Coupling material and mechanical design processes via computer model calibration

Carl Ehrett*
School of Mathematical and Statistical Sciences, Clemson University,
D. Andrew Brown
School of Mathematical and Statistical Sciences, Clemson University,
Evan Chodora
Department of Mechanical Engineering, Clemson University,
Mingzhe Jiang
Department of Chemical and Biomolecular Engineering, Clemson University,
Christopher Kitchens
Department of Chemical and Biomolecular Engineering, Clemson University,
and
Sez Atamturktur
Department of Architectural Engineering, Pennsylvania State University

July 3, 2019

observations of reality?
parameter values?

Abstract

Computer model calibration typically operates by choosing parameters in a computer model so that the model's output faithfully predicts reality. By using desired performance targets in place of observed data, we show that calibration techniques can be repurposed to wed engineering design and material ~~design~~ discovery, two processes that are ~~typically~~ carried out separately. This allows materials to be designed with specific engineering targets in mind while quantifying the associated sources of uncertainty. We demonstrate our proposed approach by "calibrating" material design settings to performance targets for a wind turbine blade and by estimating the system's Pareto front with quantified uncertainties.

conventionally
OR
traditionally

performance

ok!

Keywords: Gaussian processes, material design, optimization, Pareto optimality, Uncertainty quantification, wind turbines

*The authors gratefully acknowledge *please remember to list all relevant funding sources in the unblinded version*

1 Introduction

Real-world optimization problems typically involve multiple objectives. This is particularly true in the design of engineering systems, where multiple performance outcomes are balanced against budgetary constraints. Among the complexities involved in optimizing over multiple objectives is the effect of uncertainties in various aspects of the problem. Design is guided by models known to be imperfect, systems are built using materials with uncertainty regarding their material properties, variations occur in the construction of designed systems, and so on. These imperfections, uncertainties and errors cause ~~there to be~~ uncertainty also in the solution to a given design problem.

In traditional engineering design, one designs a system after choosing a material with appropriate properties for the project from a ~~general use~~ database of known materials. ~~These materials are themselves developed without a specific end-use in mind~~. As a result, the design of the system is constrained by the initial material selection. By coupling material ~~design~~ discovery and engineering system design, we can combine these two traditionally separate ~~design~~ processes under the umbrella of a unified multiple objective optimization problem.

wood for example was not "developed". I think we can remove this

engineering

In this paper, we cast the design problem in the framework of computer model calibration. In traditional calibration, one aligns the computer model output to observations of the real system by estimating unknown parameters in the model. Here, we instead align the computer model to performance and cost targets by finding design variables that optimize the model output with respect to those targets.

In addition to optimizing to a specific set of targets, in many situations it is helpful to this is confusing. we need a different word choice here.

maybe move this sentence

have a comprehensive picture of optimal outcomes without committing to specific targets. For example, in a system in which there is a trade-off between cost and performance, which region of the model range is considered desirable will depend upon the budgetary

pareto front

constraints of the project. ~~Decision-makers in such a scenario are well-served by having a complete picture of the curve describing the optimal performance at any budget.~~ More generally, in a system with multiple outputs, one wants to estimate the Pareto front of the model range; i.e., the set of points in the model range that are *Pareto optimal.* A point is Pareto optimal if and only if, in order to improve any one of its elements, some other element must be made worse off. For example, if a bivariate system in a minimization problem has exactly three output points $a = (2, 0)$, $b = (2, 1)$, and $c = (1, 10)$ then a and c are each Pareto optimal, but b is not, since there is a point (namely a) that is less than or equal to b in every output and strictly less than b in at least one output. We show that our proposed methodology can be used to estimate the Pareto front of a system with ~~uncertainty quantification.~~ quantified uncertainties.

Our proposed methodology uses the Bayesian framework first established as a means for computer model calibration by Kennedy and O'Hagan (2001). This area is furthered by Higdon et al. (2004), who undertake model calibration with quantification of the related uncertainty. They explicitly incorporate uncertainty regarding the computer model input, the bias of the computer model, and uncertainty due to observation error. The approach of Higdon et al. (2004) is further refined and exemplified by Williams et al. (2006). Loeppky et al. (2006) offer a maximum-likelihood-based alternative to the Bayesian approach advocated by Kennedy and O'Hagan, intending thereby to improve the identifiability of the calibration parameters in the face of model discrepancy. Bayarri et al. (2007) extend the approach of Kennedy and O'Hagan, allowing for simultaneous validation and calibration of a computer model (using the same training data). Bayarri et al. (2007) apply this methodology to functional data using a hierarchical framework for the coefficients of a wavelet representation. Similarly, Paulo et al. (2012) apply the approach of Bayarri et al. (2007) to computer models with multivariate output. Brynjarsdóttir and O'Hagan (2014) demonstrate the importance of strong priors on the model discrepancy term when undertaking calibration.

Common to those approaches is the conception of calibration as using real observations to get a posterior distribution on unknown parameters $\boldsymbol{\theta}$ such that the posterior predictive distribution of the model approximates the real system. By contrast, in our proposed methodology, we use artificial observations (representing our design goals targets?) to get obtain? a posterior distribution on design variables $\boldsymbol{\theta}$ such that the posterior predictive distribution of the model approximates (moves towards? OR reaches?) our design ~~goals~~ target. We describe how, with little added computational cost, the methodology provides an initial rough estimate of the Pareto front for the system, which can be used to select downselect ? artificial observations more stringent ? that promote strong Bayesian learning about the optimal settings for the design variables $\boldsymbol{\theta}$. Repeated applications of the procedure can then be used to produce a more thorough estimate of the Pareto front with quantified uncertainties.

We apply our proposed methodology both to ~~an artificial~~ a proof-of-concept example and to the problem of finding material design settings to optimize the performance and cost of a wind turbine blade of fixed outer geometry. The wind turbine blade in question is to be constructed using a composite material. One design variable targeted for optimization is the *volume fraction*, which is the ratio of the *filler* to *matrix* used in the composite material. ~~In a composite, the matrix holds the filler together; an example would be concrete, in which a filler of loose stones is combined with a matrix of cement.~~ Another design variable is the thickness (in mm) of the shear web used in the blade. Our material design goal is to reduce the cost per square meter of the composite material, the rotation (in radians) of the blade when under load, and the deflection (in meters) of the blade tip when under load.

definitely remove

exactly, this is the "goal". Specific values be the "targets". That is why we should be saying "target" in page 4.

In Section 2, we review the calibration framework that serves as the basis for our proposed design optimization approach. In Sections 3 and 4, we apply our proposed methodology to the example involving simulated data and to wind turbine blade design. In Section 4, we show how our approach can be used to produce an estimate of the Pareto front of the wind turbine blade system while quantifying associated uncertainty. Section 5 concludes with discussion of the results and thoughts about future directions.

2 Calibration for design

2.1 Gaussian process emulators for calibration

In this work, when an emulator is needed we assume the use of a Gaussian process (GP) emulator. Just as a multivariate Gaussian random variable is characterized by its mean vector and covariance matrix, a Gaussian process is fully characterized by its mean function $\mu : D \to \mathbb{R}$ and covariance function $C : D \times D \to \mathbb{R}$, where D is the domain of the process. Thus for any points $\mathbf{x}, \mathbf{y}$ in the domain of the Gaussian process, $\mu(\mathbf{x})$ gives the mean of the

Gaussian process at $\mathbf{x}$, and $C(\mathbf{x}, \mathbf{y})$ gives the covariance between the values of the Gaussian process at points $\mathbf{x}$ and $\mathbf{y}$. The distribution of the process at any finite number of points is multivariate Gaussian with mean vector and covariance matrix determined by $\mu(\cdot)$ and $C(\cdot, \cdot)$. In principle, model calibration need not rely on a GP emulator, or any other sort of emulator; one could (e.g.) complete a full Bayesian analysis via Markov chain Monte Carlo (MCMC; Gelfand and Smith, 1990) by running the relevant computer model at each iteration of the chain. In Section 3 we assume fast-running computer code for the simulated example. However, computer models are frequently too computationally expensive to allow for such expenditure (Van Buren et al., 2013, 2014). Instead, a computationally tractable emulator can be constructed using a sample of output from the computer model.

Hemez Atamturktur 2012 is another good referece?

GPs are popular prior distributions on computer model output for three reasons. Firstly, because their use does not require detailed foreknowledge of the model function's parametric form. Secondly, GPs easily interpolate the computer model output, which is attractive when the computer model is deterministic and hence free of measurement error. This is usually the case, although some attention in model calibration (e.g., Pratola and Chkrebtii, 2018) has focused specifically on stochastic computer models. Thirdly, GPs facilitate uncertainty quantification through the variance of the posterior GP. This section provides brief background on Gaussian processes and their use in regression broadly, and in computer model calibration specifically.

