编号 _____

中国运筹学会科学技术奖

运筹应用奖推荐表

被推荐项目名称	无导数优化算法、软件及其工业应用
主要完成人	张在坤
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推荐人或单位	中科院数学与系统科学研究院---香港理工大学应用数学联合实验室
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中　国　运　筹　学　会　制

被推荐项目的主要完成人	张在坤
工 作 单 位	香港理工大学应用数学系

被推荐项目的主要学术创新点和应用成果

工业应用中很多优化问题的目标或约束函数没有显式表达式，无法提供导数 (一阶信息)。求解此类问题需要仅使用函数值而不依赖导数的方法，即无导数优化方法。

张在坤博士长期致力于无导数优化算法的研究与软件的开发。**他和他的团队开发的无导数优化软件累计下载超过 25 万次。其中，COBYQA 将作为"Highlight of This Release"纳入 SciPy 1.14.0 (注：SciPy 每日有数百万次下载)，而 PRIMA 和 PDFO 已成为空客等研发的工业设计软件 GEMSEO 的优化引擎。他的算法和软件被国内外多家单位应用，包括英特尔、复旦大学专用集成电路与系统国家重点实验室、法国 IRT 研究所(法国航天局、空客等共建的工业研究中心)。**

主要学术创新

1. 基于子空间技术的大规模无导数优化方法。高维问题是无导数优化领域由来已久的挑战。为应对这一挑战，张在坤在其博士论文 (袁亚湘院士指导) 中提出了一个子空间无导数优化框架，进而设计了 NEWUOAs 算法和软件。该框架创新性地将函数值用于发现有效子空间，再建立子空间模型，将可解问题维数从几百提高到上万。

2. 基于随机化技术的低复杂度无导数优化方法。张在坤与合作者提出了一类基于随机子空间的直接搜索方法。无论问题维数多高，该类方法只需每步随机选取一个常数维子空间进行搜索即可收敛，有效降低了算法总体复杂度对维数的依赖，提高了可解问题的维数。相关论文获 Computational Optimization and Applications 2019 年最佳论文奖。

3. 基于 Powell 对称 Broyden 修正的无导数序列二次规划方法。张在坤指导博士研究生 Tom M. Ragonneau 首次将 Powell 对称 Broyden 修正模型与序列二次规划融合，设计了 COBYQA 算法，并发布了开源软件包。该算法能够求解一般的非线性约束无导数优化问题，且性能远超此前在工业界流行的 COBYLA (Powell 1992)。

主要应用

1. 开源无导数优化软件。基于前述研究，张在坤及其团队投入大量精力和资源开发了以下无导数优化软件并将其开源。这一过程耗时极长：保守估计，张在坤本人在无导数优化软件开发中投入的时间已超过一万小时，编码量超过 10 万行。**由于开源软件庞大的用户社区，这些软件的潜在影响力远超大多数具体应用项目。**

1) COBYQA (http://www.cobyqa.com)。该软件将作为“Highlight of This Release”纳入 SciPy 1.14.0。继 Nelder-Mead 单纯形方法、Powell 共轭方向法、Powell 的 COBYLA 算法之后，COBYQA 是 SciPy 收录的第四个无导数优化算法。

2) PRIMA (http://www.libprima.net)。该软件提供了 Powell 的无导数优化算法的现代化、模块化的实现，并修正了 Powell 代码中的 bug。PRIMA 已被接入空客等开发的工业软件 GEMSEO，并即将被纳入 SciPy。

3) PDFO (http://www.pdfo.net)。该软件累计下载量超过 **25 万次**，是工业软件 GEMSEO 的主要优化引擎之一。

4) NEWUOAs (http://www.sprima.net)。**英特尔**首席工程师 (Principle Engineer) Mika Nyström 博士将 NEWUOAs 纳入系统编程语言 Modula-3 的开源编译器 CM3。

2．5G 基站芯片设计。英特尔首席工程师 (Principle Engineer) Mika Nyström 博士团队将张在坤的 NEWUOAs 应用于**英特尔旗舰产品** Atom P5900 5G 基站芯片的设计开发。相比之前的算法，NEWUOAs 提供了**一百多倍的加速**，可在数小时内求解此前耗时数周的问题。Mika Nyström 博士开具的应用证明评论说 NEWUOAs 极大地简化了芯片设计中的软件验证流程 (“massively simplify our verification software flow”)，使得他们可以处理此前无法解决的问题 (“problems that were practically out of reach”)；NEWUOAs 已经成为他最常用的数值算法 (“I find myself reaching for NEWUOAs more often than any other numerical algorithm”)。

3．高维模拟电路优化。复旦大学专用集成电路与系统国家重点实验室曾璇教授 (长江学者、国家杰青) 团队成功将张在坤的子空间无导数优化框架和 NEWUOAs 应用于高维模拟电路智能优化。结合曾璇教授团队提出的高斯模型增强技术，新的方法可以求解一些前人无法求解甚至无法想象的大问题，解决了长期困扰模拟电路优化领域的优化维度高、仿真时间长的瓶颈问题。**NEWUOAs 已被纳入专用集成电路与系统国家重点实验室开发的高维模拟电路智能优化工具中。**

4．飞机零部件与架构设计。法国 IRT 研究所 (法国航天局、空客等共建的工业研究中心) 将张在坤开发的 PRIMA 与 PDFO 软件应用于飞机零部件与架构设计等“关键应用 (critical applications)”。IRT 团队负责人 Anne Gazaix 博士和 François Gallard 博士开具应用证明表示 PRIMA 为他们的应用领域“带来了根本性的改变 (changes the game)”。**空客等开发的工业设计软件 GEMSEO 已将 PRIMA 与 PDFO 作为优化引擎接入其中。**

鉴于其广泛的工业应用和实际影响，张在坤团队的成果作为 **Impact Case** 在“中科院数学与系统科学研究院---香港理工大学应用数学联合实验室”长期展示。

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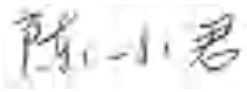
推荐人/推荐单位对推荐表上述内容的客观性和真实性负责。 推荐人签名：    或推荐单位盖章：_____ (陈小君，讲座教授、实验室主任) 2024 年 5 月 28 日

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中国运筹学会科学技术奖

运筹应用奖申报表

申报项目　　无导数优化算法、软件及其工业应用

申报人　　张在坤

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项目目标

在芯片设计、计算核物理、航空器制造、人工智能等众多工业与工程领域，很多问题的目标或约束函数是由复杂系统或昂贵仿真定义的**黑箱**，没有解析表达式，更不能提供导数 (一阶信息)。求解此类问题需要仅使用函数值而不依赖导数的方法，即无导数优化方法。

伴随着人工智能的蓬勃发展，无导数优化问题变得愈加常见，这极大刺激了无导数优化领域的发展。此外，鉴于我国在高端芯片、工业软件等关键领域的迫切需求，无导数优化的战略重要性日益凸显。我的课题组长期致力于无导数优化算法的研究和软件的开发。我们的目标如下。

