Probabilistically Perfect Cloning of Two Pure States: A Geometric Approach

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We solve the long-standing problem of making n perfect clones from m copies of one of two known pure states with minimum failure probability in the general case where the known states have arbitrary a-priori probabilities. The solution emerges from a geometric formulation of the problem. This formulation also reveals a deeper connection between cloning and state discrimination. The convergence of cloning to state discrimination as the number of clones goes to infinity exhibits a phenomenon analogous to a second order phase transition.

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It is impossible to always clone quantum states perfectly [1–3]. This leads to advantages for quantum systems over classical ones in some communications protocols of practical relevance. A common example is stronger security in cryptographic key distribution, with recent works showing more applications [4, 5]. Developments in cloning, including probabilistically perfect [6] and approximate cloning [7–11] provide anchors for better understanding quantum theory as a whole, such as the relationship between the no-cloning and no-signaling theorems [12], and fundamental limits on quantum measurements [14–17]. In particular, cloning's relationship with the fundamental limits of state discrimination will be central to this Letter. For reviews citing recent developments, applications and experiments see [18, 19].

When knowledge of the states' preparation is available, perfect cloning is probabilistically possible. With the first result in probabilistic cloning, Duan and Guo [6] considered the problem of producing perfect clones of linearly-independent pure states and focused on the two state case. They found the maximum average success rate when both states are equally likely, and set this success probability as an upper bound for arbitrary prior probabilities. While other work has been done on this problem, there has until now been no general solution. In this Letter we obtain the general analytic solution and use this to examine cloning's relationship with state discrimination.

There are a number of reasons why one might want to solve the general problem with arbitrary a-priori probabilities. (i) The solution to the equal prior problem is obtained using only symmetry arguments, with no need for optimization. (ii) A general solution would check the robustness of the equal priors case against variations of the prior probabilities around 1/2. This gives control over errors that are unavoidable for any physical realization. (iii) One could consider a discrimination protocol consisting of optimal cloning followed by optimal Unambiguous

Discrimination (UD) of the produced clones, which we will call "discrimination by cloning." Surprisingly this is optimal for equal a-priori probabilities and for any number of clones (see below). This suggests that the equalpriors case is very special and can provide a deceptive view of cloning. (iv) In the limit of infinitely many clones, the optimal strategy prepares the clones according to the outcomes of UD of the input states. This is a particular case of a "measure and prepare" protocol, which we will call "cloning by discrimination." Since the UD measurement varies over the range of prior probabilities (a 3-outcome generalized measurement vs a 2-outcome projective measurement), this hints at a similar situation for optimal cloning that can only be revealed by solving the general problem.

Our solution shows that discrimination by cloning as outlined in (iii) is sub-optimal for unequal prior probabilities (unless one state is never sent). This indicates that the equal prior case is not representative of state dependent cloning. Additionally, contrary to the suggestions in (iv) above, our solution leads to a failure probability that is a smooth function of the priors. However, the strategy converges to cloning by discrimination as $n \to \infty$, implying a discontinuous second derivative and revealing a phenomenon similar to a second order phase transition.

We can imagine a state dependent probabilistic cloner as a machine with an input port, an output port and two flags that herald the success or failure of cloning. The input $|\psi_i^m\rangle = |\psi_i\rangle^{\otimes m}$, i=1,2 (m identical copies of either $|\psi_1\rangle$ or $|\psi_2\rangle$) is fed through the input port for processing. In case of success n perfect clones $|\psi_i^n\rangle = |\psi_i\rangle^{\otimes n}$ are delivered through the output port with conditioned probability p_i . Otherwise, the output is in a refuse state. Conditioned to the input state being $|\psi_i^m\rangle$, the failure probability is $q_i = 1 - p_i$.

For cloning, optimality is usually addressed from a Bayesian viewpoint that assumes the states to be cloned

are given with some a-priori probabilities η_1 and η_2 , $\eta_1 + \eta_2 = 1$. Then a natural cost function for our probabilistic machines is given by the averaged failure probability

$$Q = \eta_1 q_1 + \eta_2 q_2. \tag{1}$$

Accordingly, the optimal cloner minimizes the cost function Q. Our aim is to find that optimal cloner and the minimum average failure probability Q_{\min} for arbitrary priors η_1 and η_2 .

