Information-geometric optimization with natural selection

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Evolutionary algorithms, inspired by natural evolution, aim to optimize difficult objective functions without computing derivatives. Here we detail the relationship between population genetics and evolutionary optimization and formulate a new evolutionary algorithm. Optimization of a continuous objective function is analogous to searching for high fitness phenotypes on a fitness landscape. We summarize how natural selection moves a population along the non-euclidean gradient that is induced by the population on the fitness landscape (the natural gradient). Under normal approximations common in quantitative genetics, we show how selection is related to Newton’s method in optimization. We find that intermediate selection is most informative of the fitness landscape. We describe the generation of new phenotypes and introduce an operator that recombines the whole population to generate variants that preserve normal statistics. Finally, we introduce a proof-of-principle algorithm that combines natural selection, our recombination operator, and an adaptive method to increase selection. Our algorithm is similar to covariance matrix adaptation and natural evolutionary strategies in optimization, and has similar performance. The algorithm is extremely simple in implementation with no matrix inversion or factorization, does not require storing a covariance matrix, and may form the basis of more general model-based optimization algorithms with natural gradient updates.

INTRODUCTION

Finding the optimal parameters of a high dimensional function is a common problem in many fields. We seek protein conformations with minimal free energy in biophysics, the genotypes with maximal fitness in evolution, the parameters of maximum likelihood in statistical inference, and optimal design parameters in countless engineering problems. Often derivatives of the objective function are not available or are too costly, and derivative-free algorithms must be applied.

Evolutionary optimization algorithms (EA) use a population of candidate solutions to generate new candidate solutions for the objective “fitness” function. In particular, genetic algorithms (GA) and evolution strategies (ES) are two classes of EAs most directly inspired by the Wright-Fisher and Moran models from population genetics [1,2]. GAs are initialized with some population of genotypes, representing candidate solutions, and use some form of stochastic reproduction, incorporating a bias known as selection. Among the different selection schemes, fitness-proportionate selection is equivalent to natural selection in population genetics.

Stochasticity of reproduction may be helpful in overcoming local optima, and noise in fitness. In population genetics, stochasticity of reproduction is known as genetic drift, and has the important effect of scaling the strength of selection inversely with the magnitude of stochasticity [2]. Stochasticity also causes the loss of many genotypes, even if they have high fitness. For example in the strong selection weak mutation regime of the Moran model, the probability that a single genotype will sweep a population (fixation) is proportional to its selective advantage, and there is a 99% chance a genotype with a one percent fitness advantage will go extinct [2].

Some form of deterministic selection in optimization is desirable to not waste computational effort, and without stochasticity a population based algorithm will still be robust to noise in fitness since a population effectively integrates information over some region of the fitness landscape. Some ES and GAs use deterministic rank based selection which removes individuals below some threshold. However, such truncation selection is very coarse, and does not affect proportionally the genotypes that survive.

Many population based algorithms, including ES and estimation of distribution algorithms (EDA), are based on drawing a population of candidate solutions from a parameterized distribution \( P(\theta) \) and iteratively updating the parameters \( \theta \). The basic approach is to move the parameters in the direction of the mean fitness: \( \nabla F \). To account for the uncertainty of the parameters many algorithms move the parameters in the direction of the natural gradient \( 1^{-1} \nabla F \), where \( g^{-1} \) is the inverse of the fisher information, which can be estimated from the population. The popular covariance matrix adaptation ES algorithm (CMA-ES) [5,6] and related natural evolution strategies (NES) [7,10] parameterize a population as a normal distribution, and use samples from the distribution to update the mean and covariance with a natural gradient descent step. More generally, natural gradients describe ascent of the fitness landscape in terms of information geometry, and their use characterizes a wide class of information-geometric algorithms [11]. These algorithms differ from GAs and population genetics, in that there are no selection or mutation operators applied directly to individuals in a population.