The use of GPs to produce a computationally efficient predictor of expensive computer code given observations of code output at $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_n)^T$ is advocated by Sacks et al. (1989) and explored at length by Santner et al. (2003). Since computer code is typically deterministic, these applications differ from the focus of O'Hagan (1978) in that the updated GP is induced to interpolate the computer output $\boldsymbol{\eta} = (\eta(\mathbf{x}_1), \cdots, \eta(\mathbf{x}_n))^T$. Kennedy and O'Hagan (2001) use GPs for computer model calibration. Kennedy et al. (2006) showcase this use of GP emulators for uncertainty and sensitivity analyses. Bastos and O'Hagan (2009) describe both numerical and graphical diagnostic techniques for assessing when a GP emulator of a computer model is successful, as well as this verb applies here? ~~discussion of~~ likely causes of poor diagnostic results. While most work in the area of GP emulation uses stationary covariance functions and quantitative inputs, efforts have been made to branch away from these core assumptions. Gramacy and Lee (2008) use treed partitioning to deal with a nonstationary computer model. Qian et al. (2008) explore methods for using GP emulators that include both quantitative and qualitative inputs.

Whether or not an emulator is used, in the framework implemented here one may consider a computer model to be of the form $\eta(\mathbf{x}, \boldsymbol{\theta})$, where $(\mathbf{x}, \boldsymbol{\theta})$ comprise all inputs to the model. The vector $\boldsymbol{\theta}$ denotes the collection of design variables. The vector $\mathbf{x}$ is the collection of all other inputs that are known and/or under the control of the researcher. We call $\mathbf{x}$ the *control inputs*. Thus, the model is

$$y(\mathbf{x}) = \eta(\mathbf{x}, \boldsymbol{\theta}) + \delta(\mathbf{x}) + \epsilon(\mathbf{x}), \tag{1}$$

where $y(\mathbf{x})$ describes a model outcome at control inputs $\mathbf{x}$, $\delta(\cdot)$ describes the model discrepancy (the systematic bias of the model as an estimate of the response) and $\epsilon(\cdot)$ is a mean-zero error, often assumed to be i.i.d. Gaussian.

To employ an emulator, suppose that we have inputs $\{(\mathbf{x}_i, \mathbf{t}_i)\}_{i=1}^n \subseteq \mathbb{R}^p \times \mathbb{R}^q$ scaled to the Cartesian product of the $p-$ and $q-$dimensional unit hypercubes, and that we have completed computer model runs $\eta(\mathbf{x}_i, \mathbf{t}_i)$ for $i = 1, \cdots, n$. Define the GP prior for modeling $\eta(\cdot, \cdot)$ as follows. Let the mean function $\mu(\mathbf{x}, \mathbf{t}) = c$, where c is a constant. Set the covariance function in terms of the marginal precision λ_η and a product power exponential correlation function:

$$C((\mathbf{x}, \mathbf{t}), (\mathbf{x}', \mathbf{t}')) = \frac{1}{\lambda_\eta} \prod_{k=1}^{p} \exp\left(-\beta_k^\eta |x_k - x_k'|^{\alpha_\eta}\right) \times \prod_{j=1}^{q} \exp\left(-\beta_{p+j}^\eta |t_j - t_j'|^{\alpha_\eta}\right) \quad (2)$$

where each β_k describes the strength of the GP's dependence on one of the elements of the input vectors $\mathbf{x}$ and $\mathbf{t}$, and α_η determines the smoothness of the GP. The model is completed by specifying priors for the hyperparameters c, λ_η, α_η, and β_j^η for $j = 1, \ldots, p+q$, though in practice these are often set to predetermined values.

2.2 Design to target outcomes

the goal is to increase stiffness or reduce cost.
target is the specific value

Call ~~design goals (such as performance and cost~~ design targets (treated as observations in the design procedure we propose below) "target outcomes", and call that procedure, which uses a Bayesian model calibration framework with target outcomes in place of real observations, "calibration to target outcomes" (CTO). Thus target outcomes are a sort of artificial data, and the calibration procedure is carried out as if these artificial data had been observed in reality. Just as in traditional calibration, in which the result of the procedure is a distribution on the calibrated parameter $\boldsymbol{\theta}$ to approximate the observed data, in CTO the result is a distribution on the design parameter $\boldsymbol{\theta}$ which induces the model to approximate the performance and cost targets. The posterior predictive distribution is thereby pushed toward the target outcomes. Herein, The model used is assumed to yield accurate results within the design domain. Future work in this area will address the case of models that are known

maybe move to conclusions?

or suspected to suffer from systematic bias. maybe move to conclusion

The tools of model calibration founded in the work of Kennedy and O'Hagan (2001) retain their advantages under our proposed methodology. Most centrally, calibration to target outcomes $\mathbf{y}$ produces not merely a point estimate $\mathbf{t}^*$, but rather a posterior distribution of $\mathbf{t}|\mathbf{y}$ reflective of remaining uncertainty about the appropriate value of $\mathbf{t}^*$. Such uncertainty may have its source in parameter uncertainty (uncertainty about the values of model inputs other than the design variables), model form uncertainty (uncertainty about how closely the code approximates reality), and that which traditional calibration would consider observation error. Of course, targets are not actually observations, so the concept of observation error does not cleanly transfer. However, a similar uncertainty would be that due to how close reality *can* come to our target outcomes. The Bayesian model calibration framework allows for the quantification of all of these uncertainties. Furthermore, by the use of informative priors on the model discrepancy and observation error, the identifiability concerns of the Kennedy-O'Hagan approach can be mitigated (Bayarri et al., 2007; Tuo and Wu, 2016).

* when applied in the context of "design", KOH approach does not have identifiability concern, I'd argue

~~In general~~ Ideally?, target outcomes should aim only a little beyond what is realistically achievable; only as much as is necessary to ensure the targets are at least as ambitious as any true optimum in the system. Three reasons why one should go only a little beyond that are as follows: Firstly, if target outcomes are set to be too farfetched, then the procedure can become computationally unstable due to underflow and round-off error, since any value of $\boldsymbol{\theta}$ within its support will have extremely low likelihood. Secondly, increasing the distance of the target outcomes from the optimal region reduces the identifiability of that region.

I think this is a little lengthy.
I also don't know how one can achieve what you argue here.

CTO finds the region of the parameter space with output closest to the target outcomes. If the entire feasible performance range is far from the target outcomes, then the optimal region will in relative terms be only a little closer than the rest of the model range. This is the same effect as when the variance of the observation error is much larger than the variance of the prior distribution on a parameter; i.e., the posterior is much more strongly determined by the prior than the likelihood, resulting in limited Bayesian learning about quantities of interest. A third reason to keep target outcomes close to the model range is that the targets lose their interpretability when they take on values that are implausible or impossible.

The issue is we do not always know what is "realistically achievable." That is whole another evaluation.

When a target cannot be selected (for example, because priorities regarding cost and performance trade-offs have not yet been settled), design can be carried out using each point in a grid over the region of plausible target values. For instance, one can design to performance targets under each point of a grid of "known" costs, rather than designing with a specific desired cost. In doing so, we present a comprehensive picture of optimal parameter distributions and resulting performance under a range of costs, which could inform the process of setting a budget.

this description is rather long-winded

It is common to plug in the MLEs of the GP covariance hyperparameters λ_η and β^η in (2) instead of including them in a full Bayesian analysis (Kennedy and O'Hagan, 2001; Santner et al., 2003; Qian et al., 2008; Paulo et al., 2012). keep In our proposed methodology, that is not merely a convenience, but rather is essential to. This is because in a full Bayesian analysis, the posterior distributions of λ_η and β^η would depend upon target outcomes which are not real observations of the system. The resulting emulator would be trained

what if the emulator was first trained based on simulator output alone and then the hyper-parameters are set "constant" during the subsequent calibration.

not only on the simulator output, but also on our performance and cost targets~~, which will~~. since ~~typically be (intentionally) unrealistic. As argued by Liu et al. (2009), it is preferable to~~

...essential to avoid training a computer model emulator using data which do not arise from that model (such as the design targets). Therefore, we use values found by maximizing the log likelihood of the observations of the simulation with respect to λ_η and $\boldsymbol{\beta}^\eta$. We set the GP to have constant mean $c = 0$, which works well when (as here) the GP is not used for extrapolation (Bayarri et al., 2007). We set $\alpha_\eta = 2$, which assumes that the model output is infinitely differentiable.

We similarly model the discrepancy term $\delta(\cdot)$ as a GP, also with mean zero, and with covariance function $C_\delta(\mathbf{x}, \mathbf{x}') = \lambda_\delta^{-1} \prod_{k=1}^{p} \exp\left(-\beta_k^\delta |x_k - x_k'|^{\alpha_\delta}\right)$. This is included in the model to capture systematic discrepancy between target outcomes and the feasible model range. We use priors $\rho_k^\delta \sim \text{Beta}(1, 0.3)$, where $\rho_k^\delta = \exp(-\beta_k^\delta/4)$ for $k = 1, \ldots, p$. A Gamma prior is appropriate for λ_δ, with strength determined by the amount of prior information available. With sufficient prior information, though, we can set λ_δ to be constant. Details surrounding the choice of prior for λ_δ are discussed below. As with the covariance function of $\eta(\cdot, \cdot)$, we set $\alpha_\delta = 2$.

