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Statistical mechanics of the maximum-average submatrix problem

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Abstract. We study the maximum-average submatrix problem, wherein given an $N \times N$ matrix J , one needs to find the $k \times k$ submatrix with the largest average number of entries. We investigate the problem for random matrices J , whose entries are i.i.d. random variables, by mapping it to a variant of the Sherrington–Kirkpatrick spin-glass model at fixed magnetisation. We analytically characterise the phase diagram of the model as a function of the submatrix average and the size of the submatrix k in the limit $N \rightarrow \infty$. We consider submatrices of size $k = mN$ with $0 < m < 1$. We find a rich phase diagram, including dynamical, static one-step replica symmetry breaking (1-RSB) and full-step RSB. In the limit of $m \rightarrow 0$, we find a simpler phase diagram featuring a frozen 1-RSB phase, where the Gibbs measure comprises exponentially many pure states each with zero entropy. We discover an interesting phenomenon, reminiscent of the phenomenology of the binary perceptron: there are efficient algorithms that provably work in the frozen 1-RSB phase.

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Keywords: cavity and replica method, phase diagrams,
typical-case computational complexity

Supplementary material for this article is available [online](#)

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We consider the maximum-average submatrix (MAS) problem, that is the problem of finding the $k \times k$ submatrix of an $N \times N$ matrix J with the largest average number of entries. This is a natural combinatorial optimisation problem that has been researched in the mathematical and data science literature [1], primarily in the context of biclustering [2]. Theoretical works have focussed on the case where J is a random matrix (*i.i.d.* standard Gaussian entries), the size of J is large ($N \rightarrow \infty$) and the size of the submatrix $k \ll N$ [3–5].

From a statistical physics point of view, the MAS problem is a natural variant of the well-known Sherrington–Kirkpatrick (SK) model [6] with spins $\sigma_i \in \{0, 1\}$ at fixed magnetisation. The statistical physics of disordered systems and the related replica method [7] have been widely used to assess other combinatorial optimisation problems, such as graph partitioning [8], matching [9], graph colouring [10], K -satisfiability of Boolean formulas [11], and many others. As far as we are aware, the MAS problem has not been examined from the statistical physics point of view. Filling this gap is the main purpose of this paper.

Our results reveal the exact phase diagram of the MAS problem when $k = mN$, N is large and m is finite. We unveil that at large values of m as the submatrix average increases, the system undergoes a continuous phase transition to a full replica symmetry breaking (RSB) phase [7]. At intermediate values of m , the phase transition becomes discontinuous, passing through a dynamical one-step RSB (1-RSB) and static 1-RSB phases to a full-RSB one [7]. At yet lower m , the full-RSB phase then vanishes and the maximum average is obtained by the 1-RSB solution. In the limit of $m \rightarrow 0$, the MAS

problem behaves in a way related to the random energy model [12] presenting frozen 1-RSB [13, 14].

We also find that in the limit $m \rightarrow 0$, the phase diagram presents a region where polynomial algorithms are proven to work [4] yet according to our results, the equilibrium behaviour of the problem is given by the frozen 1-RSB phase that is considered algorithmically hard [15]. One other such problem is known in the literature—the binary perceptron. For the binary perceptron, an explanation of the discrepancy between equilibrium properties and algorithmic feasibility has been proposed with respect to out-of-equilibrium large-local-entropy regions of the phase space that are not described within the standard replica solution [16]. This finding has been used to discuss learning in artificial neural networks [17] and propose new algorithms [18]. The analogy of the behaviour between the binary perceptron and the MAS problem is therefore interesting as it may serve to shed light over the fundamental question of algorithmic hardness. From the point of view of the mathematics of spin glasses, the perceptron problem is difficult to handle due to the effective bipartite structure of the correlations. The MAS problem instead belongs to a class of problems for which the exactness of the replica calculation has been established rigorously in [19].