Here, we point out that the natural gradient used in information-geometric optimization also appears in natural selection. Under normally distributed phenotypes,
As is done in multivariate quantitative genetics, we show how selection is related to Newton’s method in optimization. Then, we describe how intermediate levels of selection are best for optimization, and how mutation and recombination generate new variants without having to explicitly sample from the distribution. Finally, we develop a proof of principle quantitative genetic algorithm (QGA) which combines selection, recombination, and a form of adaptive selection tuning that shrinks the population towards an optimum. In contrast to GAs, QGA has deterministic selection, and compared to CMA-ES and NES, it is much simpler and does not store a covariance matrix.

**NATURAL SELECTION GRADIENT**

We begin by considering a population of infinite size, but with a finite number of unique phenotypes. Each unique variant \( i \) has a continuous multivariate phenotype \( x_i \) (a vector), with frequency \( p_i \) and growth rate, or fitness \( f(x_i) \), independent of time and frequencies. In the context of optimization, phenotypes are candidate solutions, and fitness is the objective function to be maximized. Classical replicator dynamics, leaving out mutation and genetic drift, describe the change in frequencies as

\[
\frac{dp_i}{dt} = p_i (f(x_i) - F),
\]

with mean fitness \( F = \sum_i p_i f(x_i) \). In stochastic descriptions, these dynamics describe the expected changes due to selection.

In the absence of other processes, frequencies can be integrated over time resulting in

\[
p_i(t) = p_i(0) \frac{1}{Z_t} e^{f(x_i) t},
\]

with normalization \( Z_t \) ensuring the probabilities sum to one. At long times, the phenotype distribution will concentrate on high fitness phenotypes until the highest fitness phenotype reaches a frequency of unity. The change in mean fitness equals the fitness variance (Fisher’s theorem), and higher moments evolve as well. As an example we show 100 variants in a quadratic fitness landscape and how their frequencies change over time (Fig. 1).

Remarkably, replicator dynamics can be rewritten in terms of information geometry [12]. Frequencies can be considered as the parameters of a discrete categorical distribution, and selection moves them in the direction of the covariant derivative [13, 14], (also known as the natural gradient [11]),

\[
\frac{dp}{dt} = g^{-1} \nabla_p F,
\]

where \( p \) is the vector of (linearly independent) frequencies, \( \nabla_p F \) is the vector of partial derivatives, and \( g^{-1} \) is the inverse of the fisher information metric of the categorical distribution, which defines distances on the curved manifold of probability distributions (see appendix A). Selection changes the frequencies in the direction of steepest ascent in non-euclidean coordinates defined by the geometry of the manifold of the distribution.

The natural gradient is independent of parameterization, and therefore, if the distribution over \( x \) can be approximated by another distribution, selection will change those parameters in the direction of their natural gradient. This can be demonstrated by projecting onto a normal phenotype distribution, as is assumed in classic multivariate quantitative genetics. The population mean \( \mu \) and population covariance matrix \( \Sigma \) parameterize the distribution, and selection changes the mean as (15, 16, appendix A)

\[
\frac{d\mu}{dt} = \Sigma \nabla_\mu F,
\]

where \( \Sigma^{-1} \) is the associated Fisher information metric. Similarly, the covariance follows a natural gradient with a more complex metric (appendix A). If phenotype covariance reaches zero, then the population is monomorphic and there is no selection. However, an alternative

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**Figure 1.** A) An example of 100 variants in a 2D phenotype space on a quadratic fitness landscape (blue contours). B) Frequencies evolve over time according to eq. (2) with \( t = 0.2 \) (red), \( t = 1 \) (green) and \( t = 5 \) (blue).
population genetics model in the strong selection weak mutation regime can search a fitness landscape with limited diversity, with the mutation covariance matrix serving as a metric (Appendix B).