I am not sure what you are referring to here.

Let $\boldsymbol{\eta} = (\eta(\mathbf{x}_1, \mathbf{t}_1), \cdots, \eta(\mathbf{x}_n, \mathbf{t}_n))^T$ be the vector of completed runs of the simulator, $\mathbf{y} = (y(\mathbf{x}_{n+1}), \cdots, y(\mathbf{x}_{n+m}))^T$ the target outcomes we wish to induce the system to achieve, and $\mathcal{D} = (\boldsymbol{\eta}^T, \mathbf{y}^T)^T$. Then $\mathcal{D}|\boldsymbol{\theta}, \widehat{\lambda_\eta}, \widehat{\boldsymbol{\rho}^\eta}, \lambda_\delta, \boldsymbol{\rho}^\delta$ is distributed as multivariate normal with mean 0 and covariance $\mathbf{C}_\mathcal{D}$, a matrix with i, j entry equal to $C((\mathbf{x}_i, \mathbf{t}_i), (\mathbf{x}_j, \mathbf{t}_j)) + I(i, j > n) \cdot (C_{obs}(\mathbf{x}_i, \mathbf{x}_j) + C_\delta(\mathbf{x}_i, \mathbf{x}_j))$ where $C_{obs}(\cdot, \cdot)$ reflects the acceptable deviation from targets (reminiscent to observation error in model calibration), ?? ~~serves as "observation error" of our own target outcomes, since in a typical case one can at best identify a small region within which the choice of any particular point as a target outcome would be arbitrary due to our acceptable~~

this reads clearer to me.

You can also say "deviation from targets that can be tolerated"

~~tolerance~~. Thus, $C_{obs}(\mathbf{x}_i, \mathbf{x}_j) = \sigma^2 \delta^K_{ij}$, where δ^K is the Kronecker delta and σ^2 is chosen to

for acceptable deviation from targets?

reflect the desired tolerance ~~level~~, such that targets within σ of each other are considered to be roughly equivalent. The appropriate setting for σ^2 will differ across applications. For our applications, we set $\sigma^2 = 0.05$ (with target outcomes standardized to have mean zero and prior standard deviation 1). Notice also that $C_{obs}(\cdot, \cdot)$ serves to add a nugget to the covariance matrix produced by $C_\delta(\cdot, \cdot)$. Aside from easing matters computationally (by improving the conditioning of the covariance matrix), the addition of such a nugget can improve the quality of the fit of the GP discrepancy δ (Gramacy and Lee, 2012). Setting a uniform prior on the design variables $\boldsymbol{\theta}$, the joint posterior density under the model is

$$\pi(\boldsymbol{\theta}, \lambda_\delta, \boldsymbol{\rho}^\delta | \mathcal{D}, \widehat{\lambda_\eta}, \widehat{\boldsymbol{\rho}^\eta}) \propto \pi(\mathcal{D} | \boldsymbol{\theta}, \widehat{\lambda_\eta}, \widehat{\boldsymbol{\rho}^\eta}, \lambda_\delta, \boldsymbol{\rho}^\delta) \times \pi(\lambda_\delta) \times \pi(\boldsymbol{\rho}^\delta). \quad (3)$$

Markov chain Monte Carlo methods are useful for estimating features of the posterior distribution.

we did not use this word much before. sounds a little out of the blue here.

In order to successfully locate the optimal design region, it is necessary either to place an informative prior on the marginal precision λ_δ of the discrepancy $\delta(\cdot)$, or else to specify λ_δ outright. Otherwise, the optimal region of the design variable space will suffer from poor identifiability. This longstanding concern was raised in the discussion of Kennedy and O'Hagan (2001), as well as by Bayarri et al. (2007), Tuo and Wu (2015), and Plumlee (2017). How informative one's prior on λ_δ will be depends upon how much one knows about the true Pareto front prior to undertaking CTO. For instance, if in a univariate case it is known with some confidence that the true optimum is nearly constant as a function of the other model inputs, and that it occurs in the interval [10, 11], then a constant target outcome of 9 could be used with an informative prior tailored to this prior knowledge of

but the conventional sense of identifiability does not apply in design. am I missing something here?

?? ok!

I thought this was enumerated at first ;;

there is some of this in the previous para

the approximate resulting discrepancy.

Where the prior on λ_δ cannot be chosen to be *accurate* (due to insufficient prior knowledge of the Pareto front) it should be chosen to *overestimate* the precision. Otherwise, underestimation of λ_δ may lead to poor identifiability of the optimal design region by granting the model too much flexibility in systematically deviating from the targets. ~~This is because λ_δ affects the expected distance of the target outcomes from the posterior predictive distribution. Thus, underestimating λ_δ can result in there being little penalty in leaving the region of the model range that is closest to the target outcomes. When setting a prior that overestimates λ_δ, the posterior distribution of λ_δ becomes less reliable than when an accurate prior is used. Nonetheless, even when λ_δ must be overestimated, the posterior distribution of $\boldsymbol{\theta}$ will still peak at the optimal design region, since overestimation of λ_δ forces the mean-zero discrepancy to be small and thereby only increases the penalty of leaving the optimal region.~~ Thus, while relying on vague knowledge of the optimum does interfere with one's ability to estimate the true discrepancy of the model from the target outcomes, one may still locate the posterior mode(s) of $\boldsymbol{\theta}$ and thereby the optimal settings for the model. However, if λ_δ is too highly overestimated, then MCMC may become trapped in a local mode, leading to convergence problems. In short, while the proposed methodology is forgiving of overestimation of λ_δ, the identifiability of the optimal design region(s) is best served by supplying as informative of a prior as possible.

In situations where one lacks the prior knowledge necessary to select target outcomes near the Pareto front and an accurate prior for λ_δ, an alternative is to use a "preliminary round" of CTO to *estimate* the Pareto front. For example, consider again the univariate

A

I would get rid of this.

this seems repititive

I am not sure if any of this is helpful. Too much speculation it feels like.

I am getting confused with this. In equation 1, you indicate the discrepancy but you do not explain it. Then later you say model is assumed to be accurate and the role of discrepancy will be investigated later. I am fairly puzzled with is sentence.

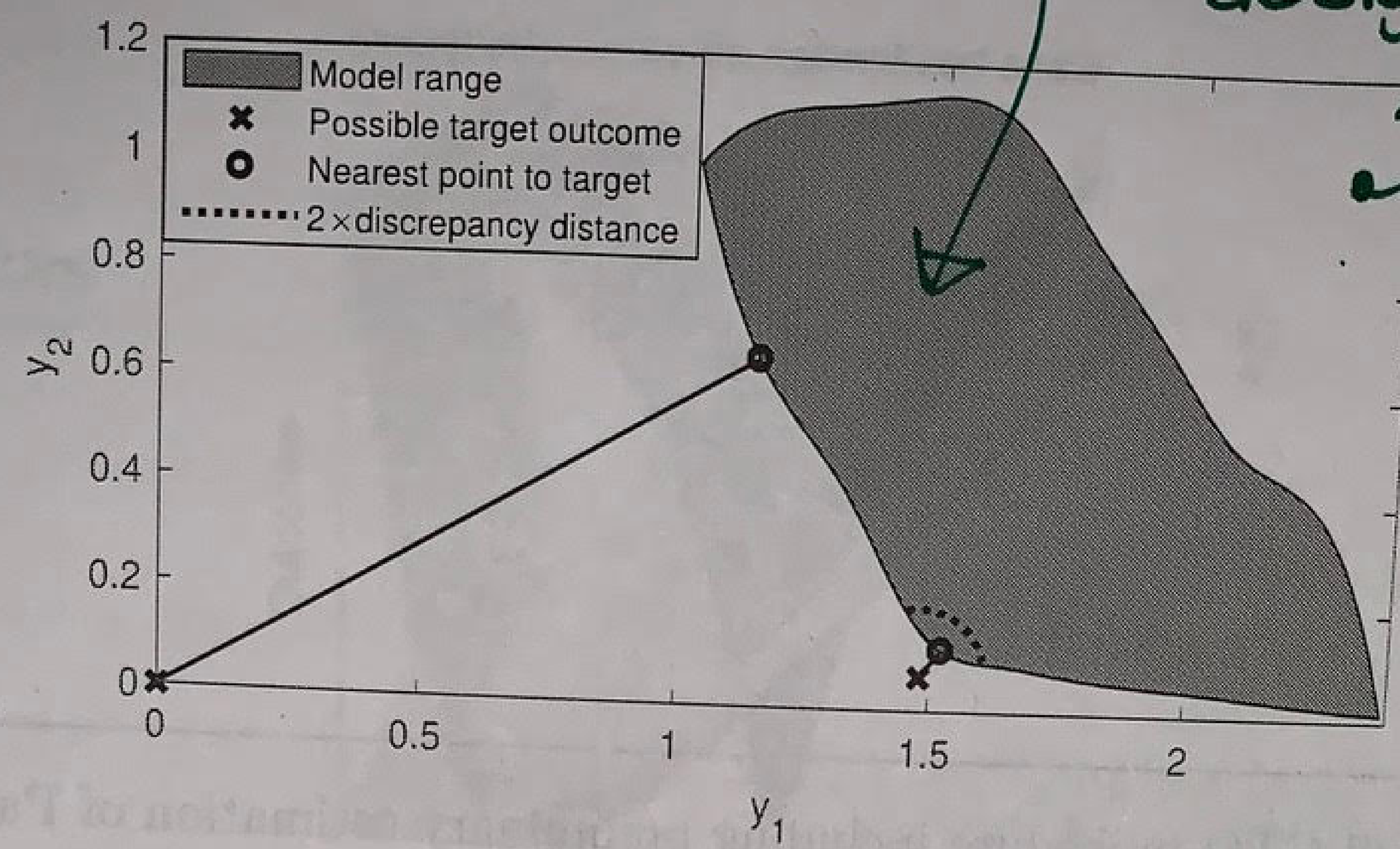
A

there is some more of this in the previous page

I would remove all of this.

