breeding values (EBVs) would normally be extracted, together with the appropriate pedigree entries, from a third-party database, such as DATAPLAN®.

Running *Example1.csv* through the online dialogue

The following is a detailed description of an OPSEL job selecting a fixed-size breeding population, illustrated by processing *Example1.csv:*

1. Start OPSEL by double-clicking on *OPSEL.exe*
2. Accept the conditions of use on the splash screen by typing "*y*", then pressing Enter
3. The description on the next screen is a summary of the information in this user guide on how to prepare the pedigree file. Note that the "root" name of the input file, in this case "*Example1*", is used by OPSEL when referencing all other files, using different extensions appended to the root.
4. Enter the name of the candidate file containing the pedigree and breeding-value data: *Example1.csv.*
5. Specify that OPSEL is to use the "equal contributions" option by entering 0.
6. OPSEL reports the current working directory and asks if the MILP solver "*dsOpt.exe*" is in this folder. If so, just answer "*y*", otherwise enter "*n*" and OPSEL will ask you to specify the full path location of *dsOpt.exe.*
7. Specify the desired census size of the selected population, in this case 50.
8. OPSEL now needs to know the constraint on diversity of the selected population. This can be specified either as group coancestry, or as Status Number. In this case, specify the constraint on maximum group coancestry as 0.015 (which is equivalent to a Status Number of $1/(2 \times 0.015) = 33.33$).
9. The solver will work on the problem until it finds the optimum solution, or until the time threshold is reached. The default threshold is 7 200 seconds and is appropriate for this example.
10. The branch-and-bound search is limited by default to 10 000 nodes. Again, this default is appropriate for this example.
11. OPSEL will continue the optimization until the solution is within a specified "gap" from the theoretical optimum. A smaller gap threshold will require more time to execute, but there is no guarantee that a better solution will be found. The default of 0.5% is appropriate for this example.
12. By default, OPSEL will store the solution in a text file, but you can specify comma-separated values here, if you wish. Doing so will make it easier to read the solution with Excel.
13. OPSEL now proceeds to formulate the MILP and to build the input for dsOpt. A call to *dsOpt.exe* is made, and you will see its progress in a separate DOS command-line window.

14. Once dsOpt has completed the optimization, control is returned to OPSEL which interprets the output. OPSEL will ask you if you want to store your responses to the online dialogue to run later from the command line; provide a filename, such as *Example1.cntl.*
15. Check the folder where you started OPSEL and you will find the following additional files:

    Example1_in.txt – the input prepared by OPSEL for dsOpt.

    Example1_in.sol – the raw solution generated by dsOpt.

    Example1_solution.csv or *Example1_solution.txt* – the solution combined with the initial candidate list, in either comma-separated format or as a text file, as specified by the user.

The columns in the file are:

Individual – ID of the individual genotype.

Female – ID of the individual's mother.

Male – ID of the individual's father.

EBV – the genetic value of the individual (supplied by user).

Freq – selected individuals are indicated by 1, all others by 0.

Max – the constraint on the maximum contribution for each individual (either 0 or 1).

Example1_log.txt – a log file that contains summary statistics about the problem and its solution.

Running *Example1.csv* from the command line

OPSEL can also be run from the command line by specifying the various job parameters in a separate text file. The simplest way to do this is to run through online dialogue and save the parameters in a text file, such as (see step 14 above). A sample version of *Example1.cntl* is provided in the OPSEL distribution package and can be modified with any text editor.

Open a Command Prompt window -- usually found in the Accessories folder. Navigate to the location of *opsel.exe* and the parameter file. Launch OPSEL by entering *opsel.exe*, followed by the path to the parameter file, for example:

C:\opsel>opsel.exe example1.cntl

SELECTING A SEED ORCHARD OR CLONE-MIX POPULATION – EXAMPLE2.CSV

Prepare the candidate list

In this example, we wish to select a seed orchard where the frequency of individual genotypes optimizes the number of ramets of each. The orchard site has 2 800 planting positions. The candidate population consists of founder plus-trees and their F1 progeny, for which EBVs are available.

Not all candidates are capable of producing large numbers of scions, so there are limitations on the number of grafts that can be made for any given individual: some founders no longer exist, so they cannot be used in the orchard; the F1 progeny are still rather small and can produce perhaps no more than

50 grafts; while other founders are large and well represented in existing orchards and archives, and so can contribute virtually unlimited numbers of grafts. The 5th column of the candidate list file contains the constraint on the maximum number of contributions permitted for each individual; in this case 0, 50 or 2 800, as appropriate.

We can also “force” an individual to be represented a minimum number of times. For this example, we have identified individual 294 as a key genotype that we plan to use in the future as a reference pollen source, so we definitely want to include in this orchard. In the optional 6th column of the candidate list, we specify a minimum contribution from this individual of 25 ramets. There is no such minimum constraint for the other individuals, so their minima are all set to 0.

