Simplifying deflation for non-convex optimization with applications in Bayesian inference and topology optimization

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Abstract

Non-convex optimization problems have multiple local optimal solutions. Non-convex optimization problems are commonly found in numerous applications. One of the methods recently proposed to efficiently explore multiple local optimal solutions without random re-initialization relies on the concept of deflation. In this paper, different ways to use deflation in non-convex optimization and nonlinear system solving are discussed. A simple, general and novel deflation constraint is proposed to enable the use of deflation together with existing nonlinear programming solvers or nonlinear system solvers. The connection between the proposed deflation constraint and a minimum distance constraint is presented. Additionally, a number of variations of deflation constraints and their limitations are discussed. Finally, a number of applications of the proposed methodology in the fields of approximate Bayesian inference and topology optimization are presented.

1 Introduction

Non-convex optimization problems are used in numerous applications including: machine learning, mechanical design, economics, and the design of clinical trials, among many other applications. One of the fundamental challenges of non-convex optimization is the existence of multiple local minimizers. Local first and second order optimization algorithms often get stuck in a particular local minimizer without any guarantees that this is the best solution that can be found. The ability to explore multiple local minimizers is often important in practice to find better solutions or to provide more diverse choices to decision makers if all the choices are nearly equally good or the optimization objectives cannot capture users’ preferences completely. For example, multiple car body designs can be reported and the decision-makers can choose one based on the subjective aesthetic appeal.

Despite the popularity of using standard non-convex optimization techniques with various random or heuristic restart strategies to find multiple optima [Rinnooy Kan and Timmer 1987, Kaelo and Ali 2006, Arnoud et al. 2019], these methods can be computationally inefficient because they don’t protect against converging to the same solution from different starting points. In contrast, deflation-based methods [Papadopoulos et al. 2021] have the benefit of provably converging to distinct solutions under certain assumptions, even when starting from the same initial guess. However, originally developed for solving nonlinear equation system [Brow and Gearhart 1971, Farrell et al. 2016], adapting deflation to non-convex optimization problems requires significant adaptation of the
non-convex optimization algorithm [Papadopoulos et al., 2021], which prevents it from being used with a broader class of problems, algorithms and applications.

In this paper, we propose a simple, yet effective and provably correct way of making use of deflation by reformulating the non-convex optimization problem, instead of adapting the backend optimization algorithm. We then prove the equivalence of this approach to a minimum distance constraint under certain assumptions. The proposed approach has the benefit of (1) being simpler to implement since it’s a formulation change rather than an algorithmic change; (2) being more flexible allowing the use of arbitrary optimization algorithms that are suitable for the problem class at hand. We show a number of examples from different applications, each using deflation together with the most suitable and/or popular optimization algorithm for the respective application, which is not achievable by previous deflation-based approaches.

One limitation of the proposed approach is that it requires the handling of a non-convex, inequality constraint even if the original problem was unconstrained. However, one way to workaround this limitation is demonstrated in the examples section.

2 Related work

Systematic multi-start. Systematically restarting the optimization multiple times from random or deterministically diverse [McKay M. D., 1979, Kucherenko and Sytsko, 2005] initial solutions is a common strategy to find multiple local minimizers in non-convex optimization. Some popular algorithms following this approach are the multi-level single-linkage (MLSL) algorithm [Rinnooy Kan and Timmer, 1987], the controlled random search (CRS) [Kaelo and Ali, 2006] algorithm, and the TikTak algorithm [Arnoud et al., 2019]. However, all the approaches above can be computationally expensive and wasteful since restarting the optimization algorithm from a different initial solution may not give a different local minimizer.

Divide and conquer Other similar algorithms rely on sub-dividing the search space into smaller hyper-rectangles to narrow down the search space for each sub-problem. Algorithms in this category include the StoGo algorithm [Gudmundsson, 1998] K. Madsen and Zilinskas, 1998] and the DiViding RECtangles (DIRECT) algorithm [Jones et al., 1993, Gablonsky and Kelley, 2001]. However, these approaches don’t scale well with the number of decision variables $m$ since the number of fixed size hyper-rectangles one can divide an $m$ dimensional solution space into grows exponentially with $m$.

Hyperparameter and bilevel optimization. Alternatively, techniques from hyper-parameter optimization [Li et al., 2018, Falkner et al., 2018] or bilevel optimization [Sinha et al., 2018] can be used to optimize the starting point of the lower level optimization algorithm. One can compose a global search algorithm such as an evolutionary algorithm [Gendreau and Potvin, 2010] and a local search algorithm together to create an algorithm that can explore different initial solutions and find best local minimizers in different neighbourhoods. This family of global-local algorithms is also sometimes termed memetic algorithms [Moscato and Cotta, 2010].

Global metaheuristics. Beside their use in memetic algorithms, global metaheuristic optimization algorithms [Gendreau and Potvin, 2010] can also be used as standalone algorithms but these algorithms don’t tend to scale well to large problems since they usually don’t exploit the often available gradients and sometimes Hessians of objective and constraint functions.