In our formulation, similar to that in [6], the Hilbert space $\mathcal{H}^{\otimes m}$ of the original m copies is supplemented by an ancillary space $\mathcal{H}^{\otimes (n-m)} \otimes \mathcal{H}_F$ that accommodates both the additional n-m clones as well as the success/failure flags. Then, a unitary transformation U (time evolution) from $\mathcal{H}^{\otimes m} \otimes \mathcal{H}^{\otimes (n-m)} \otimes \mathcal{H}_F$ onto $\mathcal{H}^{\otimes n} \otimes \mathcal{H}_F$ is defined through [6]

$$U|\psi_i^m\rangle|0\rangle = \sqrt{p_i}|\psi_i^n\rangle|\alpha_i\rangle + \sqrt{q_i}|\Phi\rangle, \quad i = 1, 2.$$
 (2)

Here the ancillas are initialized in a reference state $|0\rangle$. The states of the flag associated with successful cloning $|\alpha_i\rangle$ are constrained to be orthogonal to the refuse state $|\Phi\rangle$ for certainty in the outcomes of the projective measurement on the flag space \mathcal{H}_F . Although for optimal cloning $|\alpha_1\rangle = |\alpha_2\rangle$, we need to consider a more general setup where these two states are different to include the cloning-by-discrimination protocol whereby UD is used to identify the input state and then the clones are prepared accordingly [23]. For UD the success flag states must be distinguishable, so $\langle \alpha_1 | \alpha_2 \rangle = 0$. Taking the inner product of each equation with itself shows that our probabilities are normalized: $p_i + q_i = 1$. Similarly, by taking the product of the two equations in (2), we find the unitarity constraint

$$s^m = \sqrt{p_1 p_2} \, s^n \alpha + \sqrt{q_1 q_2},\tag{3}$$

where the overlaps $s = \langle \psi_1 | \psi_2 \rangle$ and $\alpha = \langle \alpha_1 | \alpha_2 \rangle$ can be chosen to be real valued without any loss of generality. Furthermore, we can choose $0 \le s \le 1$. We note that for optimal cloning one has $\alpha = 1$, whereas $\alpha = 0$ for cloning by discrimination. If Eq. (3) is satisfied, it is not hard to prove that U has a unitary extension on the whole space.

Before attempting to minimize Q, we need to gain geometric insight into the meaning of the unitary constraint. The following points turn out to be important: (a) For fixed s, n and m Eq. (3) defines a class of smooth curves on the unit square $0 \le q_i \le 1$ (e.g., solid, dashed or dotted curves in Fig. 1). (b) All these curves meet at their endpoints, $(1, s^{2m})$ and $(s^{2m}, 1)$. (c) At the endpoints the curves become tangent to the vertical and horizontal lines $q_1 = 1$ and $q_2 = 1$ respectively, provided $\alpha \ne 0$. (d) For $\alpha = 0$ the curve is an arc of the hyperbola $q_1q_2 = s^{2m}$ (dashed line in Fig. 1). (e) Each of these curves and the segments joining their end points

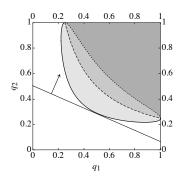


FIG. 1: Unitarity curves in Eq. (3) and the associated sets S_{α} in Eq. (4) for values of α positive (solid/light gray), zero (dashed/medium gray), and negative (dotted/dark gray). The figure also shows the optimal straight segment $Q = \eta_1 q_1 + \eta_2 q_2$ and its normal vector (η_1, η_2) . Plotted for s = 0.5, m = 1, n = 2, $\alpha = 0.8$, 0, -0.8.

with the vertex (1,1) are the boundary of the sets (any of the gray regions in Fig. 1)

$$S_{\alpha} = \{ (q_1, q_2) : \sqrt{p_1 p_2} \, s^n \alpha + \sqrt{q_1 q_2} - s^m \ge 0 \}. \tag{4}$$

They satisfy $S_{\alpha} \subset S_{\alpha'}$ if $\alpha < \alpha'$. (f) Moreover, the sets S_{α} are convex if $\alpha \geq 0$. In particular S_1 is convex.

At this point a geometrical picture of the optimization problem emerges (See Fig. 1). Eq. (1) defines a straight segment on the square $0 \le q_i \le 1$ with a normal vector in the first quadrant parallel to (η_1, η_2) . For fixed apriori probabilities, the average failure probability Q is proportional to the distance from this segment to the origin (0,0). Since S_1 is convex and the stretch of its boundary given by Eq. (3) with $\alpha = 1$ is smooth, a unique point (q_1, q_2) of tangency with the segment (1) exists for any value of the priors and finite n. It gives Q_{\min} and defines the optimal cloning strategy.