1）设计求解高维问题的无导数优化算法。高维问题是无导数优化领域由来已久的

挑战。主流的观点认为无导数方法至多能求解几百维的问题。我们的目标是把可解问题维数提高到上万。

2）设计求解一般非线性约束问题的无导数优化算法。实际应用中，大部分无导数优化问题带有约束，且约束函数本身也可能是黑箱函数。求解黑箱约束问题的算法十分有限。工业上非常流行的 COBYLA (Powell 1992)求解器已有 30 多年历史。我们将基于更现代的优化理论和技术设计更高效的算法。

3）开发稳定、高效、易用、可扩展的通用无导数优化软件。无导数优化领域较成熟的软件包大多缺乏维护和更新，且均为国外团队开发。在西方对我国战略领域实施软件禁用的背景下，开发自主可控的无导数优化软件尤为迫切。基于我们在这领域长期的积累，我们将开发稳定、高效、易用、可扩展的通用无导数优化软件。我们致力于为学界提供标杆求解器，为业界提供开箱即用的无导数优化工具。

项目技术方案概述

1．项目内涵的运筹学问题

无导数优化一直以来都受到不少著名学者 (如 M.J.D. Powell、袁亚湘院士、A.R. Conn、J. Nocedal、Ph. Toint 等) 的关注，取得了一大批理论和算法成果。然而，以下课题仍亟待研究。本项目将围绕这些课题展开。

1）高维无导数优化问题的求解。已有的无导数优化算法大多针对几十或几百维问题。然而，在机器学习、人工智能领域，高维无导数优化问题不断涌现，如何求解这些问题成为无导数优化领域不得不面对的挑战。

2）一般非线性约束无导数优化问题的求解。大部分已有的无导数优化算法针对目标函数为黑箱的情形设计。然而，实际应用中很多无导数优化问题的约束也包含黑箱函数。求解黑箱约束无导数优化问题算法十分有限，代表性的工作有 COBYLA (Powell 1992) 和 SOLNP+ (Ge et al 2022) 等。此类问题仍待更深入的研究。

3）通用无导数优化软件的开发。工业应用中流行的无导数优化软件 (如 COBYLA、NOMAD) 大都缺乏更新，且代码风格古典，不易使用，更难维护或扩展。工业界急需稳定、高效、易用、可扩展的通用无导数优化软件。

2．难度和挑战

1) 高维无导数优化问题：维数灾难。到目前为止，最有效的一类无导数优化方法

是基于二次插值模型的信赖域方法。这类方法通过插值函数值建立黑箱函数的二次逼近，以此为模型进行信赖域迭代。然而，二次模型的自由度与维数平方成正比，这从根本上限制了此类方法可解问题的维数。

2) 一般非线性约束无导数优化问题：黑箱约束的处理。实际应用中，很多无导数优化问题的约束没有显式表达式。不仅如此，有的约束函数不可量化，不能提供具体的约束违反度，仅能提示约束是否满足。处理此类约束是无导数优化特有的挑战。

3) 通用无导数优化软件：极高的人力和时间成本。要开发**符合工业标准**的**跨平台**通用优化软件，开发者必须同时具备多种能力：既要理解数值算法，又要设计软件架构，还要掌握计算技术（包括计算机语言、开发与调试工具、操作系统、硬件体系结构等），远非普通研究生或软件工程师能胜任。除此之外，无导数优化算法需要兼顾信赖域模型管理和信赖域迭代，一般流程十分复杂，导致代码量大、开发周期极长。以 Powell 的 NEWUOA 求解器为例，它的开发历时近三年，且历尽挫折 (Powell 在 NEWUOA 的论文中提到 "The development of NEWUOA has taken nearly three years. The work was very frustrating")。更重要的是，开发可靠的软件需要长期的调试和工程积累。不经过长达数年的严苛测试与实践检验，任何代码都不足以成为软件。这一过程所需的人力和时间投入远超多数科研项目。保守估计，**张在坤本人在本项目的软件开发中投入的时间已超过一万小时，编码量超过 10 万行**。

3．采取的分析方法或建立的模型

1) 基于子空间技术的大规模无导数优化方法。为求解高维无导数优化问题，张在坤在其博士论文 (袁亚湘院士指导) 中提出了一个子空间无导数优化框架，进而设计了 NEWUOAs 算法和软件。该框架创新性地将函数值用于发现有效子空间，再在子空间中求解原问题，将可解问题维数从几百提高到上万。具体来说，NEWUOAs 在每步迭代中用函数值插值构造一个模型梯度g_k, 然后在二维子空间

$$S_k = \mathrm{span}\{-g_k, d_{k-1}\}$$

中极小化目标函数。子空间 S_k 由袁亚湘院士与德国数学家 Stoer 于 1995 年受共轭梯度法启发提出，其中 d_{k-1}是上一个迭代步。袁和 Stoer 的方法要求g_k为精确梯度，张在坤将其拓展到近似梯度的情形，从而适用于无导数优化。

2) 基于随机化技术的低复杂度无导数优化方法。张在坤与合作者提出了一类基于随机子空间的直接搜索方法。不管问题维数 n 多大，该类方法每步迭代在 Grassmann 流形 Gr(m, n) 上均匀地随机取一个点作为搜索空间，只要 m > 1 即可保证收敛。换言之，无论问题维数多高，该类方法只需每步随机选取一个常数维子空间进行搜索即可收敛，有效降低了算法总体复杂度对维数的依赖，提高了可解问题的维数。相关论文获 Computational Optimization and Applications 2019 年**最佳论文奖**。

3) 基于 Powell 对称 Broyden 修正的无导数序列二次规划方法。张在坤指导博士研究生 Tom M. Ragonneau 首次将 Powell 对称 Broyden 修正模型与序列二次规划 (SQP) 融合，设计了 COBYQA 算法，并发布了开源软件包。该算法能够求解一般的非线性约束无导数优化问题，且性能远超此前在工业界流行的 COBYLA (Powell 1992)。与 COBYLA 采用的线性插值模型不同，COBYQA 每次迭代通过求解二次插值问题

$$\min \|Q - Q_{k-1}\| \quad \text{s.t. } Q(y) = f(y),\ y \in Y_k$$

来建立目标和约束函数的二次插值模型，其中f为目标或约束函数，Q_{k-1}为f的上一个模型，Y_k为当前插值点集，而 $\|\bullet\|$ 为二次多项式空间中的某个 (半) 范数。无法量化的约束用 extreme barrier 来处理。最后，COBYQA 用这些二次模型建立 SQP 信赖域子问题进行迭代。

4．方法和技术的创新点

1）软件创新。软件开发是本项目的重中之重。本项目最大的成果是开发了一系列符合工业标准、面向工业应用的无导数优化软件，即 COBYQA、PRIMA、PDFO 和 NEWUOAs。这些软件的代码量超过 10 万行，下载量超过 25 万次，已被英特尔、复旦大学专用集成电路与系统国家重点实验室、法国 IRT 研究所等用于求解工业与工程中的关键问题。我们将在“取得的主要应用效果”一节做更多介绍。

2) 理论与算法创新。

2.1) 提出了一个十分广泛的子空间无导数优化框架，并建立了其收敛性。指出函数值应当用于发现有效子空间，再在该子空间上建立模型，大大降低了模型复杂度对空间维数的依赖，有效提高了可解问题的维数。