case, supposing now that we know only that the optimal output is approximately constant somewhere in the range $(0, 20)$. One could perform CTO directly with constant target outcome below the known model range (e.g., -1) and prior on λ_δ that weakly pulls the posterior predictive distribution toward the lower end of its range (e.g., exponential with rate 2). If the true optimal output turns out to be close to the lower end of its known range, this will likely work well. However, if the optimal output turns out to be sufficiently high, the optimal region of the parameter space could suffer from poor identifiability. To avoid this, one can instead perform CTO still with constant target outcome -1 but with a prior on λ_δ that deliberately exploits the identifiability problems of the Kennedy-O'Hagan framework in order to explore large regions of the parameter space – say, exponential with rate 0.1. Though the resulting posterior distribution will have greater density in the optimal region(s) than would a uniform sampling, it will likely not center in the optimal region, instead covering a larger area of the model range. The resulting posterior predictive distribution can be filtered to retain only its Pareto front, and this can be used as an estimate of the true Pareto front in the vicinity of the target outcome. The preliminary estimate allows one to select a new set of target outcomes that is known to lie near the optimal region, along with an accurate and informative prior on λ_δ that reflects the estimated distance between the new target and the optimal region. Performing CTO with these new targets and prior will result in a posterior distribution that concentrates on the optimal region, and the resulting posterior predictive distribution will allow one to estimate the optimal output with appropriate quantification of the uncertainty. The full CTO process, including preliminary estimation of the Pareto front, is given in Algorithm 1.

this is what is referred to as "design space"



this figure is worth 1000 words. Many of the paragraphs could perhaps be replaced with one helpful figure too.

Figure 1: Two potential choices of target outcomes. The distance from $(0, 0)$ to the farthest point in the model range is only 2 times the distance to the nearest point. By contrast, for the point (1.32,0.065), the dotted line shows the small region of the model range within 2 times the distance to the nearest point.

why 2 times?

An illustration of the benefits of preliminary CTO appears in Figure 1. Suppose that, prior to undertaking CTO, we know only that the model outputs are positive. Then $(0, 0)$ is a natural choice to use as a target outcome. However, in this case, that choice of target outcome will yield three problems. Firstly, the model range is distant from $(0, 0)$. As a result, the optimal region is, relative to the size of the model range, not much closer to the target outcome than other regions of the model range. Indeed, the farthest point in the entire model range is only 2 times farther from $(0, 0)$ than is the nearest point. This leads to very poor identifiability of the optimal region, since large portions of the model range are roughly as close to $(0, 0)$ as is the optimum. Secondly, the optimal region determined by the choice of $(0, 0)$ is somewhat arbitrary. Notice that in this example the entire "left" and "bottom" edges of the model range comprise the Pareto front. The point closest to $(0, 0)$ is

do you mean "design space"?

do we know this for sure?

not intrinsically superior to any other point on the Pareto front. Its uniqueness lies solely in being nearest to the origin, and that choice of target outcome was itself driven merely by our ignorance of the design space ~~model range~~. Thirdly, since we don't know the exact design space ~~model range~~, we are not in a position to set an informative prior for λ_δ. By contrast, suppose now that we have performed preliminary CTO and have available a rough estimate of the Pareto front, empowering us to choose another point as our target outcome – for example, the point $(1.32, 0.065)$ pictured in Figure 1 targets a point of diminishing returns where allowing y_1 to increase further leads to diminishing returns in reducing y_2. Alternatively, one could select $(1, 0.015)$, since this is the minimum of each model output, and thus will optimize to a region minimizing the sum of squared increases in each output over its minimum. Either choice of new target outcome would answer all of the above problems. Firstly, each point is much closer to the model range, leading to greater identifiability. Secondly, these choices of target outcome and resulting optima are not arbitrary, but rather are driven by articulable goals informed by an estimate of the Pareto front. Thirdly, with a rough estimate of the Pareto front we can supply a strong (or even degenerate) prior for λ_δ. Note also that when an emulator is used, a preliminary round of CTO can use the same set of model observations as the subsequent CTO for the training points of the emulator. So performing preliminary CTO does not add to the total budget of model runs, and can thus be a computationally cheap supplement to CTO.

We initially set the target outcomes to $(0, 0, 0)$, constant as a function of x. We then estimated the Pareto front via a preliminary round of CTO with $\lambda_\delta \sim \text{Exp}(1)$ in order to estimate the standardized distance of the target outcome from the Pareto front. We filtered the resulting posterior predictive distribution to retain only the Pareto optimal points. Rescaling so that each model output y is replaced with $y^* = (y - \mathbb{E}(y))/\sqrt{\mathbb{V}(y)}$, the distance from the Pareto front to the target outcome is 16 units. This is large compared to the size of the design space ~~model range~~, at roughly four times its diameter. As a result, the use of $(0, 0, 0)$ as a target outcome would lead to poor identifiability of the optimal region. ~~This is because the target outcome is approximately the same distance from any point in the~~ design space ~~model range, relative to the distance from the target outcome to the optimal region. Therefore in order~~ To ~~to~~ improve identifiability of the optimal region, we updated the target outcome to lie along the line connecting the original target outcome to the nearest point of the estimated Pareto front, but now closer to the latter. We chose a distance of one unit away, as this is roughly the sample standard deviation of the distances from each model output to the sample mean. We thereby approach the estimated Pareto front closely (relative to the size of the model range) while remaining confident that the new target outcome of $(0.71, 0.71, 17.92)$ still outperforms the true Pareto front. This confidence is based on the observation that $F(\mathbf{x} - (0.71, 0.71, 17.92)^T) \geq 0.95$, where $\mathbf{x}$ is the nearest point of the estimated Pareto front and F is the cdf of the tolerance $\epsilon \sim \mathcal{N}(\mathbf{0}, 0.05I)$. We then set the marginal precision of the discrepancy function $\lambda_\delta = 1$ for subsequent CTO, corresponding to a degenerate prior informed by the estimated distance of the new target outcome from the Pareto front. For comparison, we also performed CTO directly, without the use of preliminary CTO. To

too much repetition

do so, we used our original target outcome of $(0, 0, 0)$ with a Gamma(10,10) prior deliberately overestimating λ_δ. Notice that although the Gamma prior from direct CTO and the degenerate prior $\lambda_\delta = 1$ from full CTO have the same means, this is an overestimation only in the case of direct CTO, since the two posterior explorations used different target outcomes. Figure 3 shows the resulting posterior distributions of the two design procedures, including the marginal distributions of the design variables. The marginals in each case show substantial Bayesian learning compared to the prior (uniform) distribution of the design variables. CTO successfully maps the contours of the optimal region in each of the two cases, and peaks near the true optimum. However, the benefits of preliminary CTO are apparent in the greater spread of the posterior distribution from direct CTO. The marginals are much more sharply peaked after using preliminary CTO, with much lighter tails. Thus relying on an estimate of the Pareto front when selecting target outcomes for CTO can greatly reduce uncertainty about the optimal settings for $\boldsymbol{\theta}$ and for the resulting performance and cost outcomes for the system. This simulation example illustrates that CTO can be used directly with little foreknowledge of a system's Pareto front, but that greater identifiability of the optimal region can be achieved using preliminary CTO.