For a finite amount of time, the frequencies have Boltzmann form and the parameters trace a path on the manifold of distributions following the natural gradient. Exponential weights lead to natural gradient updates and are found in many optimization algorithms beyond GAs, such as simulated and population annealing [17][18]. In contrast, CMA-ES/NES use a population to update the parameters of a normal distribution in a natural gradient step, and do not track frequencies.

**SELECTION AS A SECOND ORDER UPDATE**

To underscore how natural gradients are inherently second order optimization methods, we show how natural selection is related to a second order gradient update when phenotypes are normally distributed. The normal approximation is valid for quadratic fitness landscapes, or when the Taylor expansion of \( f(x) \) around the mean phenotype \( \mu \) to second order is a good approximation. The mean and covariance change as (Appendix B)

\[
\begin{align*}
\mu_t - \mu_0 &= t \Sigma_0 \nabla f \\
\Sigma_t^{-1} - \Sigma_0^{-1} &= t C
\end{align*}
\]

where subscripts indicate dependence on time, \( \nabla f \) are the partial derivatives of \( f(x) \) evaluated at \( \mu_0 \), \( C \) is the curvature, that is the negative of the matrix of second derivatives, evaluated at \( \mu_0 \). The change in mean is a finite natural gradient step, while the covariance aligns itself with the curvature with increasing time. Combining the two equations yields

\[
\mu_t - \mu_0 = \left( \frac{1}{t} \Sigma_0^{-1} + C \right)^{-1} \nabla f. \quad (5)
\]

For large \( t \), \( \mu_t - \mu_0 \to C^{-1} \nabla f \), corresponding to an iteration of Newton’s method, as long as the normal approximation holds (see below). For small and intermediate \( t \), selection functions as a form of regularized Newton’s method, where \( t \) determines how much to weigh the prior, that is the initial distribution. Since \( \Sigma_t \) is always positive-definite, the population cannot converge to a saddle point in fitness, which is possible in Newton’s method.

**INTERMEDIATE SELECTION IS MOST INFORMATIVE**

Natural selection moves the distribution along a manifold shaped by the fitness landscape. However, selection does not introduce any new phenotypes, and reduces diversity by biasing frequencies towards high fitness phenotypes. Diversity can be quantified by population entropy \( S_t = - \sum_i p_i(t) \log p_i(t) \), which summarizes the distribution of frequencies. The exponential of entropy \( K_t = e^{S_t} \) defines an effective number of variants, such that \( 1 \leq K_t \leq K_0 \), and \( K_0 \) is the number unique variants under uniform initial conditions \( p_i(0) = 1/K_0 \). Diversity shrinks rapidly as selection increases, depending on the starting point \( K_0 \) (Fig. 3).

There is an inherent tradeoff in choosing the strength of selection \( t \), in that small \( t \) weakly biases the frequencies towards high fitness, and large \( t \) has a low effective number of variants. If the variants are regarded as samples drawn from an underlying distribution, fewer samples leads to higher error in estimating parameters, such as mean and covariance.

For large \( t \) and small \( K_t \), the normal approximation breaks down, and eqn. 5 does not hold even if fitness is purely quadratic. The breakdown of normality is reflected in the moments of the fitness distribution. The gap between the mean and maximum fitness \( F^* - F \), known as genetic load, shrinks as selection increases, but under normal phenotype distributions, \( F^* - F \to D^2/2 \) where \( D \) is the dimensionality of phenotypes (Appendix C). Fitness has units of \( t^{-1} \), as evident from eqns. 1 and 2. The unit-less approximate scaled load \( t(F^* - F) \) where \( F^* \) is the maximum observed fitness, is zero when mean fitness approaches the maximum, and reaches a peak around some intermediate level of selection (Fig 2D). Similarly, the fitness variance scaled by \( t^2 \) has a peak at intermediate selection (Fig 2D) since fitness variance must be zero at high selection. Some intermediate level of selection is most informative of the curvature of the fitness landscape, in that it balances biasing towards high fitness phenotypes and the effective number of unique variants in the distribution.