We now review the mathematical results that we later connect to our analysis. All these results hold in the regime $k \ll N$. In [3], the authors proved that the globally optimal submatrix has an average equal to $A_{\text{opt}} = 2\sqrt{\log N/k}$ (log is the natural logarithm). They also conjectured, and it was later proven by [4] that the largest average submatrix (\mathcal{LAS}) algorithm—an efficient iterative row/column optimisation scheme—fails to reach the global optimum, as its fixed point—akin to local minima—has with high probability average equal to $A_{\mathcal{LAS}} = \sqrt{2\log N/k}$. The fact that the \mathcal{LAS} algorithm fails bears a natural question: is $A_{\mathcal{LAS}}$ an algorithmic threshold signalling the onset of a hard phase? In [4], the authors introduced a new algorithm called incremental greedy procedure (\mathcal{IGP}) that is able to produce submatrices with average $A_{\mathcal{IGP}} = 4/3\sqrt{2\log N/k} > A_{\mathcal{LAS}}$. Furthermore, they proved that for averages larger than at least $A_{\text{OGP}} = 10/(3\sqrt{3})\sqrt{\log N/k} > A_{\mathcal{IGP}}$, the problem satisfies the overlap gap property (OGP) [20]. This means that (i) the \mathcal{LAS} threshold $A_{\mathcal{LAS}}$ seems to be an algorithm-specific threshold and not a more general trace of an intrinsic computational-to-statistical gap, and (ii) the problem will likely exhibit a hard phase preventing algorithms to find submatrices with averages larger than at least A_{OGP} . [21] discusses additional results for $k = N^\gamma$, $0 < \gamma < 1$.

1. The model

We consider an $N_r \times N_c$ random matrix J comprising i.i.d. Gaussian entries with zero mean and unit variance. A $k_r \times k_c$ submatrix σ of J is defined by two arbitrary subsets of rows and columns I_r, I_c such that J_{ij} belongs to the submatrix σ if and only if $i \in I_r$ and $j \in I_c$, and the cardinalities satisfy $|I_r| = k_r$ and $|I_c| = k_c$. There are three versions of the MAS problem:

- **Rectangular MAS:** N_r, N_c, k_r and k_c are unconstrained. This is a problem relevant for applications [1, 2].

- **Square MAS of a square matrix:** $N_r = N_c = N$ and $k_r = k_c = k$. This version is studied in the mathematical literature [3, 4, 21].
- **The principal MAS of a symmetric matrix:** $N_r = N_c = N$, $k_r = k_c = k$, $J = J^T$ is symmetric and we consider only *principal submatrices*, that is submatrices for which $I_r = I_c$.

In the following section, we focus on the case of the principal MAS of a symmetric random matrix motivated by its close relationship to the SK model. In the supplementary data, we sketch the corresponding solution for the rectangular MAS of a random matrix and realise with surprise that the equations leading to the phase diagram of the square MAS of a square random matrix are exactly the same as the ones for the principal MAS of a symmetric random matrix. This allows us to compare our results directly to the mathematical literature, and it also means that the phase diagram provided by us applies to the non-symmetric case. We believe that the physics of the rectangular MAS problem has two more hyperparameters, namely N_r/N_c and k_r/k_c , leading to a four-dimensional phase diagram. Its exploration is left for future works.

We encode principal submatrices, that is their row/column index set I , as Boolean vectors $\sigma = \{\sigma_i\}_{i=1}^N \in \{0, 1\}^N$ such that if $i \in I$ then $\sigma_i = 1$ and vice versa. We fix the size of the submatrix to $k = mN$, which in the Boolean representation translates to the condition $\sum_i \sigma_i = mN$. We call $m \in (0, 1)$ magnetisation. The average of the entries of a submatrix σ can be then expressed as:

$$A = |\sigma| = \frac{1}{m^2 N^2} \sum_{i,j=1}^N J_{ij} \sigma_i \sigma_j. \quad (1)$$

We define $a = A\sqrt{N}$, and we will see that a is of order one in the thermodynamic limit.

We probe the energy landscape of the MAS problem by studying the associated Gibbs measure:

$$p(\sigma) = e^{\beta E(\sigma) + \beta h \sum_{i=1}^N \sigma_i} / Z(\beta, h), \quad (2)$$

where β is an inverse temperature that we use to fix the average energy, h is a magnetic field that we use to fix the magnetisation m and $Z(\beta, h)$ is the partition function. The uncommon plus sign in front of the inverse temperature is due to the fact that the problem is a maximisation problem. Thus, small temperatures correspond to large positive energies in this model. The energy function is defined as:

$$E(\sigma) = \frac{1}{\sqrt{N}} \sum_{i < j} J_{ij} \sigma_i \sigma_j = \frac{m^2 N}{2} a, \quad (3)$$

which, modulo subleading contributions coming from the diagonal term, is a multiple of the submatrix average a . Because the considered model resembles the classic SK model, note that the mapping of the Boolean spins to ± 1 spins, that is $s = 2\sigma - 1$, leads to an SK model in a random magnetic field, with couplings correlated to the magnetic field (see the supplementary data). Such a model has not been considered in the physics literature as far as we are aware.