The candidate file must be conform to the format and sort order described earlier, and must contain the following 5 columns (the 6th column “*Min*” is optional):

Indiv *Female* *Male* *EBV Max* *Min*

The estimated breeding values (EBVs) would normally be extracted, together with the appropriate pedigree entries, from a third-party database, such as DATAPLAN®.

Running *Example2.csv* through the online dialogue

The following is a detailed description of an OPSEL job selecting the genotypes and optimizing their contributions to a 2 800-tree seed orchard, illustrated by processing *Example2.csv:*

1. Start OPSEL by double-clicking on *OPSEL.exe*
2. Accept the conditions of use on the splash screen by typing Y, then pressing Enter.
3. The description of OPSEL on the next screen is a summary of the information in this user guide on how to prepare the pedigree file. Note that the “root” name of the input file, in this case “*Example2*”, is used by OPSEL when referencing all other files, using different extensions appended to the root.
4. Type the candidate-list file name containing the pedigree and breeding-value data: *Example2.csv*, and press enter.
5. Specify that OPSEL is to use the “unequal contributions” option by entering 1.
6. OPSEL reports the current working directory and asks if the SDP solver “*SDPA.exe*” is in this folder. If so, just answer “*y*”, otherwise enter “*n*” and OPSEL will ask you to specify the full path location of dsOpt.exe.
7. Specify the desired census size of the selected population, in this case 2 800.
8. OPSEL now needs to know the constraint on diversity of the selected population. This can be specified either as group coancestry, or as

Status Number. In this case, let's answer "*y*", then specify our constraint as Status Number 14 (which is equivalent to a group coancestry of 1/(2 × 14) = 0.0357).

9. OPSEL now asks if the input file contains a specification for a minimum constraint (column 6). In this example, we have set a minimum of 25 ramets from individual 294, so here we answer "*y*".
10. By default, OPSEL will store the solution in a text file, but you can specify comma-separated values here, if you wish. Doing so will make it easier to read the solution with Excel.
11. OPSEL now checks to make sure that the pedigree specification is legal (all individuals accounted for, parents precede progeny, etc.)
12. OPSEL will look in your root folder to see if there is an inverse A matrix file called "*Example2.giv*". This may have been calculated by a previous run of OPSEL, or by a third-party program such as ASReml or DATAPLAN®. Reusing an existing inverse A file can save a lot of time when the number of candidates is large. If the "*Example2.giv*" does not exist, or you decide not to reuse it, OPSEL will prepare the inverse-A matrix.
13. The input file for the SDP solver is prepared and submitted to SDPA.exe.
14. OPSEL now proceeds to formulate the SDP and to build the input for SDPA. A call to SDPA.exe is made, and you will see its progress in a separate DOS command-line window.
15. Once SDPA has completed the optimization, control is returned to OPSEL which interprets the output and provides an on-screen summary. OPSEL will ask you if you want to store your responses to the online dialogue to run later from the command line; provide a filename, such as *Example2.cntl.* When preparing the response file, OPSEL will ask if in future runs you will want to reuse the inverse A file.
16. Check the folder where you started OPSEL and you will find the following additional files:

    Example2_A.giv – the inverse A matrix in sparse format.

    Example2.dat-s – the input prepared by OPSEL for SDPA.

    Example2_sdpa-out.txt – the raw solution generated by SDPA.

    Example2_solution.csv or *Example1_solution.txt* – the solution combined with the initial candidate list, in either comma-separated format or as a text file, as specified by the user. The columns in the file are:

    Individual – ID of the individual genotype.

    Female – ID of the individual's mother.

    Male – ID of the individual's father

    EBV – the genetic value of the individual (supplied by user)

    Freq – the contributions from selected individuals are indicated by whole numbers

    Proportion – the contribution from each individual indicated as a proportion.

Max – the constraint on the maximum contribution from each individual.

Min – (if requested) the constraint on the minimum contribution from each individual.

Example2_log.txt – a log file that contains summary statistics about the problem and its solution.

Running *Example2.csv* from the command line

OPSEL can also be run from the command line by specifying the various job parameters in a separate text file. The simplest way to do this is to run through online dialogue and save the parameters in a text file, such as (see step 14 above). A sample version of *Example2.cntl* is provided in the OPSEL distribution package and can be modified with any text editor.

Open a Command Prompt window – usually found in the Accessories folder. Navigate to the location of opsel.exe and the parameter file. Launch OPSEL by entering *opsel.exe*, followed by the path to the parameter file, for example:

```
C:\opsel>opsel.exe example2.cntl
```

When things go wrong!

The user should be aware that OPSEL is in a continuing state of development. While it has already seen operational application, the limitations have not been thoroughly explored, as that will happen naturally as users attempt to apply it. Unexpected things can happen! OPSEL may provide messages that give some information on failed runs or problems with data input. If you cannot rectify a problem, please note the messages received and send your input file and problem parameters (census size and constraint on group coancestry) to: tim.mullin@skogforsk.se

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