**RECOMBINATION EFFICIENTLY GENERATES DIVERSITY**

While selection moves the mean phenotype toward an optimum at the cost of reducing diversity, diversity can be restored by mutation and recombination processes that add new variants to the population. Biologically, mutations and recombination are changes in genotypes and their effect on phenotypes depends on the genotype-phenotype map. Mutations generate new variants that can rise to some frequency after selection if beneficial, and the expected cost or benefit of a mutation depends on the fitness landscape.

As an alternative to specifying a genotype-phenotype map, we define a mutation as a small stochastic normally distributed change in phenotype space. Intuitively, if the mutational distribution is similar to the curvature of the fitness landscape then the cost should be minimal. However, there is no reason to expect such an alignment, and if a population is on a high dimensional ridge, then a mutation is very likely to fall off the ridge and be very costly. For normally distributed populations and mutations, the expected fitness cost is proportional to the effective number of directions which
are deleterious (Appendix D).

From an optimization perspective, mutations are very inefficient in that they rarely generate good solutions by being poorly aligned with the fitness landscape. However, recombination has the remarkable property of being adaptive to the fitness landscape. In population genetics models with genotypes, recombination is known to quickly break down correlations between sites in a genome until linkage equilibrium is reached. Under these conditions the phenotype covariance and expected fitness of recombinated offspring is the same as the parent population (19, 20). If the population is on a high dimensional ridge and the population covariance is aligned, recombinated solutions would also be aligned with the ridge. However, linkage equilibrium can only be reached on fitness landscapes without interactions between genetic sites, which excludes most fitness landscapes, including quadratic fitness-phenotype maps.

For the purposes of optimization, we are free to define any recombination operator. GAs typically use recombination in the form of a crossover operator, similar to genetic recombination. However, a naive application of crossover to phenotypes would destroy any covariance in the population. Here we define recombination of phenotypes that preserves covariance. A pair of distinct phenotypes, chosen by weighted random sampling with weights \( p_1(t) \) and \( p_2(t) \) can be recombined as

\[
 x' = \mu_t + \frac{1}{\sqrt{2}} (x_1 - x_2),
\]

which has the same expectation \( \mu_t \) and covariance \( \Sigma_t \) as the parent population. This recombination operator preserves normal statistics, and is a way of sampling from an implicit normal distribution without estimating its parameters. This operator resembles the mutation operator in differential evolution optimization, which also preserves normal statistics for certain parameter values [21]. However, the error in the mean and covariance can be large when diversity is low due to sampling noise, and the number of unique recombinants can be too limited. We improve the quality of recombination by generalizing to a stochastic sum over the entire population

\[
x' = \mu_t + \sum_i \eta_i \sqrt{p_i(t)}(x_i - \mu_t),
\]

where \( \eta_i \) is an instance of a standard normal random variable. This operator also conserves normal statistics, tuned by strength of selection \( t \), and efficiently generates new variants without storing a covariance matrix. In comparison, CMA-ES/NES must store a covariance matrix, which may be challenging in large problems.

**QUANTITATIVE GENETIC ALGORITHM**

**Algorithm 1 Quantitative genetic algorithm**

1: choose hyperparameter \( S \)
2: draw population \( x_i \) for all \( i \) from initial normal distribution
3: repeat
   4: find \( t \) such that \( S = -\sum_i p_i(t) \log p_i(t) \)
   5: sample standard normal variates \( \eta_i \) for all \( i \)
   6: add to population \( x' \leftarrow \sum_i \eta_i \sqrt{p_i(t)}(x_i - \mu_\infty) + \mu_\infty \)
7: until convergence criteria met

We define a proof-of-principle **quantitative genetic algorithm** (QGA), as it is related to quantitative genetics,
and is also a genetic algorithm that is quantitative in the sense that it tracks frequencies of types. QGA iterates between increasing selection to move the distribution up the natural gradient, and phenotype recombination to generate variants. To simplify matters, we generate only one variant per iteration, and choose uniform initial conditions $p_i(0) = 1/K_0$ for all variants, even after a new variant is generated. This differs from population genetics models where new variants are introduced at a small frequency. In our algorithm, variants are never removed, but their frequencies become small when they become irrelevant.

