Institution: University of Dundee		
Unit of Assessment: UoA 10 Mathematical Sciences		
Title of case study: The development of commercial optimization software		
Period when the underpinning research was undertaken: 2000-2012		
Details of staff conducting the underpinning research from the submitting unit:		
Name(s):	**Role(s) (e.g. job title):**	**Period(s) employed by submitting HEI:**
Roger Fletcher Sven Leyffer	Professor of Mathematics Postdoctoral Researcher	1973 - 2016 1999 - 2002
Period when the claimed impact occurred: Ongoing		
Is this case study continued from a case study submitted in 2014? Y		

1. Summary of the impact

Research conducted at Dundee led to the development of the *filter method* and associated software, which offers a radically different approach to solving large and complex optimization problems. The *filter method* is utilised globally by tens of thousands of industry users and as a teaching tool in higher education. Its use as a key enabling design software by The Boeing Company has contributed to benefits valued at many tens of millions of US dollars per year. Commercial application of the method through BARON and via TOMLAB has enabled commercial and industrial users to find feasible solutions to over 50,000 complex optimisation problems. The *filter method* is central to teaching tools used by more than 75 universities around the world through licensing agreements.

2. Underpinning research

Optimization problems are defined as those that seek to maximise or minimise a certain function usually of many variables (an objective function), subject to equality and inequality constraints on the values that can be taken by those variables. When either the objective function or the constraints are nonlinear, the process of solving these problems is called nonlinear programming (NLP). Quadratic Programming (QP) is a special case of NLP in which the objective function is quadratic in its dependent variables (and the constraints are linear). A typical method for attacking NLP problems is to solve an iterative sequence of approximate QP problems – this is called Sequential Quadratic Programming (SQP).

In **[R1]** Professor Roger Fletcher and Dr Sven Leyffer introduced the concept of the filter as a new way to solve NLP via SQP methods. In follow-up papers **[R2-R4]**, **Fletcher**, **Leyffer** and co-workers refined the heuristics in their filter method and used novel arguments to deliver a mathematically exact proof of convergence and expanded its application to other iterative methods (Sequential Linear Programming - SLP) **[R4]**. Before the introduction of the filter method, the usual procedure for solving an NLP problem was to use a 'penalty function' to induce convergence of an intermediate iterative method (e.g., SQP, SLP); sequential iterations were required to continuously improve the value of the penalty function. Often this requirement could considerably slow down the speed of convergence of the scheme making it computationally impractical for problems typical of those found in industry and business. In the filter method, the objective function and the constraint violation function are regarded as two distinct functions, and iterations can be accepted if they improve either one of these functions. This is a much less restrictive condition and allows faster convergence of the NLP solver. The generality of the filter method allows for its use in many contexts, such as trust region, line search and interior point methods.

A wide variety of test results for large scale NLP showed the effectiveness and robustness of the filter method in comparison to other commonly implemented codes. Based on the work published in **[R1-R4]**, production quality codes, *filterSD* and *filterSQP* for NLP, and *bqpd* for Quadratic Programming (QP), were created by the Dundee team and made available for distribution. For example, using *filterSQP* to solve the many NLP sub-problems generated in the Branch and Bound method for mixed integer nonlinear programming (MINLP), considerably extended the range of problems that can be solved.

The introduction of the filter idea evoked considerable interest in optimization circles and nearly 20 years on, mini-symposia and workshops are still devoted to its implementation and development. During this time, the filter method won particular praise for its novelty and effectiveness: explicit reference to development of the method was made in subsequent awards to **Fletcher** (**RF**) and **Leyffer** (**SL**): **RF** Elected Fellow of the Royal Society, 2003; **RF** Royal Gold Medal from the Royal Society of Edinburgh, 2008; **RF** and **SL** Lagrange Prize in Continuous Optimization from the Mathematical Programming Society and the Society for Industrial and Applied Mathematics (SIAM) 2006; **RF** and **SL** Elected Fellows of SIAM, 2009; **SL** Farkas Prize from the INFORMS Optimization Society, 2016.