We note in passing that the inclusion hierarchy of the sets S_{α} provides a simple geometrical proof that $\alpha = 1$, i.e., $|\alpha_1\rangle = |\alpha_2\rangle$, is indeed the optimal choice. On the other hand, we recall that for cloning by discrimination we have $\langle \alpha_1 | \alpha_2 \rangle = \alpha = 0$ (or $p_i = 0$). From points (b) and (c) above, it follows that for any finite n and arbitrary priors η_1 and η_2 this protocol is strictly suboptimal, i.e., $Q_{\min} < Q_{\text{UD}}$, where the subscript "UD" is a reminder that the failure rate of cloning by discrimination is that of UD. One could say that optimal cloning is incompatible with discerning the identity of the input states for any finite number of clones. However, optimal cloning and UD become one and the same in the limit $n\to\infty$, where $s^n\to 0$ and the curve (3) collapses to the hyperbola $q_1q_2 = s^{2m}$, as it does for $\alpha = 0$. We will come back to this point below.

A more quantitative analysis requires finding a convenient parametrization of the curve (3). To this end, simpler and more manageable expressions are derived if the symmetry under $q_1 \leftrightarrow q_2$ is preserved. We write

 $\sqrt{q_i} = \sin \theta_i$ for $0 \le \theta_i \le \pi/2$. By further introducing the variables $x = \cos(\theta_1 + \theta_2)$ and $y = \cos(\theta_1 - \theta_2)$ we manage to linearize the constraint (3), which now reads as $2s^m = (1+s^n)y - (1-s^n)x$. A natural parametrization for this straight line is given by

$$x = \frac{1 - (1 + s^n)t}{s^{n-m}}, \qquad y = \frac{1 - (1 - s^n)t}{s^{n-m}}, \tag{5}$$

where again we have taken the most symmetrical choice. Because of the symmetry of this procedure, the parameters x and y are invariant under $q_1 \leftrightarrow q_2$ (equivalently, under $\theta_1 \leftrightarrow \theta_2$). Thus, the two mirror halves of the curve (3) under this transformation are mapped into the same straight line (5). By expressing q_i as a function of t only half of the original curve is recovered. The other half is trivially obtained by applying $q_1 \leftrightarrow q_2$.

The allowed domain of t in Eq. (5) follows from that of x and y, readily seen from their definition to be the region $|x| \le y \le 1$. Hence, we have

$$\frac{1-s^{n-m}}{1-s^n} \le t \le 1. \tag{6}$$

After putting the various pieces together one can easily get rid of the trigonometric functions and express Eq. (3) in parametric form as

$$q_i = \frac{1 - xy - (-1)^i \sqrt{1 - x^2} \sqrt{1 - y^2}}{2}, \quad i = 1, 2.$$
 (7)

Fig. 2 shows examples of the unitary curve (3) for (a) n=2 and (b) n=5. In both cases m=1. For larger n=1 the curves closely approximate the hyperbolae $q_1q_2=s^{2m}$ (dashed lines) for small and moderate values of s, while for s close to one the hyperbolas remain closer to the vertex (1,1), but still retain the same end points. As mentioned previously, in the limit $n\to\infty$ all curves become hyperbolic.

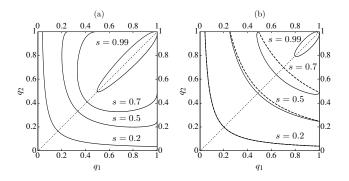


FIG. 2: Unitarity curves for different values of s and for (a) $m=1,\ n=2$ and (b) $m=1,\ n=5$. The curves are symmetric under mirror reflexion along the (dotted) straight line $q_1=q_2$, i.e., under the transformation $q_1\leftrightarrow q_2$. The dashed lines in (b) are the hyperbolae $q_1q_2=s^{2m}$.

Now we can return to the minimization of the average failure probability Q. Despite the apparent simplicity

of the problem, finding the minimum Q as an explicit function of η_1 or η_2 involves solving a quartic equation without a simple form [24]. Instead, we will derive the parametric equation of the curve (η_1, Q_{\min}) . This, along with our complete description of the unitary curve (3), provides a full account of the solution.