A critical problem of EAs is how to increase, or sometimes decrease, selection over the course of optimization to make sure it ends extremely closely distributed around the optimum. One choice is a fixed schedule of increases in selection, as in simulated annealing and population annealing. However, choosing a good rate is challenging as increasing selection too quickly will lead to premature convergence, and increasing selection too slowly wastes resources. In addition, a constant rate may not work well when different parts of the fitness landscape have different curvatures.

It is clear that some intermediate level of selection is needed, although the peak in scaled genetic load or fitness variance is not necessarily the right balance. We implement an adaptive strategy that keeps diversity fixed and lets selection vary on its own. After a variant is generated, population entropy will typically increase by a small amount since entropy is an extensive quantity. Then we choose a new $t$ such that the entropy is at a target value $S$, a hyper-parameter. This way the population adapts to keep the diversity constant, with high fitness variants driving selection higher as they are found. If $S$ is too small the algorithm can still converge prematurely outside of the local quadratic optimum.

For generating variants, we use a modified recombination operator which replaces $\mu_t$ in Eq. 7 with the best variant seen thus far $\mu_\infty$. Shifting the mean of recombinants was found to perform much better in benchmarks (see below and Fig. SS1). We provide an implementation of QGA (Alg. 1) online, with minor implementation details including a rudimentary test for premature convergence described in Methods.

**QGA PERFORMANCE**

We demonstrate QGA on two simple test functions, and a suite of functions from a benchmarking library. Optimization of a 5 dimensional quadratic function (Fig. 3A,B) converges to the optimum for large $S$, and converges outside of the optimum for smaller $S$. Selection strength $t$ increases exponentially with the number of evaluations when the algorithm is converging. On a non-convex 2 dimensional Rosenbrock function (Fig. 3C,D,E) selection is tuned according to the curvature of the landscape over the course of the optimization. Initially, selection increases rapidly as the population falls into the main valley, then selection slows down as it moves along the flatter part of the valley floor, and finally speeds up again as it converges to a quadratic optimum.

To more rigorously assess performance, we tested
QGA on noiseless test functions from the blackbox optimization benchmark library [22] (implemented in [23]), which implement an ensemble of ‘instances’ of each function with randomized locations of optima. On 5 dimensional quadratic and Rosenbrock functions, the chance of convergence to the optimum, and the average number of function evaluations is sensitive to the hyperparameter $S$, with low $S$ leading to premature convergence, and high $S$ leading to a high number of function evaluations (Fig. [S1] red lines). Performance is significantly improved with the modified recombination operator which replaces $\mu_t$ in Eq. [7] with the best variant seen thus far $\mu_{\infty}$. This modified algorithm is able to make larger steps towards optimum with lower values of $S$ without prematurely converging (Fig. [S1] blue lines).

We tested QGA on all 24 noiseless test functions with the modified recombination operator over many values of $S$ and compare to CMA-ES [23] (Fig. 4). Overall the performance of QGA with a good choice of $S$ is very similar to CMA-ES, which may be expected due to their fundamental similarities. Both algorithms perform well on functions with strong global structure, where quadratic approximations may work well, and perform worse on functions with highly multimodal structure. QGA has higher chances of convergence of some of the multimodal functions (F15-F22). For the step ellipsoidal function (F7), QGA fails completely due to our test for premature convergence (see Methods), although CMA-ES also performs poorly.

For these benchmarks, QGA requires more fine tuning of its hyper-parameter than CMA-ES. However, QGA is simpler conceptually and in implementation compared to CMA-ES and NES. Those algorithms are somewhat complex and involve matrix inversions or decompositions, as well as adaptive learning rate schemes. QGA does not require any linear algebra and does not store a covariance matrix explicitly, which may make it possible to use on higher dimensional problems, where storage of a covariance matrix may be an issue. Additionally, QGA naturally incorporates information from the history of the optimization, whereas CMA-ES/NES has “generations” of samples and incorporates past information more heuristically.