We will compute all thermodynamic observables through the *quenched free entropy*, that is $\Phi = \lim_{N \rightarrow \infty} \mathbb{E}_J \log Z(\beta, h)/N$ where \mathbb{E}_J denotes averaging over the distribution of J . We will show that the free entropy can be expressed as a variational problem for the *overlap* order parameter, which is defined as $q = N^{-1} \sum_{i=1}^N \sigma_i^a \sigma_i^b \in [0, m]$ for two replicas of the system σ^a and σ^b .

2. Replica analysis of the free entropy

We compute the quenched free entropy Φ using the replica formalism [7], that is by using the replica trick $\mathbb{E}_J \log Z = \lim_{n \rightarrow 0} (\mathbb{E}_J Z^n - 1)/n$, computing $\mathbb{E}_J Z^n$ for integer values of n and performing an analytical continuation to take the $n \rightarrow 0$ limit. We perform the analytical continuation under the 1-RSB ansatz, in which we assume that the Gibbs measure decomposes into a two-level hierarchy of pure states. This hierarchy is characterised by two overlaps: the average overlap between microstates belonging to the same pure state q_1 and the one between microstates belonging to different pure states q_0 . The Parisi parameter p acts as a temperature controlling the trade-off between the free entropy of a single pure state, and the entropy of pure states [22]. After a derivation that follows the steps standard to the replica method [7, 23], we obtain the following variational free entropy:

$$\begin{aligned} \Phi_{1\text{-RSB}}(m, q_0, q_1, p) &= -\frac{\beta^2}{4} [m^2 + (p-1)q_1^2 - pq_0^2] \\ &\quad + \frac{1}{p} \int Du \log \left[\int Dv \left[1 + e^{\beta H(u,v)} \right]^p \right], \\ H(u, v) &= h + \frac{\beta}{2} (m - q_1) + \sqrt{q_0}u + \sqrt{q_1 - q_0}v, \end{aligned} \quad (4)$$

where Du and Dv denote the integration against a standard Gaussian measure. The variational free entropy depends on the submatrix size/magnetisation m , the intra-state overlap q_1 , the inter-state overlap q_0 and the Parisi parameter p . To obtain the equilibrium free entropy, we extremise the variational free entropy over m, q_0 and q_1 . The Parisi parameter must be set to one if the resulting complexity (whose definition we provide in the following) is positive; otherwise, the variational free entropy must also be extremised over p .

Under the 1-RSB ansatz, we have the following expressions for the observables to be evaluated at the equilibrium values of the order parameters. The average energy density (and the submatrix average) equals:

$$e = \frac{m^2}{2} a = \frac{\beta}{2} [m^2 + (p-1)q_1^2 - pq_0^2], \quad (5)$$

the total entropy (logarithm of the number of microstates) equals:

$$s_{\text{total}} = \Phi - \beta h m - \beta e, \quad (6)$$

and the complexity (logarithm of the number of pure states contributing to the Gibbs measure) equals:

$$\Sigma = \max \left(0, \partial_p \left[\text{extr}_{m, q_0, q_1} \Phi_{1\text{-RSB}} \right]_{p=1} \right). \quad (7)$$

If the complexity is non-zero, the total entropy decomposes as $s_{\text{total}} = s_{\text{internal}} + \Sigma$, where the internal entropy s_{internal} is the logarithm of the number of microstates contributing to each of the exponentially many pure states.