Tunneling-based multi-start. Tunneling [Levy and Gomez, 1991, Gomez and Levy, 1982, Barron and Gomez, 1991] is another heuristic technique often used to find multiple local minimizers by finding a sufficiently different starting point with a similar or better objective value as the best solution found so far. The optimization problem is then re-solved starting from this new point hoping to converge to a different solution. However, this is a 2 step approach consisting of first solving the optimization problem and then finding a new, sufficiently different initial point. And the success to find distinct minimizers depends on the success to find a sufficiently different starting point.

Exact global optimization. Beside the use of restarts, there are also some well known exact global optimization algorithms for some classes of non-convex optimization [Tawarmalani and Sahinidis, 2005, Sahinidis, 2017, Belotti et al., 2009, Vigerske and Gleixner, 2018, Wilhelm and Stuber, 2020, Nagarajan et al., 2019, 2016, Ratschek and Rokne, 2007, Gecode Team]. These approaches however tend to require the explicit analytical mathematical expressions of the objective and constraint
functions so they are not suitable for black-box non-convex optimization, and they typically don’t scale well to large problems in practice, where the exactness guarantee has an exponential computational time complexity in the number of variables.

Deflation-based multi-start. Deflation is a recently proposed technique that employs Newton-like methods to find multiple solutions of a nonlinear systems of equations [Brow and Gearhart, 1971, Farrell et al., 2016, 2020]. Assuming the underlying Newton-like algorithm converges, under certain assumptions, a deflation-based solver is guaranteed to converge to a unique solution each time the solver is started from the same initial solution. This has the promise of being much less wasteful than multi-start optimization approaches. However, one problem with deflation is that often the assumptions under which convergence to a different solution is guaranteed are not easy to verify in practice. That said, the method was shown to perform well in practical applications.

Deflation was also used in a primal-dual interior point optimization algorithm [Wright, 1997] to find multiple locally optimal designs in mechanical design optimization problems [Papadopoulos et al., 2021]. However, this deflated optimizer had to re-invent a primal-dual interior point optimization algorithm [Wright, 1997] since off-the-shelf solvers such as the Interior Point OPTimizer (IPOPT) [Wächter and Biegler, 2006] could not be used directly for reasons to be presented in this work. Not being able to use existing optimization solvers is a huge limitation of this approach since different optimization algorithms tend to be more suitable for different problems and applications.

3 Background

3.1 Sufficient optimality conditions for regular points

We aim to find multiple solutions for the following nonlinear program (NLP):

\[
\begin{align*}
\text{minimize} & \quad f(x) \\
\text{subject to} & \quad c(x) = 0, \\
& \quad l \leq x \leq u
\end{align*}
\]  

(1)

where \( l \in (-\infty, \infty)^n, u \in (-\infty, \infty)^n \) are the finite (for simplicity) lower and upper bounds of the variable \( x \). The objective function \( f : \mathbb{R}^n \rightarrow \mathbb{R} \) and the equality constraints \( c : \mathbb{R}^n \rightarrow \mathbb{R}^m \), with \( m \leq n \) are assumed to be twice continuously differentiable. Problems with general nonlinear inequality constraints \( d(x) \leq 0 \) can be converted to equality constraints by adding slack variables.

Let:

\[
\mathcal{L}(x, \lambda, z_+, z_-) = f(x) + c(x)^T \lambda + (x - u)^T z_+ - (x - l)^T z_-
\]  

(2)

where \( \lambda \in \mathbb{R}^m \) is the Lagrangian multiplier vector of the equality constraints, \( z_- \in \mathbb{R}^n_+, z_+ \in \mathbb{R}^n_+ \) are the Lagrangian multiplier vectors of the bound constraints.

If \( x \) is regular and is a local minimizer of the NLP, then \( \exists (\lambda, z_+, z_-) \) such that:

\[
\begin{align*}
\nabla_x \mathcal{L}(x, \lambda, z_+, z_-) &= 0 \quad (3a) \\
c(x) &= 0 \quad (3b) \\
l \leq x &\leq u \quad (3c) \\
z_+ &\geq 0 \quad (3d) \\
z_- &\geq 0 \quad (3e) \\
(x - u)^T z_+ &= 0 \quad (3f) \\
(x - l)^T z_- &= 0 \quad (3g)
\end{align*}
\]

and

\[
\nabla c(x)^T \nabla^2_{xx} \mathcal{L}(x, \lambda, z_+, z_-) \nabla c(x) \geq 0
\]

(4)
Equations (3) and (4) are known as the first and second order Karush-Kuhn-Tucker (KKT) sufficient conditions for optimality respectively. A point $x$ that satisfies Equation (3) is typically called a KKT point [Nocedal and Wright, 2006]. Finding multiple solutions of the NLP can be reduced to finding solutions that satisfy Equation (3), while indirectly enforcing Equation (4) via following descent directions.