2.2) 利用鞅理论与测度集中理论，建立了基于随机子空间的直接搜索方法的全局

收敛性和收敛速度。证明该类方法每一步只需在常数维随机子空间搜索即可收敛，提高了可解问题的维数。

2.3) 提出了一个无需导数的序列二次规划框架，并利用 Powell 对称 Broyden 修正模型设计了 COBYQA 算法。

5．取得的主要应用效果

1) 开源无导数优化软件。基于前述研究，张在坤及其团队投入大量精力和资源开发了以下无导数优化软件 (超过 10 万行代码) 并将其开源。**由于开源软件庞大的用户社区，这些软件的潜在影响力远超大多数具体应用项目。**

1.1) COBYQA (http://www.cobyqa.com)。该软件将作为“Highlight of This Release”纳入 SciPy 1.14.0。继 Nelder-Mead 单纯形方法、Powell 共轭方向法、Powell 的 COBYLA 算法之后，COBYQA 是 SciPy 收录的第四个无导数优化算法。

1.2) PRIMA (http://www.libprima.net)。该软件提供了 Powell 的无导数优化算法的现代化、模块化的实现，并修正了 Powell 代码中的 bug。PRIMA 已被接入空客等开发的工业软件 GEMSEO，并即将被纳入 SciPy。

1.3) PDFO (http://www.pdfo.net)。该软件累计下载量超过 **25 万次**，是工业软件 GEMSEO 的主要优化引擎之一。

1.4) NEWUOAs (http://www.sprima.net)。**英特尔**首席工程师 (Principle Engineer) Mika Nyström 博士将 NEWUOAs 纳入系统编程语言 Modula-3 的开源编译器 CM3。

2) 5G 基站芯片设计。英特尔首席工程师 (Principle Engineer) Mika Nyström 博士团队将张在坤的 NEWUOAs 应用于**英特尔旗舰产品** Atom P5900 5G 基站芯片的设计开发。相比之前的算法，NEWUOAs 提供了**一百多倍的加速**，可在数小时内求解此前耗时数周的问题。Mika Nyström 博士开具的应用证明评论说 NEWUOAs 极大地简化了芯片设计中的软件验证流程 (“massively simplify our verification software flow”)，使得他们可以处理此前无法解决的问题 (“problems that were practically out of reach”)；NEWUOAs 已经成为他最常用的数值算法 (“I find myself reaching for NEWUOAs more often than any other numerical algorithm”)。

3) 高维模拟电路优化。复旦大学专用集成电路与系统国家重点实验室曾璇教授

(长江学者、国家杰青) 团队成功将张在坤的子空间无导数优化框架和 NEWUOAs 应用于高维模拟电路智能优化。结合曾璇教授团队提出的高斯模型增强技术，新的方法可以求解一些前人无法求解甚至无法想象的大问题，解决了长期困扰模拟电路优化领域的优化维度高、仿真时间长的瓶颈问题。**NEWUOAs 已被纳入专用集成电路与系统国家重点实验室开发的高维模拟电路智能优化工具中。**

4) 飞机零部件与架构设计。法国 IRT 研究所 (法国航天局、空客等共建的工业研究中心) 将张在坤开发的 PRIMA 与 PDFO 软件应用于飞机零部件与架构设计等“关键应用 (critical applications)”。IRT 团队负责人 Anne Gazaix 博士和 François Gallard 博士开具应用证明表示 PRIMA 为他们的应用领域“带来了根本性的改变 (changes the game)”。**空客等开发的工业设计软件 GEMSEO 已将 PRIMA 与 PDFO 作为优化引擎接入其中。**

项目小组成员

序号	姓名	单位	专业职称/职务
1	张在坤	香港理工大学	博士/助理教授
2	Tom M. Ragonneau	Axians HPC (法国)	博士/工程师
3	李海天	香港理工大学	博士研究生
4	黄存昕	香港理工大学	博士研究生

应用单位意见：项目的成果、贡献、效益等

我们开发的无导数优化软件累计下载超过 25 万次。其中，COBYQA 将作为“Highlight of This Release”纳入 SciPy 1.14.0 (注：SciPy 每日有数百万次下载)，而 PRIMA 和 PDFO 已成为空客等研发的工业设计软件 GEMSEO 的优化引擎。我们的算法和软件被国内外多家单位应用，包括英特尔、复旦大学专用集成电路与系统国家重点实验室、法国 IRT 研究所 (法国航天局、空客等共建的工业研究中心)。这些单位均已出具应用证明 (**含负责人签字或单位盖章**)，对应用效果做了详细阐述，详见附件。

鉴于其广泛的工业应用和实际影响，我们的成果作为 **Impact Case** 在“中科院数学与系统科学研究院---香港理工大学应用数学联合实验室”长期展示，详见附件。

我们的工作也得到了国际同行与学界领袖的关注，包括 J. Nocedal (西北大学，SIAM Fellow，美国工程院院士，John von Neumann 奖获得者)、M. Saunders (斯坦福大

<table>
<tr><td colspan="2">学，SIAM Fellow，新西兰皇家学会荣誉会士，首届 Beale--Orchard-Hays 奖获得者)，N.I.M. Gould (英国 Rutherford Appleton 实验室，SIAM Fellow)、C. Cartis (牛津大学，SIAM Fellow)。他们都写信或发邮件对我们的工作表示赞赏和支持，详见附件。

备注: 本项目核心算法已由张在坤及其团队**编码为开源软件**。得益于庞大的用户社区，开源软件往往比具体应用项目有更为广泛和长远的影响，已成为学术界和工业界实现知识成果落地、获得经济或社会效益的重要途径，著名例子包括 Android 操作系统、Python 科学计算标准库 SciPy、大语言模型 Llama 等。英特尔等单位均为**主动使用**张在坤团队发布的成果，其应用**并非通过正式协议或横向课题实现**。故本申请将不出具“项目委托合同书”或“应用单位同意申报书”，而代之以应用证明 (含负责人签字或单位盖章)，本栏下方“应用单位负责人签名”与“单位公章”也不适用。

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申报人签名：
2024 年 5 月 28 日</td></tr>
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附　件

1. 项目委托合同书（副本）和应用单位同意申报书（加盖公章）
2. 主要应用技术报告
3. 评审鉴定材料或技术鉴定证书及知识产权证明
4. 项目应用效益证明
5. 获得其他表彰或奖励的证明
6. 其他

附 件

文件列表：

1. 英特尔首席工程师 Mika Nyström 博士开具的应用证明 (3 页)
2. 复旦大学专用集成电路与系统国家重点实验室开具的应用证明 (1 页)
3. 法国 IRT 研究所开具的应用证明 (2 页)
4. 中科院数学与系统科学研究院---香港理工大学应用数学联合实验室对张在坤团队成果的展示 (2 页)
5. J. Nocedal 写信对张在坤的工作表示支持和赞赏 (2 页)
6. M. Saunders 写信对张在坤的工作表示支持和赞赏 (2 页)
7. N.I.M. Gould 发邮件对张在坤的工作表示支持和赞赏 (1 页)
8. C. Cartis 发邮件对张在坤的工作表示支持和赞赏 (1 页)
9. COAP 2019 最佳论文奖证明 (1 页)
10. PDFO 下载量证明 (1 页)
11. COBYQA 将作为 “Highlight of This Release” 纳入 SciPy 1.14.0 (1 页)

英特尔首席工程师 Mika Nyström 博士开具的应用证明

May 27, 2024

Dr. Zaikun Zhang
TU824, Yip Kit Chuen Building
The Hong Kong Polytechnic University
Hong Kong

Dear Dr. Zhang,

You have asked me to give you some feedback on how we use your optimization algorithms and software here at Intel, and I am honored to do so. I lead a team of senior engineers in Intel's Foundry Division's Design Enablement Group. My organization is the "Emerging Technologies Research and Development Group" within this larger group, and we are based in Santa Clara, California. Your work plays a significant role in solving many of our design problems, some of which I will describe in detail below.