In comparison to GA, QGA has deterministic selection which is much more efficient than stochastic fitness proportional selection. In addition, the recombination operator preserves relevant correlations between dimensions, in contrast to typical crossover operators.

We have shown that selection steps in ES, GA, and population genetics are intimately related, and developed a way to control the increase in selection. Our method of increasing selection by fixing the population entropy is simple and adaptive, yet its implications are not entirely clear, and there may be other strategies that tune selection more efficiently. The challenge is to find observables that indicate premature convergence early enough to be able to continually adapt the diversity of the population.

Our recombination operator assumes an underlying normal distribution to be effective. Following our scheme, a more general model-based optimization with natural gradient updates would iterate between tuning selection with exponential weights, and training some chosen generative model with that weighted data. The benefit of using natural selection is that the selection step does not require any knowledge of the generative model, including derivatives with respect to its parameters. Such an algorithm may be useful in generating high fitness variants for difficult problems, including complicated discrete spaces such as in the directed evolution of proteins.

**Methods**

**Algorithm details** Inputs are the chosen target entropy $S$ (in base 2), and the mean and variance of the initial normal distribution from which $K_0 = 2^{S+1}$ variants are drawn. In the selection step, we calculate $p_i(t) = e^{f(x_i)} / Z_t$, where $Z_t = \sum e^{f(x_i)}$ and $t$ is incremented or decremented geometrically by a small value until the entropy matches $S$. In the recombination step, a new variant is generated with an unbiased version of eq. [7], where $p_i(t) \rightarrow \frac{p_i(t)}{1-\sum_i e^{f(x_i)}}$. To simplify the implementation, the list of variants is held at a fixed size $K_0$ by replacing the variant with the lowest probability with the new recombination. Selection and recombination are iterated until the desired convergence criteria are met, or the following test for premature convergence passes. Detecting premature convergence is challenging, and the adequate solution we found is based on comparing fitness values. If the relative fitness differences are comparable to the machine error, the result of recombination is that the same fitness value may appear more than once for different values of $x$. Therefore, the algorithm terminates if duplicate fitness values are found in the population. Code available at [github.com/jotwin/qga](https://github.com/jotwin/qga)

**Test functions** The test ellipsoid is $f(x) = (x_1 + 2x_2 + 3x_3 + 4x_4 + 5x_5)^2$, and populations were initialized with 200 random variants drawn from a normal distribution with mean and variance equal to all ones, so that populations are not centered on the optimum at zero. The test Rosenbrock function is $f(x) = (1-x_1)^2 + 100(x_2-x_1^2)^2$, and populations were initialized with 200 random variants drawn from a normal distribution with mean (0,1) and standard deviation (0.25, 0.25).

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Figure 4. QGA performance is similar to CMA-ES on 24 noiseless functions from the blackbox optimization benchmark library with dimension 5 and different values of target diversity \( S \), with QGA (black), and CMA-ES (red). The best choice of \( S \) maximizes the chance of convergence and minimizes the number of function evaluations. A) Successful convergence as a function of \( S \) in 100 instances with randomized optima, where success is when the lowest value found is within \( 10^{-8} \) of the true minimum after less than \( 5 \times 10^4 \) evaluations. B) Success as function of the median number of function evaluations conditional on success, with \( S \) as in A. Both algorithms had initial conditions of mean zero and three standard deviations in each dimension. F9 and F10 are the familiar Rosenbrock and ellipsoid functions respectively.