I feel like the discussion section in this paper is overly convoluted. May be do the following A) Present the results in Fig 3A. and avoid any discussion about knowing the realistic Targets

4 Application

In this section we apply our proposed approach toward designing a material to be used in a wind turbine blade of fixed geometry. The goal is to wed the typically separate tasks of material selection and material design, thereby designing a composite material to optimize performance in a turbine blade. Our computer model here uses ANSYS finite element analysis

B) And then add a seperate sub section with the methodology section to articulate how much better the results could become if the targets are realistic. Then show Fig. 3B

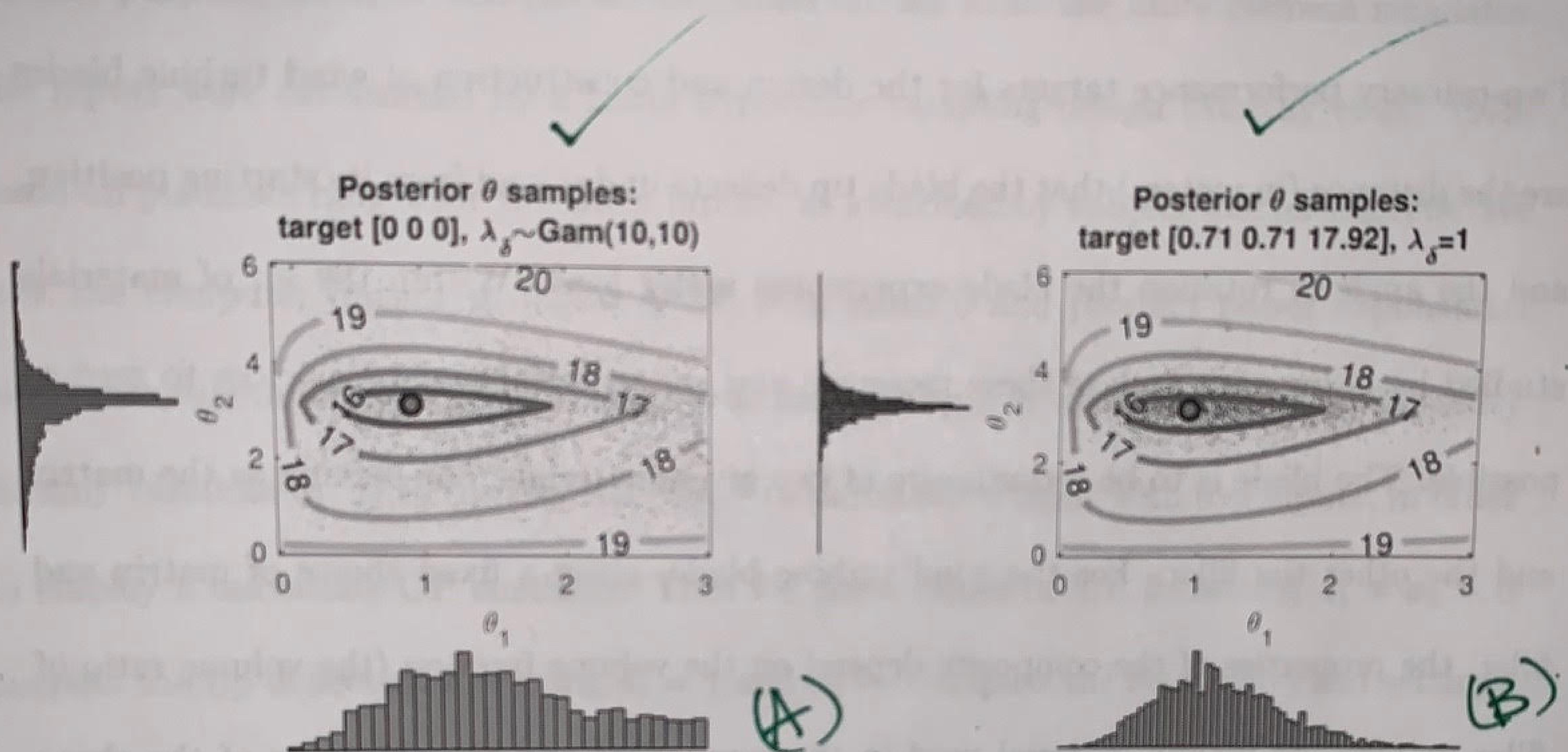


Figure 3: Posterior draws from CTO in the simulated example both without and with the use of preliminary CTO. The contours show, for each point in the design space, the Euclidean distance of the model output at that point from the original target outcome (0,0,0), averaged across the control input range [1.95, 2.05]. The large dot shows the true optimum.

software (ANSYS, Inc., 2017). It is important to observe that we assume the finite element model is an accurate representation of reality.

4.1 ~~Project background~~ Wind Turbine Blade Design

Two primary performance targets for the design and construction of wind turbine blades are the blade tip deflection ~~distance (in meters) that the blade tip deflects under load from its starting position~~, and the angle of twist? rotation ~~the blade experiences under load~~. ~~Within the set of materials studied here, we want each of~~ Herein, the objective/goal of engineering design is to keep these measures and the material cost be as ~~close to zero~~ small as possible. The blade is to be a composite of two given materials, one serving as the matrix and the other the filler. For the wind turbine blade, given a fixed choice of matrix and filler, the properties of the composite depend on the volume fraction (the volume ratio of filler material to matrix material used in the composite) and the thickness of the shear web used in the blade. The resulting material properties impact the performance of the blade, as well as its cost per square meter. The finite element model of the blade takes as inputs a triplet (h, v, k), where h is the operating temperature of the wind turbine (in kelvin), v is the volume fraction of the material, and k is the thickness of the material (in mm). The output of the model is the triplet (d, r, c), where d is tip deflection (in meters), r is rotation (in radians), and c is cost per square meter (USD) to construct the material. The wind turbine ~~should be capable of~~ is deemed to operating over the range of temperatures 230K-330K.

maybe a schematic of a wind blade will help?

not sure what area you are referring to here. It is more common to use unit length.

The temperature affects the composite material properties and hence the blade tip deflection and angle of twist.

something along those lines

4.2 Emulation of finite element model

The finite element simulator is too computationally expensive to be suitable for direct use in an MCMC routine. We employed a GP emulator in the manner of Williams et al. (2006). For this purpose, we drew 500 (trivariate) observations from the finite element simulator. The inputs were determined by a Latin hypercube sampling design (McKay et al., 1979) based on plausible ranges for the three inputs, as identified by subject matter experts. We took the computer output to follow a GP with mean 0 and product power exponential covariance function as given in (2). Since the model output is trivariate, we use two binary dummy variables a_1, a_2 to convert the model to univariate output with five inputs, in order to employ a univariate GP emulator. Thus for given values of h, v, k: setting $a_1 = a_2 = 0$ outputs the tip deflection d, setting $a_1 = 1$ and $a_2 = 0$ outputs the rotation r, and settings $a_1 = 0$ and $a_2 = 1$ outputs the cost c.

are these ranges disclosed in the paper?

I dont understand. Why not use a multivariate GP instead?

The hyperparameters λ_η, β^η ~~must be~~ are estimated to plug in to the prior. ~~To avoid our estimates being biased by the influence of the target outcomes, we estimated them prior to the design stage~~ via maximum likelihood using only the finite element model output. We used `fmincon()` (MATLAB, 2017) to maximize (with $\mathcal{D} = \eta$) over the joint (six-dimensional) support of β^η, λ_η. The result is that, following the form of Equation (2) with $p = 3$, $q = 2$, and $(x_1, x_2, x_3, t_1, t_2) = (a_1, a_2, h, v, k)$, we have $\hat{\lambda}_\eta = 0.0152$ and $\hat{\rho}^\eta = (0.9358, 0.6509, 0.6736, 0.4797, 0.9673)$, where $\rho_k^\eta = \exp(-\beta_k^\eta/4)$.

~~why not~~

OK!

4.3 Design of the wind turbine blade system

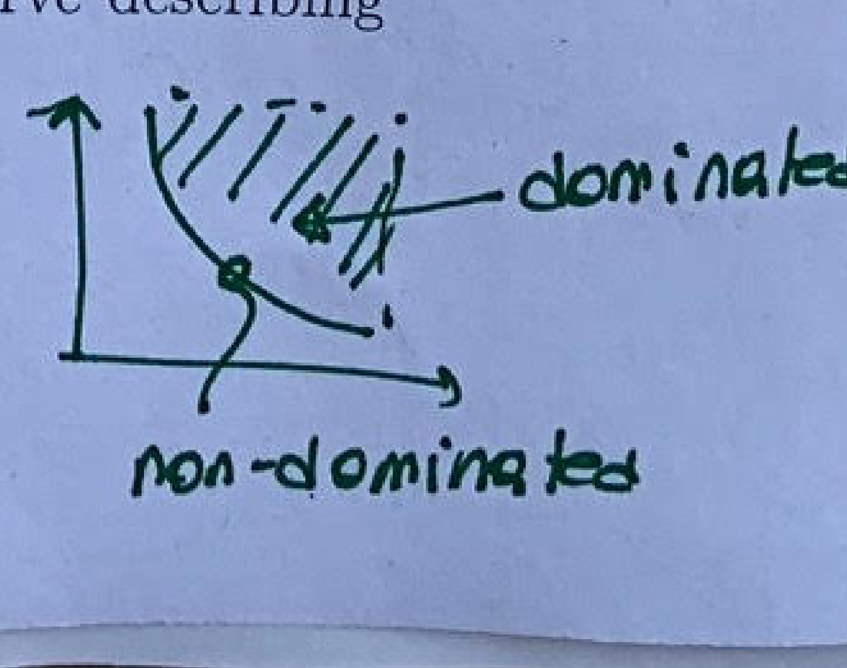
All model inputs were rescaled to [0,1]. All model outputs were standardized so that each of the three simulation responses has mean 0 and standard deviation 1. The full joint posterior density of the design variables and discrepancy function hyperparameters is given in Equation (3), using the MLEs given above.

