Supplemental material: Equivalence of primal and saddle point formulations

Central to our proposed methodology is the replacement of the following optimization functional, which we will refer to as the *primal* energy formulation

$$\tilde{E}(U) = E(U) + \sum_{i=1}^{m} \frac{d_i}{2} C_i(U)^2 \tag{1}$$

with an alternative expression that yields the same optimization solution, yet exhibits improved numerical conditioning. In Eq. 1, $U \in \mathbf{R}^n$ is the vector of free parameters that the energy $\tilde{E}$ depends on; in our image deformation problem this include the x- and y-coordinate components of all nodal displacement values, but the methodology detailed here applies to any energy of this form, regardless of application context. The term $E(U)$ is a component of the energy that has favorable (or acceptable) numerical conditioning by design. We will also assume that $E(U)$ is bounded from below and at least locally convex (in the vicinity of the solution of interest). The additional terms $d_1 C_1^2(U), \dots, d_m C_m^2(U)$ are penalty functions corresponding to the constraints $C_i(U) = 0$. A soft constraint would be associated with a low or moderate value of the respective coefficient d_i. A hard constraint would *conceptually* have an infinite penalty coefficient; in practice, a sufficiently high value would have the same effect in Eq. 1. As we will see, the alternative formulation can effectively set such penalty coefficients to infinite values, while remaining well-defined. However, even finite d_i values could lead to detrimental conditioning of $\tilde{E}(U)$ if they are disproportionately large relative to $E(U)$.

Our alternative formulation, which we refer to as the *saddle point* energy reads as follows:

$$\hat{E}(U,p) = E(U) + \sum_{i=1}^{m} \alpha_i p_i C_i(U) - \sum_{i=1}^{m} \frac{\alpha_i^2 p_i^2}{2d_i}. \tag{2}$$

Here, we have introduced a new set of independent variables $p = (p_1, \dots, p_m)$, one for each barrier term C_i. The scalar coefficients $\alpha_1, \dots, \alpha_m$ can be set to any arbitrary value; certain values will confer better numerical properties, but *any* set of values will preserve the equivalence of equations 1 and 2. The claim we will prove is that these two energies attain critical points at locations with matching values of the parameters in U. That is, if U^* is a critical point of Eq. 1, then Eq. 2 has a critical point (U^*, p^*) for some appropriate value of $p = p^*$. Conversely, if (U^*, p^*) is a critical point of the saddle point energy, then U^* is guaranteed to be a critical point of the primal energy. In the general case, we expect that U^* will be a *minimum* for $\tilde{E}$ and (U^*, p^*) will be a saddle point for $\hat{E}$ (due to its negative coefficients for the terms p_i^2), but the proof does not depend on the nature of the critical point.

This claim can be proven by examining the criticality conditions for each energy. For the primal energy to have a critical point at U^* the following must hold:

$$\left.\frac{\partial \tilde{E}}{\partial U}\right|_{U^*} = 0 \Rightarrow \left.\frac{\partial E}{\partial U}\right|_{U^*} + \sum_{i=1}^{m} d_i C_i(U^*) \left.\frac{\partial C_i}{\partial U}\right|_{U^*} = 0. \tag{3}$$

Respectively, for (U^*, p^*) to be a critical point of $\hat{E}$ the following must hold for the gradient with respect to U:

$$\left.\frac{\partial \hat{E}}{\partial U}\right|_{U^*,\, p^*} = 0 \Rightarrow \left.\frac{\partial E}{\partial U}\right|_{U^*} + \sum_{i=1}^{m} \alpha_i p_i^* \left.\frac{\partial C_i}{\partial U}\right|_{U^*} = 0 \tag{4}$$

and, at the same time, the partial derivative with respect to each p_k must be zero, thus:

$$\left.\frac{\partial \hat{E}}{\partial p_k}\right|_{U^*,\, p^*} = 0 \Rightarrow \alpha_k C_k(U^*) - \frac{\alpha_k^2 p_k^*}{d_k} = 0$$

from which we readily obtain:

$$p_i^* = \frac{d_i}{\alpha_i} C_i(U^*). \tag{5}$$

Substituting Eq. 5 into Eq. 4 yields the criticality condition (Eq. 3) for the primal energy. Conversely, if Eq. 3 holds, then by defining p^* in accordance with Eq. 5 will automatically make the remaining criticality condition for the saddle point energy (Eq. 4) hold. This concludes our proof. As a last observation, since the stated equivalence holds for any value of the d_i coefficients, we can consider the limit case of Eq. 2 with $d_i \to \infty$, making the last term converge to zero. By doing this, the saddle-point energy becomes the true Lagrangian of the constrained problem, and the p_i parameters become equivalent to Lagrange multipliers.

A less obvious aspect of this formulation is how the ability of the saddle point energy to maintain the critical points of the primal formulation is unaffected by the specific choice of the free parameters $\alpha_1, \dots, \alpha_m$. By closer examination of Eq. 4 we can see that changing a coefficient α_i to a different value $\hat{\alpha}_i$ would have been simply equivalent to a change of variable $\alpha_i p_i \leftarrow \hat{\alpha}_i \hat{p}_i$ or $p_i \leftarrow (\hat{\alpha}_i/\alpha_i)\hat{p}_i$. Thus, the two different saddle point formulations created with parameter sets α and $\hat{\alpha}$ would still have the property of matching the critical points U^* of the primal respectively) for the auxiliary variables. Since the exact value of these is unrelated to our primary objective of minimizing Eq. 1, we are free to adjust them at will, and we typically do so as to optimize the conditioning of Eq. 2.