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Appendix A: Natural selection gradient

We begin by following [13]. A population has \( i = 1 \ldots K \) variants with frequencies \( p_i \) that evolve according to

\[
\frac{dp_i}{dt} = p_i(f(x_i) - F),
\]

with fitness \( f \), phenotype \( x_i \), and mean fitness \( F = \sum_{i=1}^{K} p_i f(x_i) \). There are \( K - 1 \) independent variables, so we choose the \( K \)th variant as the reference and

\[
p_K = 1 - \sum_{i=1}^{K-1} p_i.
\]

Eliminating this variable results in

\[
\frac{dp_i}{dt} = \sum_{j=1}^{K-1} g_{ij}^{-1} \frac{\partial F}{\partial p_j},
\]

with

\[
g_{ij}^{-1} = p_i \delta_{ij} - p_i p_j
\]

where \( \delta_{ij} \) is the kronecker delta. \( g_{ij}^{-1} \) is also the covariance of a categorical distribution, and appears in the generalized Kimura diffusion equation. Note that indices are over the \( K - 1 \) variables.

The inverse of this matrix is the Fisher information metric

\[
g_{ij} = \sum_{k=1}^{K} p_k \left( \frac{\partial}{\partial p_i} \log p_k \right) \left( \frac{\partial}{\partial p_j} \log p_k \right)
\]

\[
= \sum_{k=1}^{K} \frac{1}{p_k} \frac{\partial p_k}{\partial p_i} \frac{\partial p_k}{\partial p_j}
\]

\[
= \frac{1}{p_K} + \frac{1}{p_i} \delta_{ij}
\]

If \( p_i \) describe a normally distributed phenotype \( x \), we can project onto the phenotype mean and covariance

\[
\mu = \sum_{i=1}^{K-1} p_i (x_i - x_k) + x_k
\]

\[
\Sigma = \sum_{i=1}^{K-1} p_i [(x_i - \mu)^2 - (x_k - \mu)^2] + (x_k - \mu)^2
\]

with multivariate phenotypes \( x_i \) as vectors of dimension \( D \), and shorthand for the matrix \( b^2 = bb^\top \) given a vector \( b \). The derivatives of mean fitness can be decomposed by the chain rule

\[
\frac{\partial F}{\partial p_j} = \nabla_\mu F \cdot \frac{\partial \mu}{\partial p_j} + \nabla_\Sigma F \cdot \frac{\partial \Sigma}{\partial p_j}
\]

\[
\frac{\partial \mu}{\partial p_j} = x_j - x_K
\]

\[
\frac{\partial \Sigma}{\partial p_j} = (x_j - \mu)^2 - (x_k - \mu)^2
\]

where \( \nabla_b \) is the vector of partial derivatives with respect to parameter \( b \). Combining the above equations results in

\[
\frac{d\mu}{dt} = \Sigma \nabla_\mu F
\]

\[
\frac{d\Sigma}{dt} = 2\Sigma \Sigma^\top \nabla_\Sigma F
\]
Appendix B: Selection and Newton’s method

The integrated dynamics of the frequencies are

\[ p_i(t) = p_i(0) \frac{1}{Z_t} e^{t f(x_i)}, \]

with normalization \( Z_t = \sum_i p_i(0) e^{t f(x_i)} \). The change in mean phenotype is proportional to the covariance between phenotype and fitness, (Price’s theorem)

\[ \mu_t - \mu_0 = \frac{1}{Z_t} \sum_{i=1}^K p_i(0) \left( x_i e^{t f(x_i)} - \mu_0 Z_t \right). \]

A Taylor expansion of \( f(x) \) around \( \mu_0 \) to second order is

\[ f(x) \approx f(\mu_0) + (x - \mu_0) \nabla f - \frac{1}{2} (x - \mu_0)^2 \cdot C, \]

where \( \nabla f \) is the vector of partial derivatives of fitness evaluated at \( \mu_0 \), and \( C \) is the curvature, that is the negative of the matrix of second partial derivatives evaluated at \( \mu_0 \), and we use a shorthand for the outer product, e.g., \( b^2 = b b^\top \), and \( b^2 \cdot A = b^\top A b \), for an arbitrary matrix \( A \). The expansion is more conveniently written as

\[ f(x) \approx F^* - \frac{1}{2} (x - x^*)^2 \cdot C, \]

where \( F^* \) and \( x^* \) are the approximate optimum fitness and phenotype respectively, and \( C(x^* - \mu_0) = \nabla f \).