A few years ago, I was working on a content-addressable-memory (CAM) design, for one of Intel's now flagship products, our 5G base station chip, now called Atom P5900. The challenge with memory design today is that it is difficult to design these circuits so that they are reliable in the field. We wish the designs to be digital, but they must work under the assumption that there are manufacturing variations in the underlying transistors, wires, etc. A single chip that we manufacture has on the order of ten million memory elements of the kind I am describing, each of which has 12 transistors, each of which can have variable parameters as a result of tolerances in the manufacturing process. The memory design is handled as an optimization problem, solved by wrapping a commercial circuit simulator in an optimization code. At Intel, the software we have used for many years is based on conjugate gradient descent and numerical derivatives. Since the circuit simulator itself is also quite noisy, this software flow needs to be set up very carefully to be effective, and it can only handle very simple circuits (such as a single memory element) and may entirely miss failure modes (a problem frequently encountered in practice).

My contribution to the memory-design problem involved using your algorithm NEWUOAs as a replacement for the previous, much less appropriate method. I used the Matlab code you shared with me in October 2016 as a basis for coding the algorithm in Modula-3 to fit into our optimization framework. I also evaluated Professor Powell's original NEWUOA code. The results of the evaluation were that

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your NEWUOAs code was the superior selection. For this problem, NEWUOAs had about half the evaluations of the second-best derivative-free method I investigated. In 2019, I added my coding of your NEWUOAs algorithm to the Critical Mass Modula-3 Github repository, whence it is distributed worldwide to all users of that system, and I have been maintaining this version of it for those users.

The impact of the performance of NEWUOAs as compared to prior methods was to massively simplify our verification software flow. The prior method required a senior engineer to extract a small circuit that was believed to capture the behaviors we were interested in, making a number of detailed adjustments to the circuit to vastly simplify it, while avoiding any adjustment that disturbs the failure modes we were trying to verify. After that, the engineer would have to annotate the parts of the circuit that would be variable, with only a small allowance of components that can vary (about 4--6). With NEWUOAs running the optimization, we were able to simply simulate the entire circuit design, without simplifying it at all, and we were able to use a larger number of varying components (each varying component turns into two optimization variables). The circuit's complexity went from a single memory cell to roughly 2,000, which naturally led to a slowdown of the simulator, but since so many fewer evaluations were needed, the overall performance stayed about the same. This made a big difference, because, to us, people time is much more expensive than computer time.

More recently, while working on novel ultra-low-power technologies for emerging Artificial Intelligence and other workloads, we have been studying the limits of low-power operation of fabrication technologies that are not yet public as of this writing (May 2024). We use NEWUOAs to derive test cases for technology evaluation: having designed a test circuit, the problem here is to find what we would expect to be the worst circuit out of a large set, for example the slowest circuit on a silicon die. We want to find the slowest expected circuit on a die because that would be the one circuit that determines the operating frequency and therefore the customer-visible performance of the entire die. The modeling is done through advanced statistical methods but with NEWUOAs serving to search the entire, very large, parameter space.

We have also noticed that owing to the way you coded NEWUOAs, we were able to inject quite a bit of parallelism in the optimization algorithm, and since we have a large number of processors in our data center, that led to further performance improvements. I have run practical problems where this parallelization has led to a speedup of around one hundred in terms of wallclock time, allowing us to study problems that were previously practically out of reach (the optimization that takes a couple of hours with NEWUOAs would take weeks with NEWUOA).

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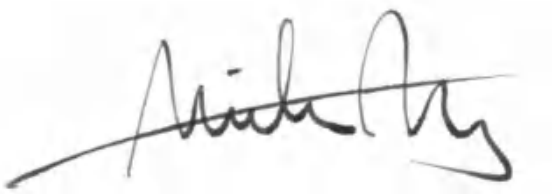
Because the function evaluations are so slow in most of my problems (as they usually involve calling out to an external circuit simulator), I find myself reaching for NEWUOAs more often than any other numerical algorithm, just to access its parallel speedup. In this respect, NEWUOAs is a significant improvement on Powell's NEWUOA algorithm.

At Intel, we also use Powell's derivative-free optimization algorithms in our work, which are available to us thanks to your maintenance and modernization under PDFO and PRIMA. These algorithms are, I believe, the best available for application workers like me. The modernization you are performing is of immense value to us who work in applications. We are not really able to use the latest publications in the specialized field of numerical optimization directly, so we rely on researchers and institutions such as yours to provide the codes in a format we can use. I have been involved in open-source projects enough myself to know that this is usually a thankless and underappreciated job. Your maintenance and modernization of these codes are serving needs far beyond your university, and I think your work deserves recognition and reward.

Finally, I want to add that I am highly looking forward to trying the COBYQA algorithm by you and your Ph.D. student Tom M. Ragonneau. I am excited to know that it will be included into SciPy 1.14.0 as a highlight of the release. This will lead to a huge impact, as SciPy is downloaded by millions of users daily. I look forward to using it in my projects.

Sincerely yours,



Mika Nyström, Ph.D.
Principal Engineer
Emerging Technologies Research & Development
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张在坤教授的子空间无导数优化方法和求解器在高维模拟电路智能优化工具的应用证明

模拟集成电路的设计传统上依赖人工完成，设计周期长、设计指标难以保证，目前没有成熟的模拟电路自动优化工具。模拟电路自动设计中的一个瓶颈问题是高维黑盒函数优化，具有函数值计算代价高昂、无法计算导数等难点，是复旦大学集成芯片与系统全国重点实验室曾璇教授（2008—2012 年实验室主任、国家杰青、长江学者）领导的电子设计自动化 EDA 团队长期攻坚的关键课题之一。

张在坤教授于 2012 年在博士论文（袁亚湘院士指导）中创新性地提出了一套子空间无导数优化框架，并设计了基于不精确梯度方向与历史迭代方向的子空间无导数优化算法 NEWUOAs，将任意高维的黑盒无导数优化问题降维到二维子空间中进行求解。曾璇教授领导的 EDA 团队与张在坤教授合作，成功地将 NEWUOAs 算法应用于模拟电路优化问题。新的方法可以求解一些前人无法求解甚至无法想象的大问题，可以将模拟电路的数百上千问题降低到 2 维，解决了长期困扰模拟电路优化领域的，优化维度高、仿真时间长的瓶颈问题。张在坤教授提出的 NEWUOAs 方法集成到了复旦大学高维模拟集成电路智能优化工具中。复旦大学高维模拟集成电路智能优化工具可以实现高维模拟电路的晶体管尺寸自动优化设计，求解大规模电路优化问题。