The initial target outcomes were set to $(0, 0, 0)$ on the original scale, constant as a function of temperature, on an evenly-spaced grid of temperature values over the range [230K, 330K]. We carried out a preliminary round of CTO with an Exp(5) prior on λ_δ, in order to estimate the Pareto front and update the target outcomes to lie close to the Pareto front and thereby improve identifiability of the optimal region. For this purpose, a total of 2,000 Markov chain realizations were drawn via Metropolis-Hastings-within-Gibbs MCMC (Metropolis et al., 1953; Hastings, 1970; Geman and Geman, 1984) in each of three chains (with random starts), of which the first 1,000 draws were discarded as burn-in. During the burn-in period, the covariances of the proposal distributions were periodically adjusted for optimal acceptance rates of around 23% for the multivariate $\boldsymbol{\theta}$ and ρ^δ (Roberts et al., 1997) and 44% for the scalar λ_δ (Gelman et al., 2013, p. 296) using the sample covariance of the preceding draws. Convergence of the three chains was verified visually and by the Gelman-Rubin statistic (≈ 1.01; Gelman and Rubin, 1992). As expected for the preliminary round of CTO, the posterior distribution of $\boldsymbol{\theta}$ was quite diffuse. We used the GP emulator to predict the model output for each realization of $\boldsymbol{\theta}$. Figure 4 displays the estimated Pareto front after filtering the posterior predictions. Though the model range is three-dimensional, the Pareto front appears to be a roughly coplanar curve describing

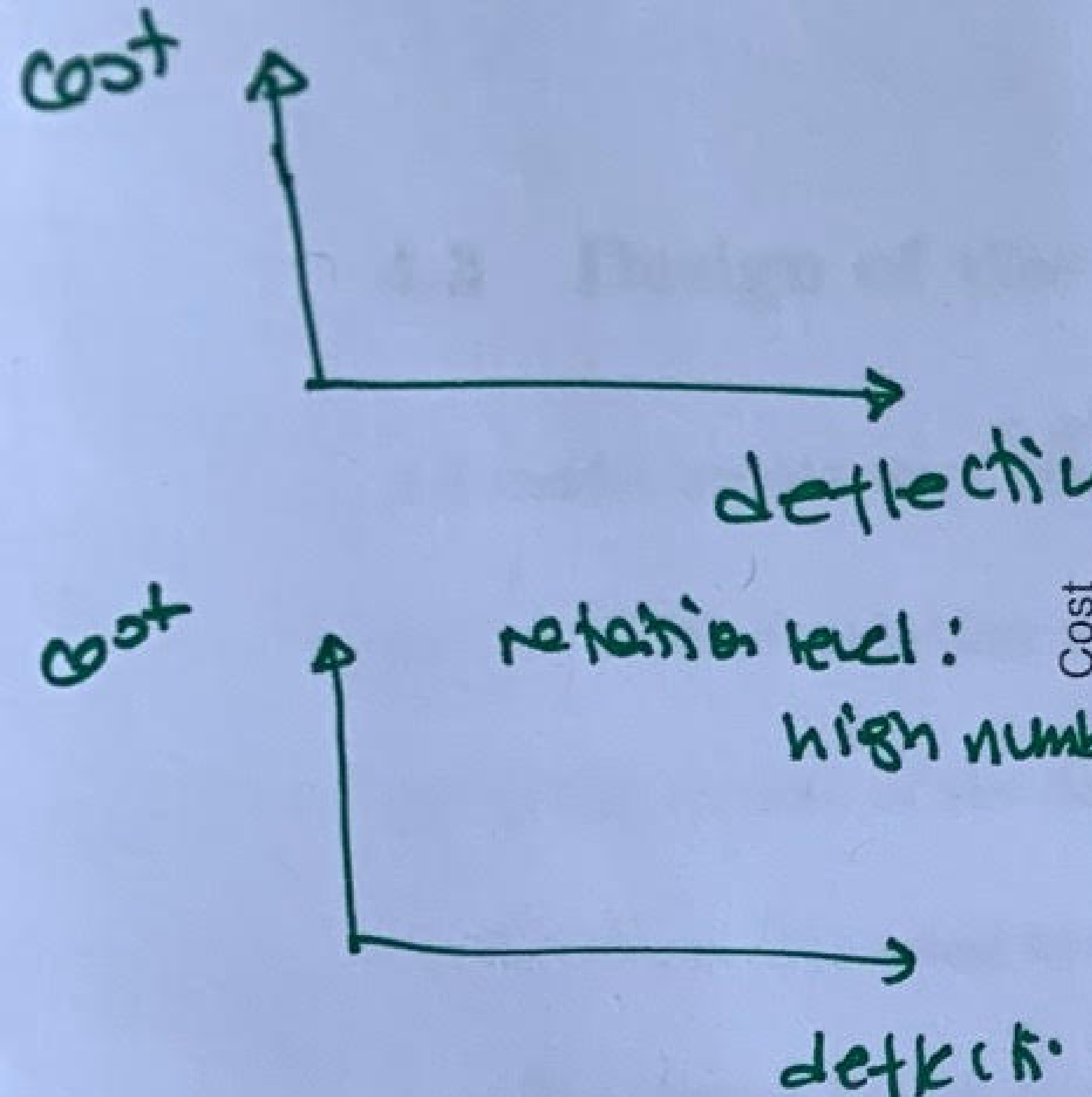
e^5?

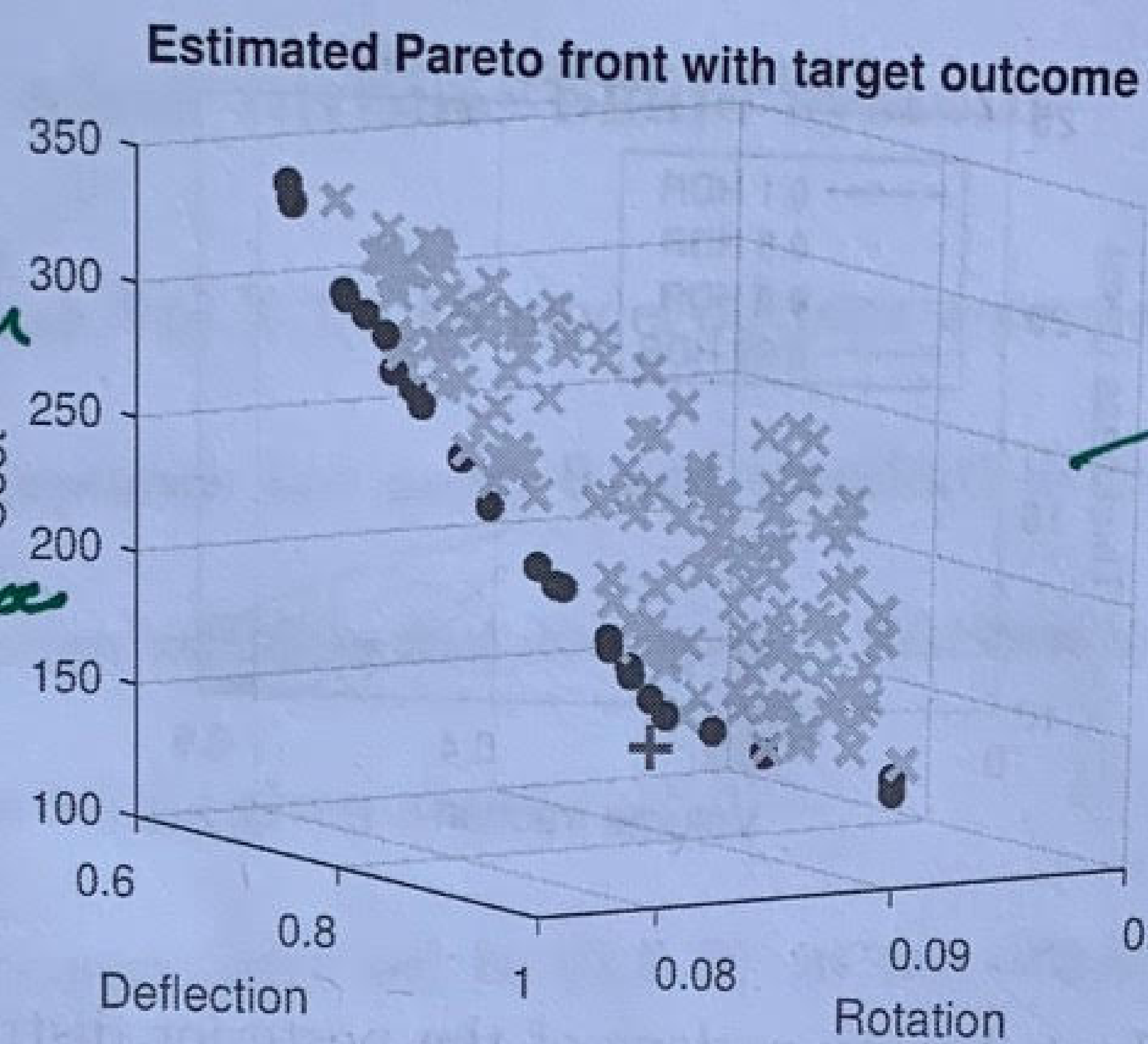
design space

what do you mea filteing? like " filteing out dominated pofomace predictios" ?