3.2 Deflation

Deflation is a technique that systematically modifies a nonlinear problem to guarantee that Newton’s method will not converge to a known root, thus enabling unknown roots to be discovered from the same initial guess [Farrell et al., 2016].

Deflation for nonlinear equation solving [Farrell et al., 2016] proved that under certain conditions, solving a system of $n$ nonlinear equations:

$$F(x) = 0$$

starting from the same initial solution $x_0$ can converge to multiple locally optimal solutions by applying a deflation operator whenever a solution is found. Let the first solution found be $x_1$. The deflation operator can then be defined as:

$$M(x; x_1) = m(x; x_1)I$$

$$m(x; x_1) = ||x - x_1||^{-p} + \sigma$$

for some power $p$ and shift $\sigma$, where $I$ is the $n \times n$ identity matrix. The deflated nonlinear system of equations is given by:

$$M(x; x_1)F(x) = 0$$

After solving the system once, one can solve the deflated system and obtain a new solution $x_2$. One of the assumptions required to prove the convergence of the proposed algorithm to a different solution $x_2$ is:

$$\lim_{x \to x_1} ||M(x; x_1)F(x)|| > 0 \quad (6)$$

To deflate away from multiple found solutions, the original method proposes multiplying the operators and solve $\prod_{k=1}^{\hat{K}} M(x; x_k)F(x) = 0$, where $\hat{K}$ is the number of found solutions. To improve numerical stability, summation instead of multiplication can also be used.

Deflation for NLP optimization To apply deflation to finding multiple solutions of NLP, one can write most of Equation (3) as $F(x, \lambda) = 0$ (see the appendix for more details) and solve for different solutions of the deflated system:

$$M(x; x_1)F(x, \lambda) = 0$$

while ensuring a descent direction is taken at every step. However, solving this nonlinear system of equations using Newton-like algorithms requires evaluating the Jacobian of the residual of the deflated nonlinear system of equations. One of the most popular existing implementations of the primal-dual interior point algorithm in IPOPT assumes the Jacobian of the top block of $F$ to be symmetric (since it’s the Hessian of the Lagrangian). This makes it difficult to reuse IPOPT with deflation directly. Arguably, this is also the main motivation for Papadopoulos et al. [2021] developing a specialized primal-dual interior point algorithm from scratch for use with deflation. For more details on the derivations relevant to this discussion see Appendix A.

4 Method

In this section, the use of deflation and the choice of the optimization algorithm to use will be decoupled by making use of a deflation constraint that only requires a change in the formulation of the optimization problem without specifying the algorithm.
4.1 Formulating deflation as a constraint

Instead of deflating the optimality conditions, one can create a new constraint and variable that enforce the same deflation effect. Let \( y \geq 0 \) be a new variable. One possible constraint to add is:

\[
m(x; x_1) = ||x - x_1||^{-p} + \sigma \leq y
\]

(7)

If after adding this constraint, the optimal solution \( x_2 \) obtained has a finite \( y \) in exact arithmetic, then \( x_1 \neq x_2 \) since \( \lim_{x \to x_1} m(x; x_1) = \infty \). One can further show that every KKT point of the new NLP with a finite \( y \) is a KKT point of the original formulation.

**Lemma 4.1.** If \((x^*, y^*)\) is a regular KKT point to the following NLP:

\[
\begin{align*}
\text{minimize} & \quad f(x) \\
\text{subject to} & \quad c(x) = 0, \\
& \quad m(x; x_1) \leq y, \\
& \quad l \leq x \leq u
\end{align*}
\]

(8)

for a finite \( y^* \), and \( m \) is bounded from below, then \( x^* \) is a regular KKT point to problem 1 and \( x^* \neq x_1 \).

**Proof.** Let the Lagrangian multipliers of the equality constraints be \( \lambda, z_+ \) be those of the \( \geq \) bound constraints, and \( z_- \) be those of the \( \leq \) bound constraints. Let the additional Lagrangian multiplier of the deflation constraint be \( \eta \). The stationary conditions of problem 8 are:

\[
\nabla_x f(x) + \nabla_x c(x)^T \lambda + z_+ + z_- + \eta \nabla_x m(x; x_1) = 0
\]

\[
\eta = 0
\]

Since \( \eta \) will be 0 at any KKT point, the stationarity conditions of problem 8 will be satisfied.

\[
\nabla_x f(x) + \nabla_x c(x)^T \lambda + z_+ - z_- = 0
\]

(10)

Additionally, the complementarity condition of the deflation constraint and the dual feasibility constraint \( \eta \geq 0 \) are trivially satisfied at \( \eta = 0 \). Since the constraints of problem 8 are a subset of the constraints of problem 8, \( x^* \) must be feasible to the original problem and the complementarity conditions of those constraints must be satisfied.

Given that \( y^* \) is finite, \((x^*, y^*)\) is feasible to the deflation constraint in problem 8 and \( m \) is bounded from below, then \( m(x^*; x_1) \) must be finite which implies that \( x^* \neq x_1 \). This completes the proof. \( \square \)

Note that the proof above can be trivially generalized to inequality constrained and even conic constrained nonlinear programs. Therefore, this deflation constraint approach is a completely generic and non-invasive way to use deflation in optimization.