除了 NEWUOAs 之外，张在坤教授与他的博士研究生开发的 PDFO、PRIMA 等软件包用更现代化、模块化的方式重新实现了 Powell 的所有无导数优化求解器。相对于其他无导数优化求解器，能用更少的函数值求解更多的问题；由于模块化设计，相关代码的可读性得到保障，也更容易进行修改和扩展。张在坤教授团队开发的这些软件包已经在复旦大学集成芯片与系统全国重点实验室研发的模拟电路智能优化工具中得到了广泛应用。

复旦大学集成芯片与系统全国重点实验室

2024 年 5 月 23 日

法国 IRT 研究所开具的应用证明

IRT Saint Exupéry
Toulouse, France
21th September 2023

Dr. Zaikun Zhang
Department of Applied Mathematics
The Hong Kong Polytechnic University
Hong Kong, China

Dear Dr. Zhang,

This letter is to provide some feedback on the optimisation software packages your team have developed, in particular PRIMA, PDFO, and COBYQA. Your packages are of major importance for industry that involves optimal design problems based on numerical simulations, which is particularly the case for the MDO (Multidisciplinary Design Optimisation) projects at IRT Saint Exupéry, France. IRT is an industrial research institute focused on advanced manufacturing technologies, greener technologies, smart technologies and methods & tools for the development of complex systems. We are co-founded by major industry players including Airbus, Safran, Thales, CNES (French national space agency), and the French state (see https://www.irt-saintexupery.com/our-members/ for a full list).

Optimisation Based on Simulation (also known as Black-box Optimisation) is a key technology in every field of science and engineering and a key element of the ongoing digital transformation of industry. However, most open source packages are based on unmaintained Fortran code from the 1980s. For example, the NLopt and SciPy packages (more than 1 million downloads per day) are largely based on obsolete implementations of L-BFGS-B, COBYLA and SLSQP, which haven't been significantly improved since their creation. These codes have known bugs and limitations that have very practical implications in terms of the solutions obtained and their robustness, and thus their potential for use by industry. This has also been the case for the widely used derivative-free optimisation (DFO) solvers in industry (COBYLA, UOBYQA, NEWUOA, BOBYQA, and LINCOA), but your PRIMA package changes the game. Thanks to your very large effort in modernizing the code, the PRIMA package now provides most reliable implementations of these solvers. Moreover, the PRIMA solvers work evidently more efficient than the classical implementation by the late Professor M.J.D. Powell, which is quite remarkable.

The CUTEst benchmark suite, which is the reference in the field, have shown that PRIMA achieves significant improvements in performance and reliability. The benchmark we use internally to compare these packages shows a similar trend for the COBYLA algorithm, which is useful to us. The modernized code is easy to modify and will allow further research into the optimisation algorithms, whereas the old implementation prevented this due to its architectural limitations: mostly a single file with many GOTO statements, which prevented important modifications.

The reliability of the PRIMA solvers is of particular importance for us. We have been using COBYLA in critical applications including optimisation of aircraft components and architecture, and design electrical systems such as car power electronics for car engines. Obviously, such applications require a high level of reliability, as the optimisation results are used to make important decisions. It is also noted that the PRIMA solvers are quite robust in the presence of noise in function evaluations, which is always the case in the aforementioned applications. PRIMA's capability of doing so is great news for the industry.

Your work on PDFO is also very important for us. The PDFO package provides a unified and user-friendly interface for the above-mentioned DFO solvers, which is very convenient for us. We note

that PDFO has been downloaded for more than 140,000 times on PyPI (https://www.pepy.tech/projects/pdfo) and 48,000 times on Anaconda (https://anaconda.org/conda-forge/pdfo), which demonstrates its success and importance. Indeed, we have included PDFO as an optimisation engine in our software GEMSEO (https://gemseo.readthedocs.io), which is a Generic Engine for Multidisciplinary Scenarios, Exploration and Optimisation, and is used by industrial partners. We also have interfaced PRIMA with GEMSEO.

A particular challenge in our applications is the general nonlinear black-box constraints. Your solver COBYQA is a major contribution in this regard. The fact that it is based on SQP certainly provides a better handling of the general constraints compared with state-of-the-art solvers such as COBYLA. It was really straightforward to connect to the GEMSEO framework and worked fine at first try. We have given it a try and compared with COBYLA on some problems we have (without derivatives), it is significantly faster, provides a better convergence. We are really impressed by the fact that COBYQA is only part of the Ph.D. thesis by Dr. Ragonneau supervised by you. It is a really big and impressive piece of work for a single Ph.D. Thanks for sharing it as open source.

We must stress our appreciation of your large efforts in developing these packages. As practitioners, we understand very well the importance and difficulty of developing such packages. The main difficulty is that it requires the combination of the following conditions:

- An advanced theoretical knowledge of numerical optimisation,
- a fine understanding of assemblies of dozens of algorithms,
- avanced know-how and experience in the development of numerical algorithms,
- the ability to identify and overcome the existing limitations of the existing complex code,
- and finally, very importantly but often overlooked, a considerable amount of time allocated to the task.

It is likely that only an expert researcher actively working in the field can meet these requirements.

It is important for us that the academic community highly recognizes and supports the development of such packages as they play a key role in pushing the boundaries of science. In particular for us, as an Institute dedicated to innovation, your advanced algorithms are of primary importance.

Thank you very much for your great work!

Yours sincerely,

Dr. Anne Gazaix
Head of the Multidisciplinary Design Optimization Center of Competence
IRT Saint Exupéry, Toulouse, France

Dr. François Gallard
Multidisciplinary Design Optimization Architect
IRT Saint Exupéry, Toulouse, France

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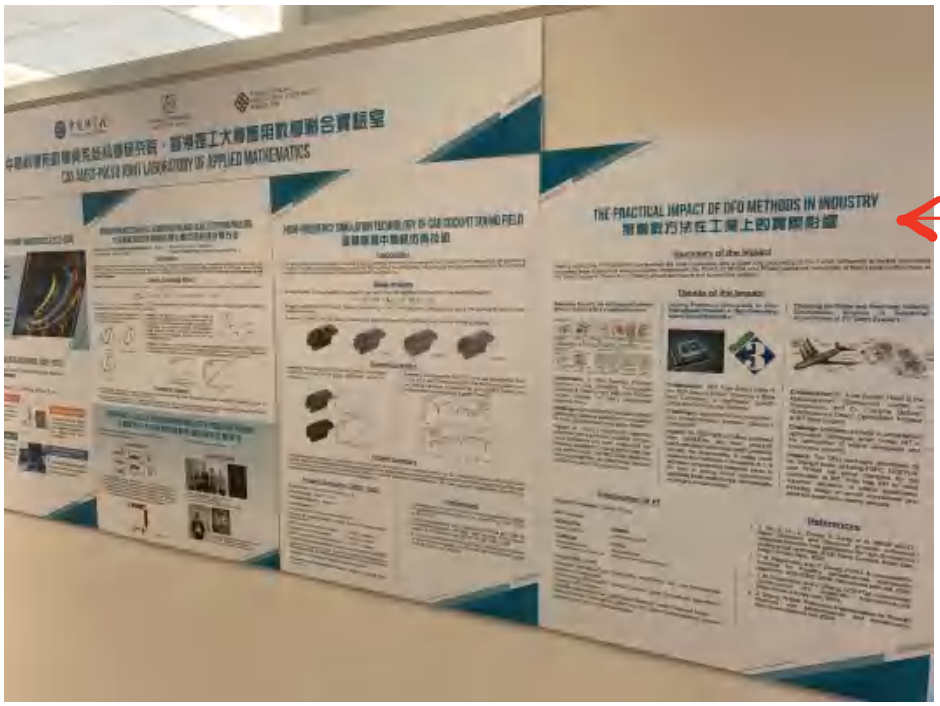
中科院数学与系统科学研究院—香港理工大学应用数学联合实验室
将张在坤团队的成果作为 Impact Case 长期展示