rotation level: low number here





in multi-objective design, it is very common to plot slices. so maybe pick 2 different cost levels and plot deflection versus rotation. OR pick a rotation level and plot cost versus deflection

also known as "dominated design"

Figure 4: Each x represents a non-Pareto optimal ~~point~~ design? drawn from the predictive distribution through preliminary CTO in the wind turbine design application. The dots indicate the estimated Pareto front. The plus sign is the target selected as the performance objective in our proposed design approach.

a trade-off in which reduced cost is achieved by allowing higher deflection and rotation. We see a distinct point of maximum curvature in the Pareto front. This location seems

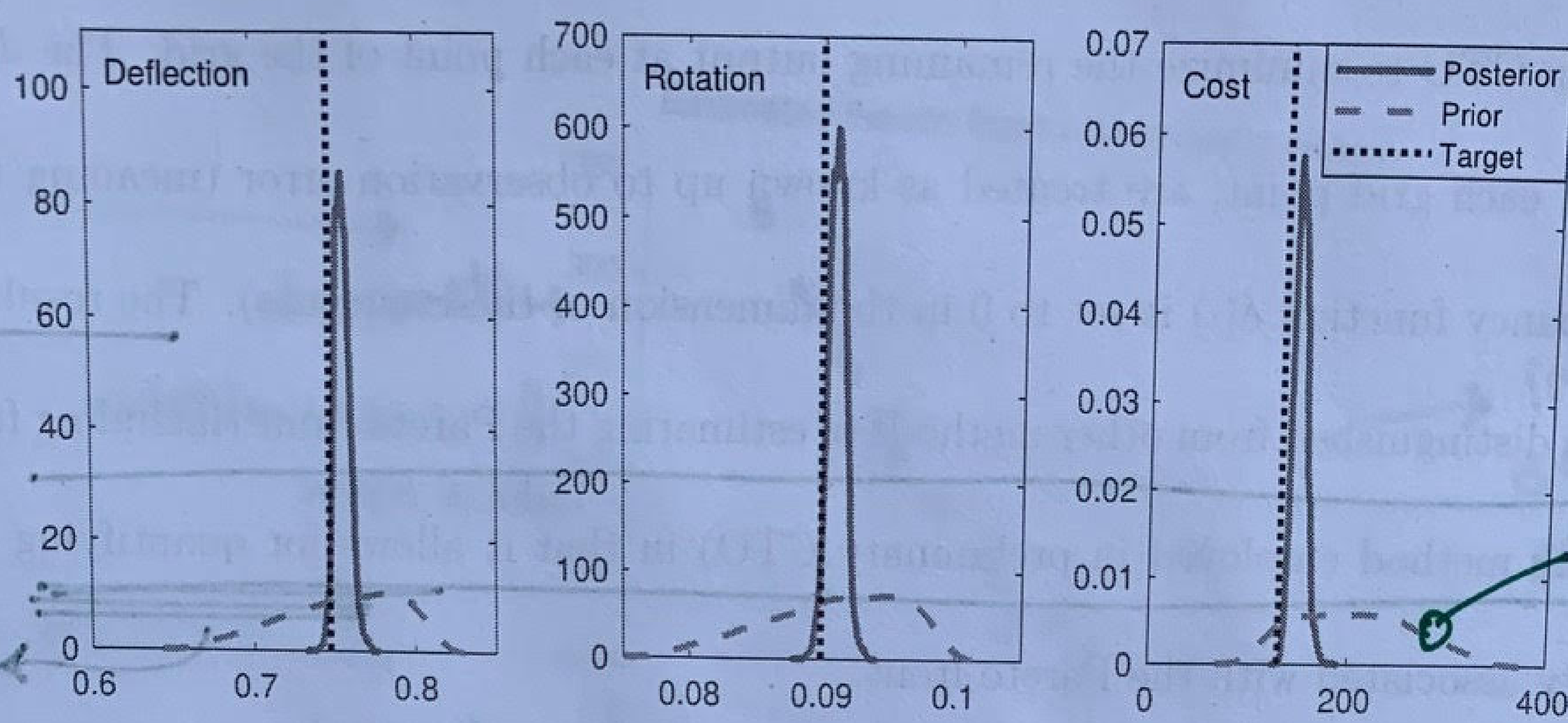
you mean the "knee point"! Not sure what point you are referring to.

to represent a point of diminishing returns in the tradeoff between performance and cost, and thus we selected this point as the target region for design. To do so, we set the point (deflection = 0.75m, rotation = 0.09 rad, cost = \$130.34) as the target outcome,

how did you calculate cost? it was not explained. Details of the FE model are missing too. We should at least refer to one of our earlier papers OR to Evan's recent paper (not submitted).

constant as a function of temperature. Based on the estimated Pareto front, the target outcome is approximately 0.2 units away on the standardized scale. Therefore, we set $\lambda_\delta = 1/0.2^2 = 25$.

In the subsequent CTO step, we employed the same MCMC approach as in the preliminary round, except that λ_δ was now fixed. The marginal posterior distribution of the design variables is shown in Figure 5 as contours of highest density regions. The contrast of



how was the prior obtained? It is not a uniform distribution.

Figure 6: Approximate prior and posterior marginal predictive densities for each of the three model outputs. Note that it is to be expected that the posteriors peak near the target (and not on it), since the target was intentionally chosen to lie outside the ~~model~~ range. feasible design space.

4.4 Pareto front estimation with uncertainties?

Goal is to reduce deflection and cost. It is very clear.

~~Often in the case of a system with multivariate output, one might not antecedently have a clear goal for design. All else being equal,~~ When ~~all outputs~~ multiple design targets are to be minimized, any point in the Pareto front is optimal relative to some set of priorities. If those priorities have not been explicitly determined prior to the design process, then no particular outcome can be targeted. ~~In determining one's priorities, it is helpful to know the Pareto front of the relevant system.~~ For example, in a system where quality is monotonically increasing in cost, depending on one's tolerance for high cost, any point in the model range might be optimal. In low-dimensional cases, CTO may be used to achieve a holistic picture of the Pareto front by optimizing to each target outcome on a grid. To do this, where the model output is $d-$dimensional, one may draw a grid over the range of $d-1$ of the model outputs

*MAYBE EXPLAIN THE IMPORTANCE OF KNOWING THE UNCERTAINTIES IN PARETO FRONT

What does this mean? are you referring to "performance"?

did you not say this already before? I would remove why is it important to retain the information about uncertainties in Pareto front?

and perform CTO to minimize the remaining output at each point of the grid. The $d-1$ outputs, at each grid point, are treated as known up to observation error (meaning that the discrepancy function $\delta(\cdot)$ is set to 0 in the dimension of these outputs). The resulting estimate is distinguished from other methods of estimating the Pareto front (including from the filtering method employed in preliminary CTO) in that it allows for quantifying the uncertainty associated with the Pareto front.

is this the only way to retain UQ information about the Pareto Front? I did not think so.

Our proposed procedure is illustrated here using the wind turbine blade application. For simplicity, rotation has been removed as a model output, leaving a system with 2-dimensional output of deflection and cost. The range of cost is known (via preliminary CTO) to be [\$96, \$352]. A 20-point grid was drawn over this range of costs. For each point c in the cost grid, we used the point (0m, \$c) as the target outcome for calibration (constant with respect to temperature). For each such point, we then updated this initial target outcome to improve identifiability using the rough estimate of the Pareto front from preliminary CTO using target outcome (0m, \$0). Note that only one round of preliminary CTO was needed for this purpose, rather than a separate instance at each grid point.

these numbers are not helpful since I dont even know how they were calculated.

The result of the strategy is to provide an estimate of the response surface with included uncertainty quantification describing, for each point in the grid, the optimal ? achievable outcome for the output not included in the grid. This enables a decision-maker to visualize the space of desirable possibilities with associated uncertaint~~y metrics~~ies. ~~They can do so without the need for rigorously predetermining their exact priorities for weighing gains in each of the outputs against one another~~. The result of applying this strategy to the wind turbine blade application is shown in Figure 7. The lefthand plot shows that the

why is it important to know these uncertainties?

where is the uncertainty originating from? not explained.