Finally, we need to investigate whether the 1-RSB result is exact in the thermodynamic limit. This is done by analysing the stability of the 1-RSB ansatz against perturbations of higher-order RSB nature. We perform the so-called type-I stability analysis (see supplementary data section I.d) and obtain the stability condition:

$$\int \text{D}u \frac{\int \text{D}v (1 + e^{\beta H})^p \left[\ell(\beta H)^2 (1 - \ell(\beta H))^2 \right]}{\int \text{D}v (1 + e^{\beta H})^p} < \frac{1}{\beta^2}, \quad (8)$$

where $\ell(x) = 1/(1 + \exp(-x))$. If this condition is not satisfied, then the 1-RSB results are just an approximation and more steps of RSB need to be considered.

We derived the variational free entropy using the replica trick. Note, however, that the proof of the full-RSB free entropy giving the exact solution in the thermodynamic limit from [19] applies to the MAS problem and thus to our setting. To apply their results to our model, we note that [19] constrains the free-entropy to fixed self-overlap $q_{\text{self}} = N^{-1} \sum_i \sigma_i^2$, whereas we constrain the model to fixed magnetisation $m = N^{-1} \sum_i \sigma_i$. Due to the choice of Boolean spins, we have that $\sigma_i^2 = \sigma_i$, so that the two constraints coincide (this is not true in general).

3. The phase diagram

After solving the above equations, we identify five distinct phases for finite $m \in (0, 1)$, and we plot them in figure 1.

- **RS phase:** For small submatrix average (corresponding to large temperatures), we observe a replica-symmetric (RS) phase, in which the extremum of the variational free entropy is attained at $q_0^* = q_1^*$. In this phase, the complexity is zero, whereas the total entropy is strictly positive. As the submatrix average increases (i.e. the temperature is lowered), the system undergoes a phase transition to an RSB phase. The nature of the transition is different for $m \leq m_c$ and $m \geq m_c$. We start by discussing the former case.
- **Dynamical 1-RSB phase:** For $m \leq m_c$, we observe a discontinuous transition at a value $a_{\text{dynamic}}(m)$ of the submatrix average from the RS phase to a dynamical 1-RSB phase, in which the extremum of the variational free entropy satisfies $q_0^* \neq q_1^*$. This transition is identified by a sharp jump of the complexity from zero to a positive value, meaning that the measure shatters into an exponential number of pure states each

with non-zero entropy. As m decreases, the appropriately rescaled internal entropy decreases, suggesting that in the $m \rightarrow 0$ limit, this phase becomes a frozen 1-RSB phase, see figure S2 in the supplementary data.

- **Static 1-RSB phase:** For $m \leq m_c$, in the dynamical 1-RSB phase, the complexity continuously decreases with the increase in the submatrix average. At the value of the submatrix average $a_{\text{static}}(m) > a_{\text{dynamic}}(m)$ at which the complexity vanishes, we observe a first-order phase transition, from the dynamical 1-RSB phase to a static 1-RSB phase ($q_0^* \neq q_1^*$, zero complexity, positive entropy).
- **The full-RSB phase:** For values $m \geq m_c$ we observe a continuous phase transition from the RS to the full-RSB phase at $a_{\text{stability}}(m)$. The transition occurs when the type-I 1-RSB stability condition (8) fails. We conjecture that this phase is full RSB due to the similarity to the SK model, in which a similar continuous phase transition to full-RSB occurs. For the values of $m_c \geq m \geq m^*$, we observe a Gardner-like phase transition at a value $a_{\text{stability}}(m)$ of the sub-matrix average from the 1-RSB phase to the full-RSB phase. This transition is reminiscent of the one known from the Ising p -spin model [24].
- **The UNSAT phase:** As the average of the matrix increases, we encounter a point at which the total entropy vanishes, denoting that the sub-matrix average has reached its maximum value $a_{\text{max}}(m)$. After this point, the total entropy becomes negative and we observe an unsatisfiable (UNSAT) phase, where no submatrix with that value of the submatrix-average exists. For $m \geq m^*$, we provide only an approximate estimate of this transition line (while all other transitions presented are exact up to the precision of the numerical solver). We estimated $a_{\text{max}}(m)$ in the 1-RSB solution, even though this ansatz is unstable in this phase, by computing the 1-RSB entropy, finding the temperature at which it vanishes, and computing the corresponding submatrix average.
It is often the case that the 1-RSB prediction for the maximum energy is numerically very close to the full-RSB prediction. Evaluation of the full-RSB equations, which are proven to yield the correct maximum average (analogous to the ground-state energy in the SK model) [19], is left for future works.
- **Tricritical points:** The phase diagram features two tricritical points. The first one, at $(m_c, a_c) \approx (0.09\text{--}0.1, 9.3\text{--}9.7)$, marks the coexistence of the RS, 1-RSB and full-RSB phases. It can be pinpointed by finding the intersection of the stability and the static transition lines. As $m \rightarrow m_c^-$, the static and dynamic transitions approach very quickly so that it is very difficult to distinguish them numerically. The second tricritical point is at $(m^*, a^*) \approx (0.0001\text{--}0.002, 100\text{--}650)$, marking the crossing between the stability and the UNSAT transition lines. For $m \leq m^*$, the 1-RSB phase is stable up to the maximum average $a_{\text{max}}(m)$. This second tricritical point is hard to pinpoint numerically and accurately. In the supplementary data, we show analytically that at least for $m \rightarrow 0$, the 1-RSB phase is indeed stable up to $a_{\text{max}}(m)$. Thus, by continuity, this second tricritical point must exist.