THE PRACTICAL IMPACT OF DFO METHODS IN INDUSTRY
無導數方法在工業上的實際影響

Summary of the Impact

PolyU's NEWUOAs DFO algorithm has enabled the Intel Corporation and a State Key Laboratory at the Fudan University to tackle previously unsolvable large-scale circuit design problems. Additionally, the PDFO, COBYQA, and PRIMA packages developed at PolyU play crucial roles at IRT Saint Exupéry in France for optimizing critical aerospace and automotive systems.

Details of the Impact

Massively Simplify the Verification Software Flow for One of Intel's Flagship Products

Collaboration: Dr. Mika Nyström, Principal Engineer of the Emerging Technologies Research & Development within the Custom Circuits Division of Intel's Accelerated Graphics Group.

Challenge: High-dimensional simulation-based optimization problems arising from circuit design for Intel's 5G base station chip (Atom P5900).

Impact: Dr. Zhang's NEWUOAs algorithm enhanced Intel's software, enabling complex circuit simulations with fewer evaluations and leveraging parallelism to reduce optimization time from weeks to hours. The NEWUOAs algorithm is now incorporated into the Critical Mass Modula-3 GitHub repository for global access.

Solving Previously Unsolvable or Even Unimaginable Problems in High-Dimensional Analog Circuit Optimization

Collaboration: Prof. Xuan Zeng, Leader of the EDA team at Fudan University's State Key Laboratory of Application Specific Integrated Circuits and Systems.

Challenge: High-dimensional, nonconvex, and computationally intensive black-box optimization.

Impact: The BBGP-sDFO method developed from NEWUOAs can solve previously unsolvable large-scale circuit design problems, reducing the dimensionality of analog circuit problems from hundreds or thousands to 2. It addresses long-standing bottleneck issues in the field of analog circuit optimization, specifically those related to high dimensionality and lengthy simulation times.

Changing the Game and Providing Reliable Optimization Engines in Industrial Applications at IRT Saint Exupéry

Collaboration: Dr. Anne Gazaix, Head of the Multidisciplinary Optimization Center of Competence, and Dr. François Gallard, Multidisciplinary Design Optimization Architect at IRT Saint Exupéry.

Challenge: Limitations and bugs in unmaintained optimization packages, which hinder IRT in the optimization of critical aerospace and automotive systems.

Impact: The DFO packages developed by Dr. Zhang's team, including PDFO, COBYQA, and PRIMA are game changers for the optimization at IRT. They help IRT to make important decisions in critical applications including design of aircraft components and electrical systems for electric vehicles.

Information of PI

Principal Investigator: Zaikun Zhang

DFO Software:

- **NEWUOAs** *www.sprima.net*
- **PRIMA** *www.libprima.net*
- **COBYQA** *www.cobyqa.com* downloaded more than 14,000 times
- **PDFO** *www.pdfo.net* downloaded more than 200,000 times

Grants (2020 - 2026)

- Scalable Derivative-Free Optimization Algorithms with Low-Dimensional Subspace Techniques
- Accelerating Optimization Methods without Using Derivatives: Algorithms, Theory, and Software
- Reliable Derivative-Free Optimization Methods under Untamed Noise
- Derivative-free Optimization Algorithms with Space Decomposition, Coarse Space Correction, and Randomization

References

1. T. Gu, X. Liu, Z. Zhang, X. Zeng, et al. BBGP-sDFO: Batch Bayesian and Gaussian process enhanced subspace derivative free optimization for high-dimensional analog circuit synthesis. IEEE Trans. Comput. Aided Des. Integr. Circuits Syst., 2023.
2. T. M. Ragonneau and Z. Zhang. PDFO: A cross-platform interface for Powell's derivative-free optimization algorithms. arXiv:2302.13246. https://www.pdfo.net, 2023.
3. T. M. Ragonneau and Z. Zhang, COBYQA: Constrained Optimization BY Quadratic Approximations. https://www.cobyqa.com, 2024.
4. Z. Zhang. PRIMA: Reference Implementation for Powell's Methods with Modernization and Amelioration, http://www.libprima.net, 2024.

J. Nocedal 写信对张在坤的工作表示支持和赞赏

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NORTHWESTERN UNIVERSITY

Dear Zaikun,

This letter is to follow up on the conversations we had in Seattle. I want to reiterate my interest in collaborating with you on the creation of new methods for derivative-free optimization. Let me put this suggestion into context, stressing the research strengths you possess, how they complement mine, and how they can naturally lead to new research directions.

First of all, your long-term effort on optimization software (Prima, PDFO) makes you the top expert on interpolation based methods. You mentioned the idea of including randomized directions within an algorithm like NEWUOA and developing a convergence theory; that would be an excellent start.

I have been very interested in the design of methods that can deal with noise in the function. I was therefore quite intrigued about your new results showing the resilience of pattern search methods in the presence of noise and the complexity results one can establish. Based on this work of yours I would like to contrast the idea of patterns with that of random searches. Your work with Gratton and Vicente sets the stage for this. That is an impressive paper that in my view shows a path forward by strongly suggesting the advantages of choosing a small number of randomized directions. Yet, it remains to be seen if these random methods really compete with interpolation-based approaches. I would like to undertake such an exploration, first from a theoretical perspective, then algorithmically and finally through software implementation. I can think of no better qualified researcher for this.

I am very impressed by your insights into complexity bounds for a variety of methods for derivative-free optimization. I believe that the direction you are proposing is more productive than the randomized subspace approaches in vogue today, and I believe that we can prove this rigorously.

We can discuss this in greater length during one of our regular zoom conferences. Let me stress, that your experience in developing the PRIMA software package provided the foundations for breakthroughs in the area of derivative-free optimization. I believe in the late Prof. Powell's approach that the ultimate test about the value of our ideas is the success of their software in practice. You have mastered this, together with the imperatives of developing a supporting theory. This balanced way of doing research has proved to be the most impactful in optimization, over the long run.

Jorge Nocedal
Walter P. Murphy Professor
Member oft he US National
Academy of Engineering

M. Saunders 写信对张在坤的工作表示支持和赞赏

Stanford | ENGINEERING
Management Science & Engineering

Michael Saunders
Professor (Research) Emeritus
saunders@stanford.edu

May 29, 2024

To Whom It May Concern

Dr Zaikun Zhang
Expert in software for numerical optimization

I am truly glad to write in commendation of Dr Zaikun Zhang's invaluable contributions to the area of numerical optimization, especially in the development of high-quality optimization software.