The concept of balancing optimality and feasibility was seen to have profound implications in many areas of optimization and has been utilized and extended by researchers since its introduction in diverse areas such as constrained and unconstrained optimization, solving systems of nonlinear equations (the idea of a multi-filter) and in derivative-free optimization. Extensions to the original work include those constructed by the Dundee team. In **[R5]** the filter method was extended to a class of mathematical programming with equilibrium constraints (MPECs) with complementary constraints leading to the development and distribution of the code *filter MPEC*. Nonmonotone filter methods were introduced in **[R6]**, work that received further praise winning the Best Paper Award for 2012.

3. References to the research

[R1] Fletcher R. and Leyffer S., (2002). Nonlinear Programming Without a Penalty Function, *Mathematical Programming*, 91(2), pp. 239-269. DOI: 10.1007/s101070100244

[R2] Fletcher R., Leyffer S. and Toint P. (2002). On the Global Convergence of a Filter–SQP Algorithm, *SIAM Journal on Optimization*, 13(1), pp. 44-59. DOI: 10.1137/S105262340038081X

[R3] Fletcher R., Gould N., Leyffer S., Toint P. and Wächter A. (2002) Global Convergence of a Trust-Region SQP-Filter Algorithm for General Nonlinear Programming, *SIAM Journal on Optimization*, 13(3), pp 635-659. DOI: 10.1137/S1052623499357258

[R4] Chin C.M. and Fletcher R. (2003). On the Global Convergence of an SLP-Filter Algorithm that takes EQP steps, *Mathematical Programming*, 96(1), pp.161-177. DOI: 10.1007/s10107-003-0378-6

[R5] Fletcher R. and Leyffer S. (2004). Solving mathematical program with complementarity constraints as nonlinear programs, *Optimization Methods and Software*, 19(1) pp.15–40. DOI: 10.1080/10556780410001654241

[R6] Shen C., Leyffer S. & Fletcher R. (2012). A nonmonotone filter method for nonlinear optimization. *Computational Optimization and Applications,* 52, pp. 583–607. DOI: 10.1007/s10589-011-9430-2

4. Details of the impact

The invention of the filter method meant that a broad range of previously computationally unfeasible optimization problems could be solved efficiently. Arguably the most challenging of the optimization problem types is MINLP, in which some of the variables are constrained to take only discrete values. Until the filter breakthrough, MINLP problems were regarded as intractable unless the number of variables was small. **Fletcher** and co-workers showed that using *filter SQP* to solve the many NLP sub-problems generated in the Branch and Bound method for MINLP, considerably extended the range of problems that can be solved.

The Boeing Company. Boeing is the world's leading aerospace company and the largest manufacturer of commercial jetliners and military aircraft. It employs over 153,000 people in more than 150 countries worldwide. *Design Explorer* is software developed by Boeing for use as its primary tool for design optimization. The Dundee filter method was first built into Design Explorer in 2002 and remains a key enabling tool for the Boeing software. The Dundee filter method enables Design Explorer to implement features that are essential ingredients of optimal design for the company. Through Design Explorer, the Dundee filter method has been implemented in a range of applications including the design of rotor blades and hypersonic vehicles. Its success and commercial value have been highlighted by the company:

> "*Design Explorer was awarded a Boeing Technical Replication Award in 2014 having generated several hundred million US dollars' worth of documented benefit to the company… In the years since [2014] Design Explorer has continued to generate benefits worth many tens of millions of dollars to Boeing each year.*" **[E5]**

Since 2014, the filter method continues to enable the application of Design Explorer to complex and computationally challenging problems. It has been used to optimize the design of the 777X airliner (first flight took place in January 2020) and resolved an issue regarding structural stiffness of a refuelling link for the KC-46 Pegasus (in-flight refuelling tanker). In 2019, Design Explorer was used to optimize the aft body shape of Boeing's new mid-range airliner planned to enter revenue service in 2025. Furthermore, using Design Explorer to optimize the design of carbon fibre-based parts is facilitating the use of this state-of-the-art manufacturing technology.

The substantial value that Design Explorer offers to Boeing ensures that it continues to be developed, with the Dundee filter method remaining a key and enduring element of the Boeing design software:

> "[The Dundee] *Filter methods are one of the key and enduring enabling technologies for Design Explorer, so the impact of the filter method at Boeing is both well-established and substantial."* **[E5]**

The continued global reach of the Dundee filter method and associated codes is further exemplified by its use by TOMLAB and BARON:

BARON Software. BARON (Branch-and-Reduce Optimization Navigator) is a suite of optimization software tools that was commercialized through The Optimization Firm in 2001. Full access to BARON software is by licence and is obtained by corporations and the academic community through routes including The Optimization Firm website **[E1]** and the open-source online server NEOS **[E2]**. The Dundee codes *filterSD* and *filterSQP* have been embedded in BARON since 2014 and 2017, respectively. Each run of BARON invokes the Dundee filter method.