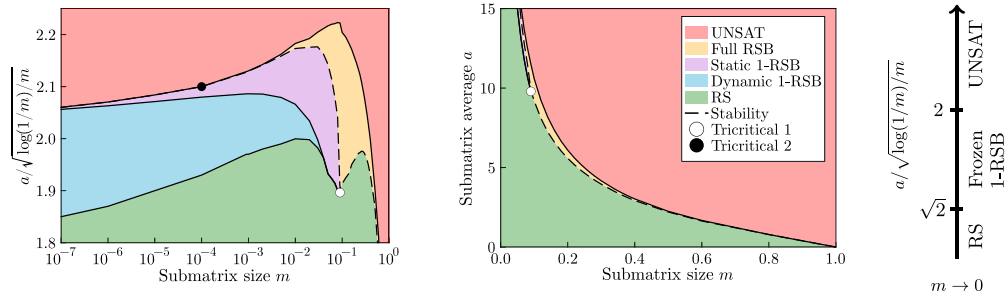


Figure 1. The phase diagram of the MAS problem as a function of the submatrix average a and the submatrix size $m = k/N$ for a linear scale in m (left), the logarithmic scale in m (centre) and $m \rightarrow 0$ (right). In the central and right panels, we rescale the submatrix average as $a/\sqrt{\log(1/m)/m}$ to highlight the limit's convergence. We identify five distinct phases. In the RS phase (green), the system is replica symmetric. In the 1-RSB phases, the replica symmetry is broken to one step and two sub-phases. A dynamical 1-RSB with an extensive number of equilibrium pure states (blue) and a static 1-RSB exists with only finitely many pure states (purple). All the phase boundaries are exact in the thermodynamic limit except the boundary between full RSB (orange) and UNSAT (red), which would require solving the full-RSB equations. In the full-RSB phase (orange), the replica symmetry is completely broken and the set of pure states manifests ultrametricity. In the unsatisfiable phase (UNSAT, red), no submatrix exists with the given values of a and m . The transition from RS and 1-RSB to full-RSB is continuous and caused by an instability of the 1-RSB ansatz (dashed line), whereas the other transitions are discontinuous. We observe two tricritical points: one at (m_c, a_c) where the system shows the coexistence of RS, 1-RSB and full-RSB phase (white marker) and one at (m^*, a^*) where the largest-average submatrices become 1-RSB stable and the full-RSB region ceases to exist (black marker). In the limit $m \rightarrow 0$, we observe only the RS, 1-RSB and UNSAT phases. The 1-RSB phase is frozen, meaning that the internal entropy of each pure state goes to zero in the $m \rightarrow 0$ limit.

4. The small magnetisation limit

We now study the phase diagram in the $m \rightarrow 0$ limit, corresponding to the $1 \ll k \ll N$ regime. The limit must be carefully taken to preserve the extensivity of the energy function in the thermodynamic limit. Indeed, we have that for fixed m and N :

$$\text{var}(E(\sigma)) = \mathcal{O}(m^2 N), \quad \# = \mathcal{O}(Nm \log 1/m), \quad (9)$$

where $\#$ denotes the logarithm of the number of microstates at fixed m and N . As $m \rightarrow 0$, the energy must be rescaled by $c(m) = \sqrt{\log(1/m)/m}$, and the entropy and complexity must be rescaled by $m \log(1/m)$. This can be achieved by considering the $m \rightarrow 0$ limit of (4) at fixed $b = \beta/c(m)$. We perform analytically the limit in the RS and 1-RSB solutions, leading to the following phase diagram.