Without any loss of generality we may assume that $\eta_1 \leq \eta_2$, or equivalently, that $0 \leq \eta_1 \leq 1/2$. Then the slope of the vector normal to the straight line (1) is less or equal to one and thus it can only become tangent to the lower half of the unitary curve (3) (see Fig. 2). The slope of this lower half increases monotonically as we move away from the line $q_1 = q_2$, where it has the value -1, and vanishes before we reach the line $q_1 = 1$. This follows from the properties (a)–(f) above and can be checked using Eq. (7). The values of t at which the slope is -1 and 0 are respectively

$$t_{-1} = \frac{1 - s^{n-m}}{1 - s^n}, \quad t_0 = \frac{1 - s^{2(n-m)}}{1 - s^{2n}},$$
 (8)

where we note that t_{-1} is the lower value of the range of t in Eq. (6). For any point $(q_1(t), q_2(t))$ with $t \in [t_{-1}, t_0]$ there is a line $Q = \eta_1 q_1 + \eta_2 q_2$ that is tangent to it, starting with $\eta_1 = \eta_2 = 1/2$ for $t = t_{-1}$ up to $\eta_1 = 0$, $\eta_2 = 1$ for $t = t_0$.

This observation enables us to derive the desired parametric expression for the optimality curve (η_1, Q_{\min}) as follows: for a given t in the range above, a necessary condition for tangency is $\eta_1 q_1' + \eta_2 q_2' = 0$, where $q_i' = dq_i/dt$. In this equation we can solve for η_1 (or η_2) using that $\eta_1 + \eta_2 = 1$. By substituting q_1 and q_2 in Eq. (1) with (7) we enforce contact with the unitarity curve and obtain the expression of Q_{\min} . The final result can be cast as:

$$\eta_1 = \frac{q_2'}{q_2' - q_1'}, \quad Q_{\min} = \frac{q_2' q_1 - q_1' q_2}{q_2' - q_1'}, \quad t_{-1} \le t \le t_0, \quad (9)$$

where t_{-1} , t_0 and q_i are given in Eqs. (8) and (7). The expressions for the derivatives q'_i are

$$q_i' = \frac{\sqrt{q_i(1-q_i)}}{s^{n-m}} \left\{ \frac{1+s^n}{\sqrt{1-x^2}} - (-1)^i \frac{1-s^n}{\sqrt{1-y^2}} \right\}. \quad (10)$$

Fig. 3 shows plots of the curves (η_1, Q_{\min}) for m=1 input copies and (a) n=2 or (b) n=5 clones, as in the previous figure. We see that Q_{\min} is an increasing function of η_1 in the given range [0, 1/2]. The values of Q_{\min} at the end points of this range follow by substituting t_0 and t_{-1} , Eq. (8), into Eq. (7). They are given by

$$Q_0 = q_2(t_0) = \frac{s^{2m} - s^{2n}}{1 - s^{2n}}, \quad Q_{-1} = \frac{s^m - s^n}{1 - s^n},$$
 (11)

where $Q_{\min} = Q_{-1}$ holds for equal priors and $Q_{\min} = Q_0$ for $\eta_1 \to 0$ (i.e., $\eta_2 \to 1$). The dashed lines in Fig. 3 (b)

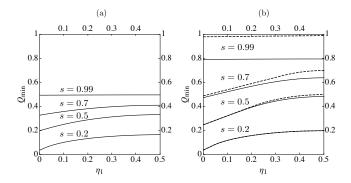


FIG. 3: Minimum cloning failure probability Q_{\min} vs. η_1 (solid lines) and UD failure probability Q_{UD} vs. η_1 (dashed lines) for the same values of m, n and s used in the previous figure.

are the well known piecewise unambiguous discrimination solution [21]:

$$Q_{\text{UD}} = \begin{cases} \eta_1 + s^{2m} \eta_2, & 0 \le \eta_1 \le \frac{s^{2m}}{1 + s^{2m}}; \\ 2\sqrt{\eta_1 \eta_2} s^m, & \frac{s^{2m}}{1 + s^{2m}} \le \eta_1 \le \frac{1}{2}. \end{cases}$$
(12)

It is apparent from these plots that the optimal cloning protocol performs strictly better than cloning by discrimination, as was proved above. However, as the number of produced clones becomes larger the difference in performance reduces. In Fig. 3 (b), for only n=5, a difference is hardly noticeable for $s \leq 0.5$. For larger overlaps it takes larger values of n to get the same level of agreement. As discussed above, in the limit $n \to \infty$ there is perfect agreement for any s < 1.

The complete UD solution in Eq. (12) emerges naturally from our geometrical approach in a straightforward manner: First, we recall that in this case the right hand side of Eq. (3) becomes $q_1q_2 = s^{2m}$ (dashed lines in Figs. 1 and 2). The maximum slopes of these curves are at their end points and all have the value $-s^{2m}$. This implies that the boundary of S_0 has a cusp at $(1, s^{2m})$. It follows that a unique point of tangency with the line (1) exists for $s^{2m} < \eta_1/\eta_2 \le 1$ (recall that we are assuming $\eta_1 \leq 1/2$). This condition gives the η_1 interval for that solution. The tangency condition, $(q_2, q_1) \propto (\eta_1, \eta_2)$, quickly leads us to the optimal failure rate in the second line of Eq. (12). For $s^{2m} > \eta_1/\eta_2 \ge 0$ tangency is not possible, and the optimal line (1) merely touches the cusp on the boundary of S_0 , so the expression of Q becomes the first line of Eq. (12). In geometrical terms, the straight line (1) pivots on the end point as η_1 varies between 0 and $s^{2m}/(1+s^{2m})$.