Since the deflation constraint approach only requires a change in the formulation optimized rather than the optimization routine, any KKT seeking nonlinear programming algorithm, e.g. the method of moving asymptotes [Svanberg, 1987, 2002] or the augmented Lagrangian algorithm [Bertsekas, 1996] can be used to solve the deflated formulation. This is a much more generic and simpler way to use deflation than deflating all of the optimality conditions.

4.2 Alternative deflation constraint

One can also avoid the introduction of an additional variable \( y \) replacing it with a large finite constant \( M \).

**Lemma 4.2.** If \((x^*)\) is a regular KKT point to the following NLP:

\[
\begin{align*}
\text{minimize} & \quad f(x) \\
\text{subject to} & \quad c(x) = 0, \\
& \quad m(x; x_1) \leq M, \\
& \quad l \leq x \leq u
\end{align*}
\]

(11)
for some finite constant $M$, the constraint $m(x; x_1) \leq M$ is satisfied at a strict inequality, and $m$ is bounded from below, then $x^*$ is a regular KKT point to problem 1 and $x^* \neq x_1$.

**Proof.** Let the Lagrangian multipliers of the equality constraints be $\lambda$, $z_+$ be those of the $\geq$ bound constraints, and $z_-$ be those of the $\leq$ bound constraints. Let the additional Lagrangian multiplier of the deflation constraint be $\eta$. The stationary conditions of problem 11 are:

$$\nabla_x f(x) + \nabla_x c(x)^T \lambda + z_+ - z_- + \eta \nabla_x m(x; x_1) = 0$$

By the complementarity slackness conditions, since the deflation constraint is satisfied at a strict inequality, $\eta$ must be equal to 0 at any KKT point. The rest of the proof is identical to the proof of Lemma 4.1.

### 4.3 Simple deflation for nonlinear systems

Much like in optimization, the following deflation equality constraint can be added to a nonlinear system of equations:

$$m(x; x_1) = y$$

solving for both $x$ and $y$. It is trivial to see that if the algorithm converges to a solution $(x^*, y^*)$ with a finite $y^*$, then $x^*$ will satisfy the original set of equations and $x^* \neq x_1$.

### 4.4 Deflating multiple intermediate solutions

In Papadopoulos et al. [2021], the deflation operator was used to deflate away from the barrier sub-problems’ intermediate solutions. This is a nice way to automatically adapt the deflation power by ensuring that we deflate away from the entire critical path of the interior point optimizer next time the system is solved. It can also be used to provide accelerated convergence by encouraging solutions to intermediate barrier sub-problems to be more different from the previous barrier sub-problems. The same approach can be used in any nonlinear programming algorithm by using a manual callback and adding new “known solutions” to the deflation operator every fixed number of iterations.

### 4.5 Deflation constraint is a minimum distance constraint

The deflation constraint is equivalent to the following distance constraint assuming finite non-zero $m > 0$ and $y > \sigma$:

$$||x - x_1||^p \geq z$$

where $z = \frac{1}{y-\sigma}$. In this case, it is clear what the deflation algorithm does. It just puts a constraint on the distance to known solutions. If the NLP optimizer approaches $z = 0$ or $y = \infty$, then the deflation operator may not be swaying the solution enough away from known solutions. When using the fixed, large $M$ formulation from equation 11 instead of $y$ tending to infinity, the deflation constraint will be satisfied at equality when deflation fails to make the algorithm converge to a different solution. The main hyperparameters that can be tuned in the deflation constraint are the distance measure used and $p$ to ensure convergence to a different solution.

### 4.6 Different distance measures

One can change the distance measure used in the deflation function to more interesting choices than a simple power of a 2-norm. The following are different ways to change the distance measure to achieve different desired effect:

1. Use a $\ell_q$ norm distance measure instead of a power $p$ of a $\ell_2$ norm, or use a power $p$ of a $\ell_q$ norm distance measure.

2. Use a positive semi-definite weight matrix $Q$ and define the distance as the generalized $\ell_2$ norm distance: $(x - x_1)^T Q (x - x_1)$. If $Q$ is diagonal, it can be used to give different weights to different deviation terms.
3. The distance measure can detect symmetries in the solution space if 2 solutions are numerically different but practically identical. In topology optimization for example, it may make more sense to define the distance measure in the pseudo-densities $\rho$ space after applying density filtering, interpolation and Heaviside projection to the solution $x$, rather than calculating distance in the $x$ space. This more accurately reflects the desire of the optimizer to obtain different designs rather than different, symmetric representations of the same design.