- **RS phase:** For sub-matrix average $a < a_{\text{dynamic}} = \sqrt{2}c(m)$, we observe a stable RS phase with zero complexity and positive total entropy. In this phase, $q_0 = q_1 = m^2$.

- **Frozen 1-RSB phase:** For sub-matrix average $a_{\text{dynamic}} < a < a_{\text{static}} = 2c(m)$, we observe a stable 1-RSB phase with $q_1 = m$, $q_0 = m^2$ and complexity $\Sigma = 1 - b^2/4$. This is a frozen phase, meaning that each of the exponentially-many pure states contributing to the measure has zero internal entropy.
- **The UNSAT phase:** For submatrix average $a > a_{\text{static}}$, the total entropy is negative, signalling the onset of the UNSAT phase.

The threshold a_{dynamic} and a_{static} coincide with the thresholds proved in [3] for, respectively, the submatrix-average of the local maxima $A_{\mathcal{L}AS} = a_{\text{dynamic}}/\sqrt{N}$ and the maximum submatrix-average achievable $A_{\text{opt}} = a_{\text{static}}/\sqrt{N}$. Thus, as a byproduct of our analysis, we obtain an equilibrium interpretation of $A_{\mathcal{L}AS}$ as a freezing transition.

The $m \rightarrow 0$ limit of the MAS phase diagram closely resembles that of the random energy model (REM) [12]. More precisely, we find that the static threshold, as well as the values of the entropy and complexity, do coincide (in the REM the static transition threshold equals $a_{\text{static,REM}} = 2$, the complexity equals $\Sigma = 1 - b^2/4$ and the internal entropy is zero for all $b > 0$). This connection is related to the fact that the MAS energy $E(\sigma)$ is a Gaussian random variable with covariance $\langle E(\sigma)E(\sigma') \rangle \propto q(\sigma, \sigma') \leq m$, which vanishes in the $m \rightarrow 0$ limit. The notable difference between the REM and the MAS problem is given by the finite value of the dynamic threshold in the MAS problem, whereas the system is frozen at all temperatures in the REM.

In [4], the authors introduced an algorithm called \mathcal{IGP} , and they proved that it can find submatrices with average A which, following our analysis, are inside the frozen 1-RSB region. This is at odds with the common belief that solutions in frozen states are algorithmically hard to find [15]. Another problem in which a similar situation happens is the binary perceptron, where the algorithmic feasibility is explained with respect to out-of-equilibrium dense regions [16, 17]. We leave for future work a deeper understanding of the out-of-equilibrium properties of the MAS problem, and more generally, the relationship between them and algorithmic tractability.

5. Conclusions

In this paper, we studied the maximum-average submatrix problem using tools from the statistical physics of disordered systems, and in particular, a mapping onto a variant of the SK model.

We unveiled the phase diagram in the large submatrix regime $k = mN$, discovering a rich phenomenology including glassy phases and phases where exponentially many pure states contribute to the equilibrium behaviour of the system.

By considering the $m \rightarrow 0$ limit, we characterised the phase diagram in the small submatrix regime $k \ll N$, shedding some light on previous results [3, 4] and highlighting a connection to the REM. We note that there exist efficient algorithms that work in the frozen 1-RSB phase, usually associated with hard-algorithmic phases, similar to what happens in the binary perceptron due to non-equilibrium phenomena.

Our findings leave many questions answered: (i) the study of the out-of-equilibrium properties of the problem and their relationship with algorithmic hardness and (ii) how

for $k \ll N$ the vanishingly small correlations between the energies combine to shift the dynamical temperature from infinite (REM) to finite (MAS).

We conclude by remarking that our techniques generalise straightforwardly to the case in which the entries of J are non-Gaussian as long as they are i.i.d. with finite first and second moments, and to the rectangular MAS problem, in which both J and the submatrices may be rectangular, possibly with different aspect ratios.

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