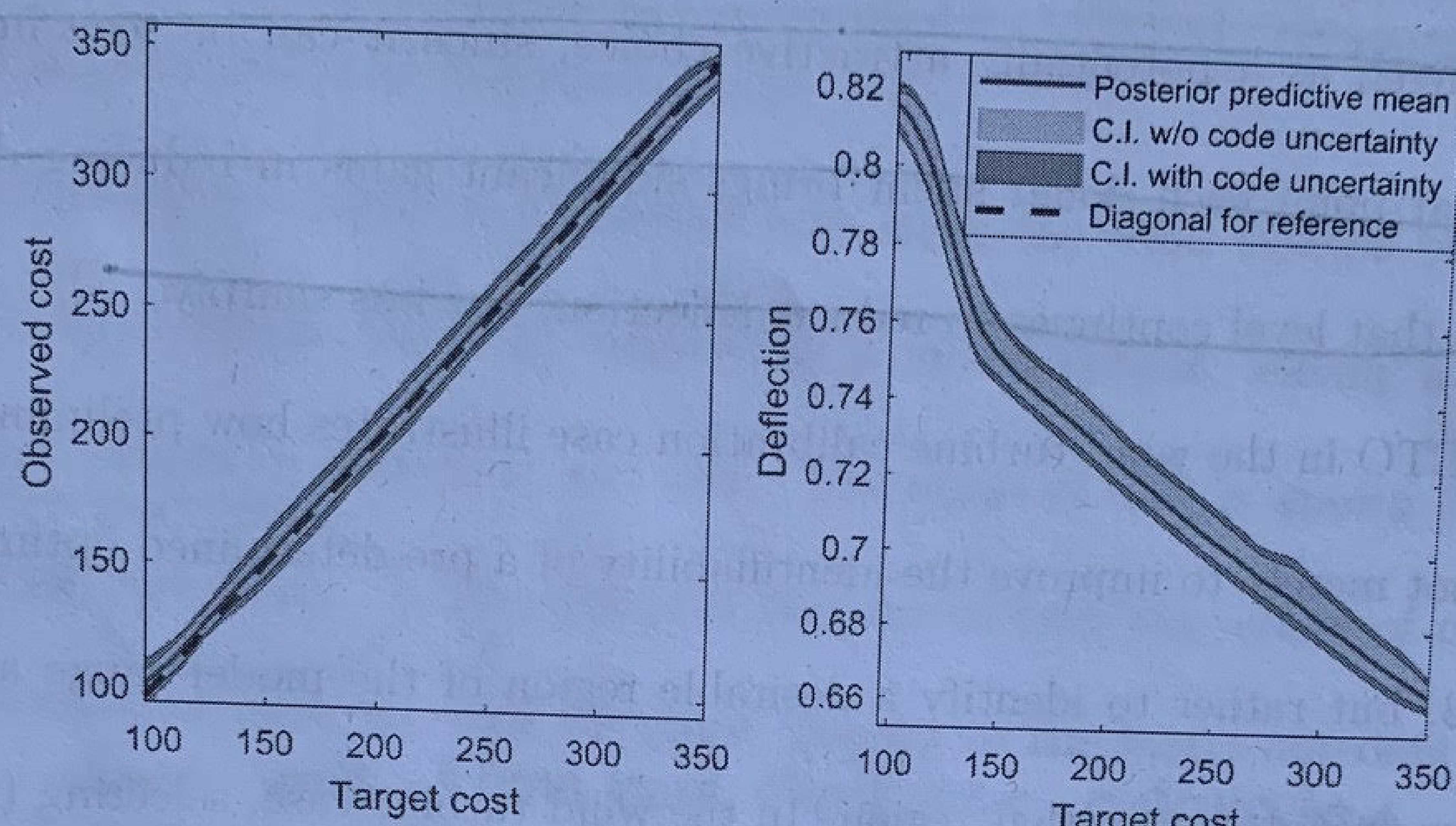


Figure 7: The lefthand plot shows the posterior predictive distribution of cost as a function of target cost, verifying that the ~~calibration~~ design process achieved the ~~“known”~~ target costs up to small error. The righthand plot shows the posterior predictive distribution of ~~optimal~~ deflection as a function of target cost, and therefore is an estimate of the Pareto front for the system with attendant uncertainty quantification.

minumum achieved?

minimum deflection achieved through design?

posterior model predictions respected the target ~~"known"~~ cost values used in the design process. The Pareto front for the system, along with associated uncertainty bands, appears in the righthand plot. ~~This plot visualizes a distribution on the optimal performance outcome for any cost that a decision maker might select as a budget for production, which would be helpful when selecting a budget. For example, the point of maximum curvature around \$140 manifests itself as a potentially attractive choice, since it can be seen in the plot that prior to that point each dollar spent brings significant gains in reducing deflection. Spending above that level continues to reduce deflection, but less sharply.~~

The use of CTO in the wind turbine calibration case illustrates how preliminary CTO may be used, not merely to improve the identifiability of a pre-determined optimal region as in Section 3, but rather to identify a desirable region of the model range and select target outcomes that design to that region. In the wind turbine case, selecting $(0, 0, 0)$ as one's target determines the optimal region to be the high-cost region toward the upper-left of Figure 4, since (on the standardized scale of model outputs) that region happens to be closest to the target. If one has substantive goals that drive one to select that target, then one is well-served by optimizing to that high-cost region. But if the target $(0, 0, 0)$ is chosen arbitrarily, then the resulting optimal region is itself determined arbitrarily. The estimate of the Pareto front provided by preliminary CTO allows us to identify regions of special interest, and to select target outcomes that that lead to clearly defined designs, as illustrated in Figure 4. The use of CTO in this case also demonstrates the value of obtaining a posterior distribution on the design variables, rather than just a point estimate. For example, Figure 5 shows not just that a reasonable point estimate of the optimal $\boldsymbol{\theta}$ is at (.58, 10.2mm), but also that if the volume fraction is lowered to 0.4 it is important to simultaneously raise the thickness to 14mm. More generally, one can see in Figure 5 an indication of the range of $\boldsymbol{\theta}$ values that achieve results near the target, which is potentially useful when one's goal is to set tolerances (rather than a specific value) for $\boldsymbol{\theta}$. Finally, the use of CTO in the wind turbine case illustrates how the method can deliver "Pareto bands", providing not merely an estimate of the Pareto front (as in preliminary CTO) but also uncertainty associated with that estimate. Such an estimate can be of use to decision-makers when deciding on performance goals subject to budgetary constraints.

I suggest we make a point to include this term in the abstract and introduction.

5 Conclusion

We have described how the computer model calibration framework established by Kennedy and O'Hagan (2001) can be adapted to address questions of engineering design. Calibration to target outcomes is a modification of that framework which undertakes design by "calibrating" a computer model not to field observations, but rather to artificial data representing performance and cost ~~goals~~ targets for the system. The procedure optionally includes a computationally cheap preliminary step that provides a rough estimate of the Pareto front, which may be used to select target outcomes that promote strong Bayesian learning. The resulting posterior predictive distribution is induced to approximate the target outcomes, so that the posterior distribution of $\boldsymbol{\theta}$ constitutes a distribution on optimal design settings for the system. Repeated applications of this methodology allow one to construct a thorough estimate of the Pareto front of the system with quantified uncertainties. Unlike other methods of Bayesian optimization (a review of which was provided by Shahriari

because this initial step is "optional," it must be taking out of the general methodology and presented separately as a potential refinement.

et al. 2016), CTO does not require the ability to evaluate model output adaptively. Instead, it can operate using a batch of observations gathered prior to (and independently of) the design process. We described the implementation of this approach in an MCMC routine along with considerations to accommodate computational instability. The use of this methodology is illustrated in the case of material design for a wind turbine blade. We have shown thereby a variety of ways in which CTO can be used to guide decision-makers in the design process. By expropriating established tools of model calibration, CTO offers a method of optimization which is sensitive to, and quantifies, all sources of uncertainty.

what were the sources of uncertainty considered in your application?

The methodology as described here treats the computer model as universally valid over the domain of the design variables. Future work in this area will include the use of a second discrepancy term capturing model bias. That is, while CTO as presented above includes $\delta(\cdot)$ to capture systematic discrepancy between the target outcomes and the true system, it assumes that the computer model is an unbiased estimate of the true system. The inclusion of a second discrepancy term to capture systematic differences between the model and the observed reality would avoid this idealizing assumption. Other possible extensions of our proposed methodology include its application to so-called "state-aware calibration" (Atamturktur and Brown, 2015; Stevens et al., 2018; Brown and Atamturktur, 2018), which would allow the optimal region of the design variables to vary as a function of the control inputs.

SUPPLEMENTARY MATERIAL

Matlab code for CTO: This includes the example model described in Section 3, along with code to perform CTO on that system and thereby reproduce Figure 3.