4. In topology optimization also, the number of design variables can be extremely large with many similar looking designs that have slightly different numerical values. A particular modification to the distance measure can therefore be useful to workaround this curse of dimensionality problem. Let $\sigma = 0$ and consider the following deflation function:

$$m(x, x_1) = \max(||x - x_1|| - r, 0)^{-p}$$ (15)

This deflation function treats all solutions in the hyper-ball of radius $r$ around $x_1$ as identical to $x_1$, i.e. the distance between them is 0. This function is smooth and twice differentiable for all $x \in \{x : ||x - x_1|| > r\}$. A KKT solution with a finite $y$ (in exact arithmetic) can be similarly shown to be equivalent to finding a new optimal solution outside the hyper-ball. This new parameter $r$ can be useful for high dimensional problems in topology optimization where 2 designs can be numerically different but visually and practically identical. Another side advantage of using $r > 0$ is that even if deflation fails to push the optimization algorithm away from $x_1$, the new solution obtained is guaranteed to be outside the hyper-ball.

5. In variational inference, the Kullback-Leibler (K-L) divergence can be used to deflate away from known distributions that locally optimize the K-L divergence to the posterior distribution.

6. In deep learning, a distance measure between the neuron values can be used instead of the weights and biases to account for symmetries in the weights.

### 4.7 Potential problems with deflation

While deflation has proven rather successful in a number of root finding and optimization applications, it is not free of limitations which need to be addressed or acknowledged when implementing or using the algorithm. The following are some common problems associated with the proposed deflation constraint most of which are also concerns when using the traditional deflation method.

1. The deflation effect may not be strong enough where the algorithm can still approach $x_1$, asymptotically increasing $y$ to $\infty$. This is similar to what can happen in the classic deflation when assumption 6 is violated.

2. The optimization is not done in exact arithmetic but rather up to machine precision. This can make the algorithm converge to a solution with a finite but large value value of $y^*$ instead of overflowing to $\infty$. Therefore, the finiteness of $y^*$ may not be a good enough indication that the algorithm has converged to a solution other than $x_1$.

3. Deflation guarantees that if convergence happens, the solution will be different. However, it doesn’t guarantee that convergence will happen to begin with. Even more so, deflating away from 1 solution is likely to push the optimizer away from other nearby locally optimal solutions if they exist. This can make it particularly challenging to fine-tune the hyperparameters of the algorithm. However arguably this can also be a desirable effect of deflation since it means that more diverse solutions are naturally more likely to be output by the algorithm.

4. Careful selection of the power $p$ and other hyperparameters used in the chosen distance measure is required.

### 5 Examples

In this section, a number of applications of deflation and non-convex optimization are showcased from machine learning and topology optimization. The main highlight of this section is that known popular algorithms were used or minimally modified to solve the deflation sub-problems. In all of the examples, the same initial solution was used in the deflation sub-problems to showcase the efficacy.
5.1 Classical variational inference

In this section, an example of the use of deflation in variational inference will be demonstrated. For simplicity, the log joint probability in variational inference is replaced by the log probability of a 1D mixture of 10 Gaussian distributions. The variational family used is a 1D Gaussian. The automatic differentiation variational inference (ADVI) [Kucukelbir et al., 2015] algorithm was used together with the decayed ADAGrad [Duchi et al., 2011] stochastic optimization algorithm from the AdvancedVI.jl package to minimize a stochastic estimator of the negative of the evidence lower bound (ELBO). Since there is no data, the negative of the ELBO is equal to the K-L divergence. Distributions.jl was used to define the mixture of Gaussians, the variational family, and the estimator of the K-L divergence objective function. The deflated variational approximation problem can be formulated using the loss function $L(\theta)$ as follows:

\[
\begin{align*}
\text{minimize} & \quad L(\theta) \\
\text{subject to} & \quad \sum_{k=1}^{\tilde{K}} m(\theta; \theta_k) \leq y
\end{align*}
\]  

(16)

where $\theta$ is the vector of parameters of the variational family and $\theta_k$ is the previously found local minimizer of the loss function from subproblem $k$, and $\tilde{K}$ is the total number of found solutions so far. $m$ and $y$ are the deflation function and variable respectively as described in the previous sections.

Since the objective is a stochastic estimator of the K-L divergence and the constraint is non-convex, a log-barrier approach [Fiacco and McCormick, 1968] is used to transform the stochastic constrained problem to an unconstrained one. The log-barrier formulation becomes:

\[
\begin{align*}
\text{minimize} & \quad L(\theta) - r \times \log \left( y - \sum_{k=1}^{\tilde{K}} m(\theta; \theta_k) \right)
\end{align*}
\]  

(17)

where $r$ is defined as a decaying coefficient approaching 0. The above problem was solved 10 times from the same initial solution $\theta_0$ each time converging to different Gaussian approximations and appending it to the list of found solutions. The distance function used between solutions in the deflation function was the analytic K-L divergence between the 2 Gaussian distributions offset by a radius $r$. Let $d(\theta) = \mathcal{N}(\mu = \theta[1], \sigma = \exp(\theta[2]))$ be the Gaussian distribution obtained from solution $\theta$. The K-L divergence based deflation function $m$ used was therefore:

\[
m(\theta; \theta_k) = \max \left( \text{div} \left( d(\theta), d(\theta_k) \right) - 1, 0 \right)^{-3}
\]  

(18)

where div is the K-L divergence between 2 Gaussian distributions. Note that the minimum radius of 1 was used to enforce convergence to a different distribution even if the convergence assumptions of deflation were violated. The optimal Gaussian distributions’ obtained and the target distribution’s probability density functions are shown in figure[1]. The results indicate that deflation was successful at generating reasonable mode-seeking approximations of the target mixture of Gaussians.