If phenotypes are initially normally distributed then they remain normal after selection with the quadratic approximation of the fitness landscape, as can be seen from the integrated replicator dynamics. The resulting mean and inverse covariance are

\[ \mu_t = \Sigma_t \left( \Sigma_0^{-1} \mu_0 + t C x^* \right) \]

\[ \Sigma_t^{-1} = \Sigma_0^{-1} + t C. \]

The change in the mean is

\[ \mu_t - \mu_0 = \Sigma_t t \nabla f \]

\[ = \left( \frac{1}{t} \Sigma_0^{-1} + C \right)^{-1} \nabla f. \]

Under strong selection in a quadratic fitness landscape the covariance shrinks to zero at a rate

\[ \Sigma_t \to \frac{C^{-1}}{t} \]

Appendix C: Genetic load

Fitness is distributed as a noncentral chi-squared distribution, since fitness is a sum of squared values that are normally distributed. The difference between the optimum and the mean fitness:

\[ F^* - F = \frac{1}{2} \sum_i p_i (x_i - x^*)^2 \cdot C \]

\[ = \frac{1}{2} \left( \Sigma_t + (\mu_t - x^*)^2 \right) \cdot C \]

which decomposes into an effective degrees of freedom \( Tr(\Sigma_t C) \), and a noncentrality parameter \( (\mu_t - x^*)^2 \cdot C \). For strong selection this fitness difference approaches zero as

\[ F^* - F \to D \frac{2}{2t} + O(t^{-2}) \]

where \( D \) is the dimension of \( x \).
Appendix D: Mutations

If mutations are normally distributed around each focal phenotype, the total covariance of all mutants will be 
the phenotype covariance plus the mutational covariance $\Sigma + \Sigma_m$. The associated mutational load is $\text{Tr}(\Sigma_m C)$, 
and if mutations are standard normal, then the mutational load is the sum of the eigenvalues of $C$, or roughly the 
number of dimensions where fitness is sharply curved and not flat.

Appendix E: Gradient step in SSWM moran model

In strong selection weak mutation dynamics $||$, a population is monomorphic (only one type), and changes type $x$ 
by mutation-fixation events. A mutant has a fitness difference $f(x') - f(x) \approx \Delta x \nabla f \equiv s$, and the probability of 
fixation is

$$P_{\text{fix}}(x'|x) = \begin{cases} 
2s & s > 0 \\
0 & s \leq 0 
\end{cases}.$$

The expected change in $x$ is

$$E(\Delta x) = \int \Delta x P_{\text{fix}}(x'|x) P_m(x'|x) dx',$$

where $P_m(x'|x)$ is the mutation distribution around $x$. For a normal mutation distribution $P_m(x'|x) = \mathcal{N}(x, \Sigma_m)$, 
$$E(\Delta x) = \Sigma_m \nabla f$$
Figure S1. QGA performance on 5 dimensional quadratic (A,B) and Rosenbrock (C,D) functions from the blackbox optimization benchmark library with different values of target diversity $S$. The best choice of $S$ maximizes the chance of convergence and minimizes the number of function evaluations. A,C) Successful convergence as a function of $S$ in 100 instances with randomized optima, where success is when the lowest value found is within $10^{-8}$ of the true minimum after less than $5 \times 10^4$ evaluations. B,D) Success as function of the median number of function evaluations conditional on success, with $S$ as in A,C. Red lines indicate standard recombination, Eq. 7, and blue lines indicate modified recombination (see text). Each population was initialized with mean zero and standard deviation of 3 in each dimension.