Zaikun and I first met in 2013 during a conference at CERFACS, Toulouse, France. Since then, we have met often in optimization and scientific computing conferences and workshops. In particular, we were both at the ICIAM 2023 conference in Tokyo, August 20–25, 2023 (along with my colleague Alexis Montoison, an expert in linear algebra, optimization, and the Julia language for scientific computing). Alexis and I and many other researchers attended Zaikun's talk about his remarkable project to revive and immortalize the extensive optimization software left behind by the late Professor M J D Powell. Zaikun's ongoing e□orts on this software are creative, tireless, and noble (worthy of a nonfiction novel!).

Zaikun's contribution to the area of numerical optimization software is truly impressive. He has produced several high-quality optimization software packages, including PDFO (http://www.pdfo.net), PRIMA (http://www.libprima.net), COBYQA (http://www.cobyqa.com), and NEWUOAs (http://www.sprima.net). PDFO has been downloaded more than 250,000 times—a remarkable achievement for any researcher and a clear demonstration of the impact of Zaikun's packages on industry. PDFO, PRIMA, and COBYQA are being used by IRT (a French industrial research institute founded by major industrial players including Airbus) to solve optimization problems in aircraft engineering. Zaikun's NEWUOAs package (developed in 2012 in his PhD thesis supervised Prof Ya-xiang Yuan) has been used by Intel Corporation on optimization problems in the design of computer chips, and has led to significant reductions in computation time, enabling Intel to tackle problems that were previously intractable. Zaikun's COBYQA package (a new trust-region SQP algorithm for solving general nonlinearly constrained optimization problems without using derivatives, co-developed by Zaikun and his former PhD student Dr Tom M. Ragonneau) will be included in SciPy as a highlight of release 1.14. The integration of PRIMA into SciPy is also underway. Along with SciPy, Zaikun's software will be installed on millions of computers worldwide. How exciting!

I can relate to my own career of algorithm and software development in numerical optimization and linear algebra. The greatest reward for software developers is learning that their solvers have proved useful for someone in academia or industry. I am very glad that

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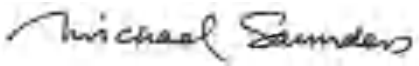
Zaikun's research has made such an impact on industry. Software development is a very important aspect of such research, and it takes much time and effort to develop high-quality software. Zaikun's success in this area is a testament to his dedication and hard work.

I visited Zaikun at the Hong Kong Polytechnic University in February/March 2024. During this visit, I learned that Zaikun in his office has numerous computers running day and night to verify the code of PRIMA (see PRIMA: Reference Implementation for Powell's Methods with Modernization and Amelioration `https://github.com/libprima/prima`) following each modernizing modification. His implementations are more efficient than the originals by Powell in terms of number of function evaluations, and he has uncovered several bugs in some established Fortran compilers and in Matlab. These are hard-won benefits for us all.

Zaikun is a talented young researcher with a strong background in optimization and numerical analysis. In 2012 he finished his PhD under the supervision of Prof Ya-xiang Yuan at the Chinese Academy of Sciences, where he published a single-authored paper in Mathematical Programming (one of our premier journals). This is a fine achievement for a young researcher, and it demonstrates his ability to conduct independent high-quality research. Most importantly, developing high-quality optimization software needs not only talent but also fortitude, dedication, and hard work. Zaikun's success in this area is a testament to all of these qualities.

I am confident that Zaikun Zhang will continue for many years to make invaluable contributions to the field of numerical optimization and its software development. His painstakingly constructed and tested software is the best possible way to bring optimization technology to Operations Research practitioners.

Sincerely,



Michael A. Saunders
Professor (Research) Emeritus
ICME and Dept of MS&E
Stanford University

N.I.M. Gould 发邮件对张在坤的工作表示支持和赞赏

Gmail

Zaikun ZHANG <zaikunzhang@gmail.com>

The PRIMA project

Nick Gould <nick.gould@stfc.ac.uk> 3 février 2023 à 15:18
À : ZHANG Zaikun <zaikun.zhang@polyu.edu.hk>

Hi Zaikun

That is marvellous! A great effort, and something that the community will be very grateful for. Yes, it is important to provide interfaces to other languages, as this is the only way you will persuade many people to use the methods. My own library, GALAHAD, has now extend to C, and is making progress in python and julia. As you say, this is a time sink, often frustrating, but ultimately rewarding. Indeed, use from other languages often reveals defects with the original fortran design, and certainly with the installation procedures.

When people ask for DFO codes, I will point them at PRIMA, a great name, by the way.

I hope all is well with you

Best wishes

Nick

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Scientific Computing Department email: nick.gould@stfc.ac.uk
G39, R71 Rutherford Appleton Laboratory phone: 0(44)1235 445801
Chilton, Oxon OX11 0QX England EU
www: http://secure-web.cisco.com/1uS0BDpRdpqCWFqg5gy5IabW7RO5l_Z2RYnqQQGHn-0urmjACg8KL9arksy5y31PNCBUZDIzA9nM3L_OsbrWvOFkLaE__LPDvOYt_NtjtsNetNJPEh-QH40xjDe89PnxMVeHZIqdLXz3rshEBHWXYowC3y06hgnygtymR8PnLLHX9nIwn2pM8MbJPuR1Kta0IG8l3dZtl95r2JWlKJeOsAScVzcx1LpXA5lYJZEGn2_bbg2cIbUaD-CsMOXb3gy7_lGPk8PyGlJOdAJc8zsxSsDeOaQ3dly9Xh_QIY2jSJXzrLXbLLqRaVSOqvNuNop01/http%3A%2F%2Fwww.numerical.rl.ac.uk%2Fpeople%2Fnimg

C. Cartis 发邮件对张在坤的工作表示支持和赞赏

Gmail

Zaikun ZHANG <zaikunzhang@gmail.com>

The PRIMA project

Coralia Cartis <cartis@maths.ox.ac.uk> 17 novembre 2022 à 06:46
À : ZHANG Zaikun <zaikun.zhang@polyu.edu.hk>
Cc : Lindon <lindon.roberts@sydney.edu.au>

Dear Zaikun - what a wonderful initiative and immense amount of work and dedication on your part !!!
This is and will be a very valuable repository and tool and bedrock of future advances, thank you for all your efforts !!!
I will have a closer look and let you know of any feedback.

I hope you can enjoy your life and have a rest after all this !….