5.2 Pathfinder algorithm for variational inference

The pathfinder algorithm [Zhang et al., 2021] is a recently proposed algorithm for approximate Bayesian inference. The pathfinder algorithm relies on multi-start optimization of the log joint probability, reusing the trajectory of intermediate solutions and gradients from the optimization to construct a Gaussian approximation per trajectory. Re-starting the optimization from a different initial point can result in a different optimal solution and trajectory, leading to a potentially different local Gaussian approximation. These Gaussian approximations are then combined and weighted in

[1] https://github.com/JuliaTopOpt/deflation_examples/
[2] https://github.com/TuringLang/AdvancedVI.jl
[3] https://github.com/JuliaStats/Distributions.jl
a mixture of Gaussians which is used to approximate the posterior distribution. For more details, please refer to [Zhang et al., 2021]. For simplicity, a target mixture of Gaussians distribution was used in the experiments instead of an unknown posterior distribution. The Pathfinder.jl package was adapted to use IPOPT [Wächter and Biegler, 2006] as an optimizer as wrapped in the Nonconvex.jl package. Instead of random restarts, the same initial solution of 0.0 was used in all the deflation-based pathfinder sub-problems. The target (blue) and approximate (orange) mixtures of Gaussians are shown in figure 2. The results are almost perfect for a target mixture of 2, 4 and 6 Gaussians. Given that all the optimization sub-problems were started from the same initial solution, this is a fairly positive result. For the target mixture of 8 Gaussians, deflation on its own (without random restarts) fails to accurately approximate the target distribution, however this is not entirely surprising.

5.3 Topology optimization - volume constrained compliance minimization

The volume-constrained compliance minimization problem from topology optimization (TO) seeks to find designs for physical structures that are as stiff as possible (i.e. least compliant) with respect to known boundary conditions and loading forces while adhering to a given material demand. It has been well studied and widely applied in mechanical, aerospace, and architectural engineering [Bendsoe and Sigmund, 2003]. However, because TO problems are high-dimensional, partial differential equation (PDE) constrained, and non-convex, finding multiple local minima that are visually different has been challenging and rarely studied, despite its practical values. A compliance-minimizing, volume-constrained TO problem can be formulated as:

\[
\begin{align*}
\text{minimize} & \quad f \cdot u \\
\text{subject to} & \quad K(x)u(x) = f, \\
& \quad \sum_{i=1}^{n} x_i = \tilde{V}, \\
& \quad 0 \leq x \leq 1
\end{align*}
\]
where $x$ is the pseudo-density of cells in the domain, $f$ the given load vector, $K(x)$ the stiffness matrix from the finite-element discretization, $\tilde{V}$ is the user-specified volume fraction. When $x_i = 0$, the corresponding cell is removed and when $x_i = 1$ the cell is kept.

We apply our deflation technique by adding an extra constraint to problem 19 using the distance measure that encourages visually different designs mentioned in Section 4.6:

$$\tilde{K} \sum_{k=1}^{\tilde{K}} m(x; x_k) = \tilde{K} \max(\|x - x_k\| - r, 0)^{-p} \leq y$$

where $\tilde{K}$ is the number of found local minima from previous deflation iterations. In our experiments, $p = 4$, $r = 20$, $y \in (0, 100)$.

Two classic topology optimization benchmark problems are tested here: a continuum MBB beam domain of dimension $120 \times 40$ and a cantilevering truss domain of dimension $40 \times 10$ (Figure 3). TopOpt.jl is used for the implementation of problem modeling, finite-element analysis, and density filters. We use the widely used Method of Moving Asymptotes (MMA) algorithm [Svanberg, 1987] to solve both the undeflated and deflated problems. Runtime results are presented in Table 1. Figure 4 and Figure 5 visualize the results of running 20 deflation iterations on both domains. The results show that the proposed deflation formulation generates visually different, near-optimal designs deterministically, all starting from the same initial guess. The runtime results suggest no significant change in the running time due to adding a deflation constraint to an already constrained optimization problem.

https://github.com/JuliaTopOpt/TopOpt.jl
Table 1: Deflated topology optimization runtime. *: deflated problem runtime is averaged over all the 20 deflation iteration.

| TopOpt problems          | x dim | undeflated | deflated* |
|--------------------------|-------|------------|-----------|
| Continuum (Figure 4)     | 4800  | 121s       | 122s      |
| Truss (Figure 5)         | 3608  | 1.9s       | 1.6s      |

Figure 3: Topology optimization domains: (a) half MBB beam continuum domain; (b) cantilevering truss domain.