> "*Each BARON run invokes Roger's optimization algorithms* [the Dundee filter method] *to solve many nonlinear optimization problems that arise as subproblems in BARON's algorithms. Roger's NLP codes allow BARON to quickly obtain feasible solutions for difficult optimization problems*" **[E6]**.

The significant reach of the Dundee filter method and associated codes is demonstrated by lower bound estimates of commercial usage offered by considering the NEOS access data:

> "*Between 1/1/2014 and 12/31/2018, more than 387,499 optimization problems were submitted to BARON through the NEOS server alone… at least 49,669 of these... were submitted by commercial users"* **[E6]**

At 17/12/20, the number of commercial jobs submitted to BARON via NEOS is over 52,000 – **[E8]**. The company confirms that the Dundee codes continue to outperform alternatives for certain classes of problem and remain an important contributing component of the success of BARON software:

> "*Roger's research work [the Dundee filter method] has resulted in algorithms and software with a tremendous impact across many fields in science and engineering."* **[E6]**

TOMLAB. TOMLAB is the premier developer and distributer of large-scale optimization software for use in conjunction with the MATLAB system. MATLAB currently has more than 3 million users worldwide. Since 2003, TOMLAB has invoked the Dundee filter method via codes developed by **Fletcher**, **Leyffer** and co-workers as part of TOMLAB's software suite. TOMLAB's CEO confirms these algorithms remain at the core of TOMLAB until this day **[E3]**.

> "*We are pleased to confirm continuing commitment to... the marketing and distribution of ... the optimization solvers bqpd, filterSQP, miqpBB and minlpBB developed by Dr. Fletcher and Dr. Sven Leyffer.*" **[E7]**

In his letter of support, TOMLAB CEO underlines the central importance of the Dundee filter method and the codes (solvers) written by **Fletcher** and Leyffer:

> "*TOMLAB Optimization Environment provides... packages with over a dozen of the most powerful products for all the major categories of large-scale optimization problems… We see these* [Dundee] *solvers as key additions to our line-up.*" **[E7]**

TOMLAB currently has more than 60 large-scale industrial/commercial users including Honeywell International, General Motors, Credit Suisse, Bank of Japan and JP Morgan **[E4]**. Moreover, it has users in research institutes across the world e.g., RIKEN-Japan, Draper Laboratories, IBM Research and NASA Ames Research Centre. Applications range from portfolio management through precision medicine to data analysis during space exploration and the Dundee solvers are invoked to solve a wide range of problems particularly those requiring MINLP. TOMLAB is also used extensively as a teaching tool in higher education. Over 75 universities worldwide are registered TOMLAB users with 26 new users registered since 2014.

> *"The majority of our clients using the* [Dundee] *algorithms are academic… There are users of the Dundee software... around the globe and very many students have been running our demo licenses.*" **[E7]**

5. Sources to corroborate the impact

Online sources of corroboration:

[E1] The Optimization Firm (2021) *BARON: The Best Solver for Mixed-Integer Nonlinear Optimization*. Available at: https://www.minlp.com/baron [Accessed 12 March 2021]

[E2] NEOS Server Optimization (2021) *NEOS Solver Statistics*. Available at: https://neos-server.org/neos/report.html [Accessed 12 March 2021]

[E3] TOMLAB Optimization (2020). *TOMLAB / MINLIP*. Available at: https://tomopt.com/tomlab/products/minlp/ [Accessed 12 March 2021]

[E4] TOMLAB Optimization (2020). *TOMLAB Customers*. Available at: https://tomopt.com/tomlab/company/customers.php [Accessed 12 March 2021]

Letters of corroboration:

[E5] Senior Technical Fellow, Boeing Research and Technology, USA

[E6] Founder, BARON Software, USA

[E7] CEO, TOMLAB Software AB, Sweden

[E8] NEOS Solver Statistics