With my best wishes - and thanks for letting me know - Cora

[Texte des messages précédents masqué]

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> uFRaXKa8r/https%3A%2F%2Fgithub.com%2Fequipez%2FPRIMA
>
> The "P" in "PRIMA" stands for "Powell", and "RIMA" means "Reference
> Implementation with Modernization and Amelioration".
>
> Thank you very much for your attention. I will be very happy to hear
> your suggestions and comments.
>
> Best regards,
> Zaikun
> --
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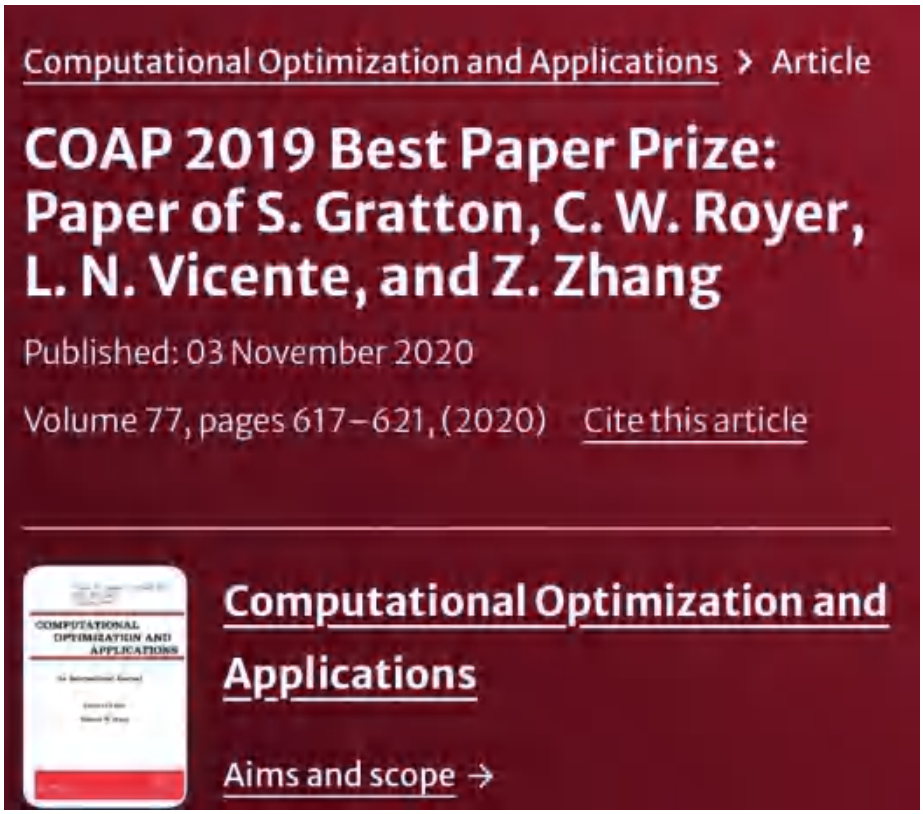
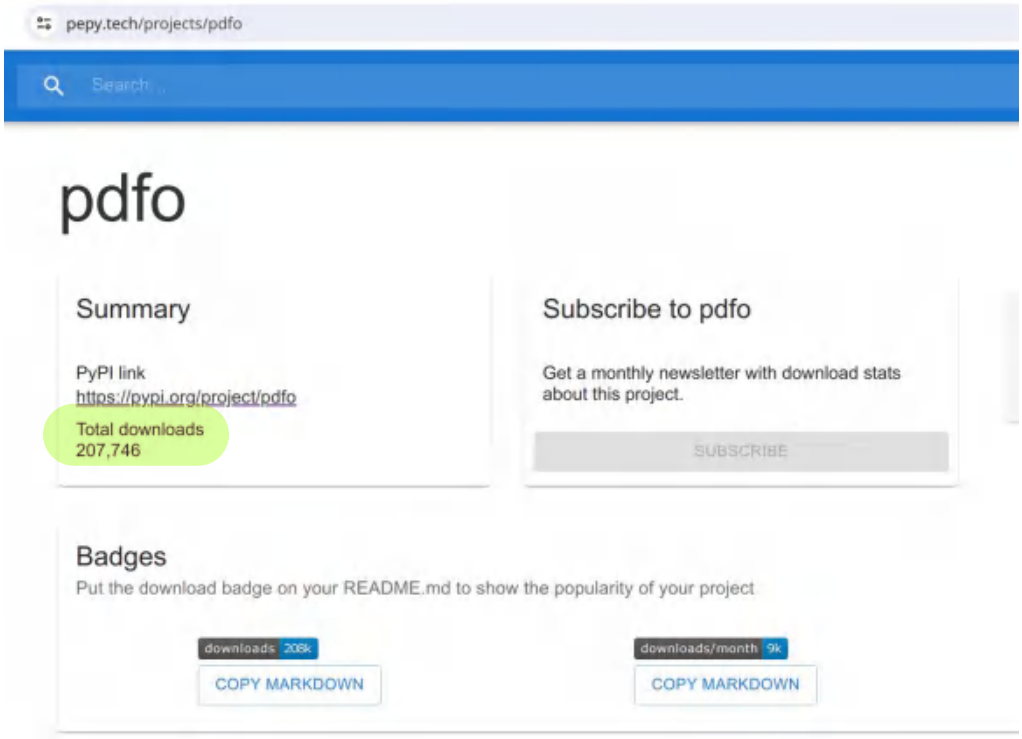
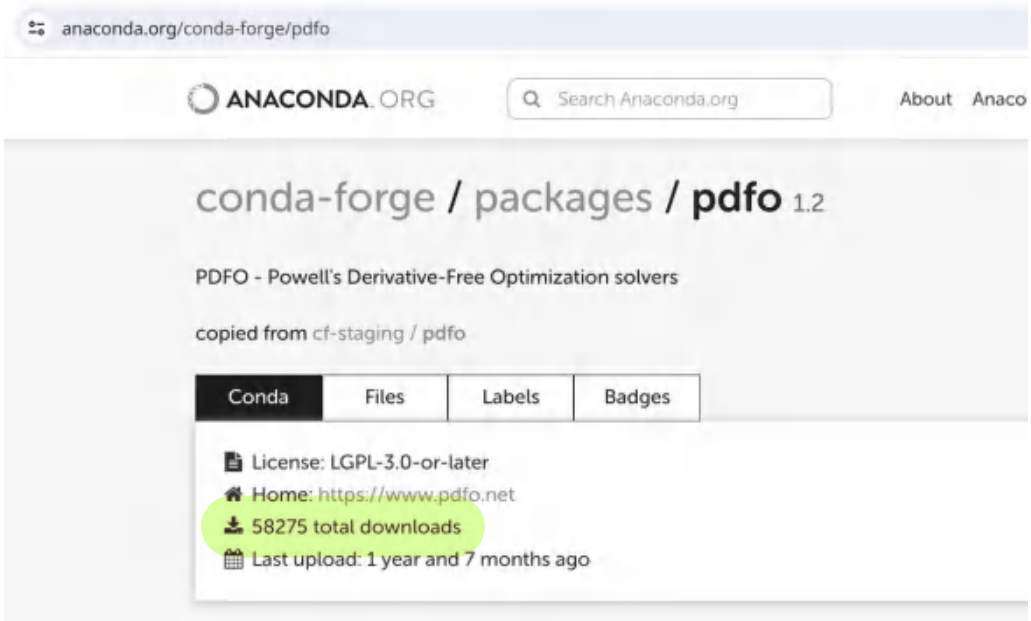
张在坤与合作者关于随机化子空间直接搜索的文章获 COAP 2019 最佳论文奖



PDFO 在 PyPi 的下载量：超过 20 万（截至 2024 年 5 月 29 日）



PDFO 在 ANACONDA 的下载量：超过 5 万（截至 2024 年 5 月 29 日）



COBYQA 将作为“Highlight of This Release”纳入 SciPy 1.14.0