6 Conclusion and future work

In this work, a new way to use deflation was proposed to find diverse solutions of non-convex optimization problems. With the proposed problem re-formulation, the deflation technique can be easily applied to any non-convex problems using existing, off-the-shelf optimizers. Promising results of applying the proposed technique on solving problems from topology optimization and variational inference are presented. We hope our work can enable applications of this simple, yet powerful idea of deflation to a broader set of problems where multiple local optimal solutions are required. In the future, we hope to make use of deflation-based optimization to enhance optimization-based machine learning algorithms such as maximum likelihood estimation, and to use it for model-based design of experiments in clinical trials to explore multiple possible designs.
Figure 4: Deflated results of the continuum half MBB beam problem. Iteration 0 is the solution found by solving the undeflated problem.

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A Deflated KKT system of NLP’s barrier subproblems

In this section, derivations for the deflated KKT system of the barrier sub-problem by the interior point method [Wright 1997] as implemented in the IPOPT software [Wächter and Biegler 2006] are presented.

A.1 KKT system of the barrier problem

In IPOPT, a log barrier method is used to guarantee that \( l \leq x \leq u \) remains satisfied at every intermediate solution if the initial solution is within the bounds. The barrier function is defined as:

\[
B_\mu(x, l, u) = -\mu \left( \sum_i \log (x_i - l_i) + \sum_i \log (u_i - x_i) \right)
\]

for some \( \mu > 0 \) which would go to \( \infty \) if any of the decision variables approaches one of its finite bounds. This creates a barrier stopping the optimizer from every reaching the finite bound. The barrier sub-problem is defined as:

\[
\begin{align*}
\text{minimize} & \quad \phi_\mu(x) = f(x) + B_\mu(x, l, u) \\
\text{subject to} & \quad c(x) = 0
\end{align*}
\]

The KKT stationarity condition is therefore:

\[
\nabla f(x) + \nabla c(x)^T \lambda - z_l - z_u = 0
\]

where \( \lambda \) is the vector Lagrangian multipliers associated with the equality constraint \( c(x) = 0 \), \( z_l \) is a vector whose \( i^{th} \) element is \( z_{li} = \frac{\mu}{x_i - l_i} \) and \( z_u \) is a vector whose \( i^{th} \) element is \( z_{ui} = \frac{\mu}{u_i - x_i} \).

Additionally, let \( Z_l \) be the diagonal matrix whose diagonal is \( z_l \), \( Z_u \) be the diagonal matrix whose diagonal is \( z_u \), \( X_l \) be the diagonal matrix whose diagonal is: \( \tilde{x}_i = x_i - l_i \) and \( X_u \) be the diagonal matrix whose diagonal is: \( \tilde{x}_i = u_i - x_i \).

The first-order KKT sufficient conditions for optimality of the barrier problem, assuming the constraint qualifications are satisfied, can be written as:

\[
\begin{align*}
\nabla f(x) + \nabla c(x)^T \lambda - z_l - z_u &= 0 \quad (21a) \\
c(x) &= 0 \quad (21b) \\
X_l Z_l 1 - \mu 1 &= 0 \quad (21c) \\
X_u Z_u 1 - \mu 1 &= 0 \quad (21d) \\
l \leq x &\leq u \quad (21e) \\
z_l &\geq 0 \quad (21f) \\
z_u &\geq 0 \quad (21g)
\end{align*}
\]

where \( 1 \) is a vector of ones. Conditions \( 21c \) and \( 21d \) ensure that the relationship between \( X_l, Z_l, X_u \) and \( Z_u \) is maintained according to the definitions of \( z_l \) and \( z_u \). In an interior point algorithm (e.g. IPOPT [Wächter and Biegler 2006]), primal-dual solutions to the equality KKT conditions are found using a Newton-like method while ensuring that the inequality conditions are satisfied by projection.

In order to solve the barrier problem for a given value \( \mu = \mu_j \), a damped Newton’s method is usually applied to the primal-dual optimality conditions. Here we use \( k \) to denote the iteration counter for the inner iterations when solving the barrier problem. Given an iterate \( (x_k, \lambda_k, z_{1,k}, z_{u,k}) \) with \( l < x_k < u \) and \( z_{1,k}, z_{u,k} > 0 \), some search directions \((d^c_k, d^\lambda_k, d^{z_l}_k, d^{z_u}_k)\) are obtained using the regularized linearization of the optimality conditions (excluding the inequality conditions):

\[
\begin{bmatrix}
W_k & A_k & -I & -I \\
A_k^T & 0 & 0 & 0 \\
Z_{l,k} & 0 & X_{l,k} & 0 \\
Z_{u,k} & 0 & 0 & X_{u,k}
\end{bmatrix}
\begin{bmatrix}
d^c_k \\
d^\lambda_k \\
d^{z_l}_k \\
d^{z_u}_k
\end{bmatrix}
=
\begin{bmatrix}
\nabla f(x_k) + A_k^T \lambda_k - z_{l,k} - z_{u,k} \\
c(x_k) \\
X_{l,k} Z_{l,k} 1 - \mu_j 1 \\
X_{u,k} Z_{u,k} 1 - \mu_j 1
\end{bmatrix}
\]