For the second case in Eq. (12), one has $q_1, p_1 \in (0, 1)$ and there are three orthogonal flag states in Eqs. (2), namely, the two success states $|\alpha_1\rangle$, $|\alpha_2\rangle$, and the failure state $|\Phi\rangle$. This 3-outcome measurement can be rep-

resented by a 3-element positive operator valued measure (POVM) on $\mathcal{H}^{\otimes m}$. For the first line in Eq. (12), $p_1 = 1 - q_1 = 0$, which leads to a 2-outcome projective measurement, as only one success flag state ($|\alpha_2\rangle$) is needed in Eqs. (2).

This two-paragraph derivation of Eq. (12) proves that the convergence of the optimal cloning failure probability Q_{\min} to that of cloning by discrimination, with rate $Q_{\rm UD}$ in Eq. (12), follows from the convergence of the general unitarity curve in Eq. (3) to the hyperbola $q_1q_2 = s^{2m}$, i.e., from $\lim_{\alpha \to 0} S_{\alpha} = S_0$. Interestingly enough, such convergence entails a phenomenon analogous to a second order phase transition. Our geometrical approach shows that the average failure probability $Q_{\min}(\eta_1)$ is an infinitely differentiable function of η_1 for finite n. However, as n goes to infinity (or at $\alpha = 0$, for the sake of this discussion) the limiting function $Q_{\text{UD}}(\eta_1)$ has a discontinuous second derivative. Moreover, the symmetry $q_1 \leftrightarrow q_2$ breaks in the "phase" corresponding to the first line in Eq. (12). A similar phenomenon arises in UD of more than two pure states [22].

It has been argued above that cloning by discrimination is strictly suboptimal (unless $n \to \infty$). One could likewise wonder if discrimination by cloning can be optimal. On heuristic grounds, one should not expect this to be so, as cloning involves a measurement and some information can be drawn from the observed outcome. However, the equal-prior and the $\eta_1 \to 0$ cases provide remarkable exceptions. For both we may write the total failure rate as $Q_{\rm C} + (1 - Q_{\rm C})Q_{\rm UD}$, where C stands for cloning. For $\eta_1 = \eta_2 = 1/2$, Eq. (11) implies $Q_C = Q_{-1}$, in which case the produced n-clone states are equally likely. The UD of these states fails with probability s^n , as follows from Eq. (12) applied to n copies. The total failure rate is then s^m , which is the optimal UD failure rate of the original input states, Eq. (12). If $\eta_1 \to 0$ then only $|\psi_2^n\rangle$ is produced with non-vanishing probability and $Q_{\rm C} = Q_0$. Failure in the second step (UD) is given by the top line in Eq. (12) applied to n copies. The total failure rate is s^{2m} , also achieving optimality.

Using our main result in Eqs. (9), and (7) one can check that these are the only cases where discrimination by cloning is optimal. These are also the only cases where no information gain can be drawn from the cloning measurement. This hints at how special these cases are and justifies the need of the derived solution for arbitrary priors to have a full account of two-state cloning.

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- [23] Likewise, we could consider a more general setup with two refuse states $|\Phi_1\rangle$ and $|\Phi_2\rangle$ in Eqs. (2). This is necessarily sub-optimal since we could probabilistically determine whether we received $|\psi_1\rangle$ or $|\psi_2\rangle$ by applying UD to the refuse states $|\Phi_i\rangle$. Sometimes we would be certain of the input state, when we can always prepare n copies of the state, thereby increasing the overall success rate of the cloning strategy.
- [24] Using the alternative change of variables $u = \sqrt{q_1q_2}$ and $v = (q_1 + q_2)/2$, the unitary constraint, Eq (3), defines a parabola on the u-v plane. Likewise, the failure rate, Eq (1), defines an ellipse with center on the v axis whose eccentricity only depends on η_1 and η_2 . The size of the ellipse and the v coordinate of its center both increase with Q. It follows that Q_{\min} emerges when the ellipse is tangent to the parabola. The intersection of these two conics can be written as a quartic equation.