(22)

where \( A_k := \nabla c(x_k)^T \) and \( W_k := \nabla^2_{xx} (f(x_k) + c(x_k)^T \lambda_k) \) is the Hessian of the Lagrangian function of the original problem. The Lagrangian terms from the bounds constraints are ignored.
because they don’t contribute to the Hessian. When the Hessian of the Lagrangian is not available, a
1-BFGS approximation [Nocedal and Wright 2006] of the Hessian can be used instead. This changes
the IPOPT algorithm from a second order algorithm to a first order one. And the Newton update
becomes a quasi-Newton update.

Instead of solving the non-symmetric system of equations above, one can instead change the system
as such:

\[
\begin{bmatrix}
W_k & A_k & -I & -I \\
A_k^T & 0 & 0 & 0 \\
X_l^{-1}Z_l,k & 0 & I & 0 \\
X_u^{-1}Z_u,k & 0 & 0 & I
\end{bmatrix}
\begin{bmatrix}
d^x_k \\
d^\lambda_k \\
d^z_l \\
d^z_u
\end{bmatrix}
= - \begin{bmatrix}
\nabla f(x_k) + A_k^T\lambda_k - z_{l,k} - z_{u,k} \\
0 \\
0 \\
0
\end{bmatrix}
\] (23)

Adding the third and fourth equations to the first one, the third and fourth blocks of coefficients of the
first equation will be eliminated.

\[
\begin{bmatrix}
W_k + \Sigma_k & A_k & 0 & 0 \\
A_k^T & 0 & 0 & 0 \\
X_l^{-1}Z_l,k & 0 & I & 0 \\
X_u^{-1}Z_u,k & 0 & 0 & I
\end{bmatrix}
\begin{bmatrix}
d^x_k \\
d^\lambda_k \\
d^z_l \\
d^z_u
\end{bmatrix}
= - \begin{bmatrix}
\nabla f(x_k) + A_k^T\lambda_k - \mu_j X_l^{-1}1 - \mu_j X_u^{-1}1 \\
0 \\
0 \\
0
\end{bmatrix}
\] (24)

where \( \Sigma_k = X_l^{-1}Z_l,k + X_u^{-1}Z_u,k \). Therefore, one can now solve for \( d^x_k \) and \( d^\lambda_k \) by solving the
following symmetric linear system:

\[
\begin{bmatrix}
W_k + \Sigma_k & A_k \\
A_k^T & 0
\end{bmatrix}
\begin{bmatrix}
d^x_k \\
d^\lambda_k
\end{bmatrix}
= - \begin{bmatrix}
\nabla f(x_k) + A_k^T\lambda_k - \mu_j X_l^{-1}1 - \mu_j X_u^{-1}1 \\
0
\end{bmatrix}
\] (25)

then use the value of \( d^x_k \) to find \( d^z_l \) and \( d^z_u \) using:

\[
\begin{align*}
d^z_l &= -z_{l,k} + \mu_j X_l^{-1}1 - X_l^{-1}Z_l,k d^x_k \\
d^z_u &= -z_{u,k} + \mu_j X_u^{-1}1 - X_u^{-1}Z_u,k d^x_k
\end{align*}
\] (26a)

A.2 Deflating the KKT system

If we define the RHS of Equation (25) as:

\[
F(x, \lambda) = \begin{bmatrix}
\nabla f(x) + A^T\lambda - \mu_j X_l^{-1}1 - \mu_j X_u^{-1}1 \\
0
\end{bmatrix}
\] (27)

Then the goal of the primal-dual optimizer then becomes solving for \( F(x, \lambda) = 0 \).

If we apply the deflation operator to the entire \( F(x, \lambda) \), we will obtain \( G(x, \lambda) = M(x; x_1)F(x, \lambda) = 0 \), whose Jacobian is:

\[
\nabla_x G(x) = m(x; x_1)\nabla_x F(x, \lambda) + diag(F(x, \lambda))1(\nabla_x m(x; x_1))^T
\]

where \( \nabla_x m(x; x_1) \) is the gradient of the deflation function, \( 1 \) is a column vector of 1s and
diag(\( F(x) \)) is a diagonal matrix with diagonal \( F(x) \). The Jacobian of this function wrt \( x \) is:

\[
\begin{bmatrix}
W + \Sigma \\
A^T
\end{bmatrix}
\] (28)

where \( W, \Sigma \) and \( A \) are defined as \( W_k, \Sigma_k \) and \( A_k \) in the last section. The top matrix is symmetric
because it is the Hessian matrix of the barrier objective function. However, \( A_k := \nabla c(x_k)^T \) in
general is not symmetric, and thus prevents the usage of efficient linear algebra algorithms for
symmetric linear system.