



Double descent in the condition number

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Abstract

In solving a system of n linear equations in d variables $Ax = b$, the condition number of the n, d matrix A measures how much errors in the data b affect the solution x . Bounds of this type are important in many inverse problems. An example is machine learning where the key task is to estimate an underlying function from a set of measurements at random points in a high dimensional space and where low sensitivity to error in the data is a requirement for good predictive performance. Here we report the simple observation that when the columns of A are random vectors, the condition number of A is highest, that is worse, when $d = n$, that is when the inverse of A exists. An overdetermined system ($n > d$) and especially an underdetermined system ($n < d$), for which the pseudoinverse must be used instead of the inverse, typically have significantly better, that is lower, condition numbers. Thus the condition number of A plotted as function of d shows a double descent behavior with a peak at $d = n$.



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The concept of condition number was introduced by Turing in 1948 [1] and has since played a key role in the theory of algorithms. The condition number of a function measures how much the output value of the function can change for a small change in the input argument. The condition number most commonly associated with $Ax = b$ is defined as the ratio of the relative error in x to the relative error in the data b . In terms of the l_2 norm on x and b , this leads to the following definition (see Box1) for the condition number of A , denoted by $\kappa(A) = \|A\| \|A^\dagger\|$, where $\|A\|$ is the operator norm of the m, n matrix A is defined in terms of the vector norm of K^n, K^m as $\|A\| = \sup_{x \in K^n, x \neq 0} \frac{\|Ax\|}{\|x\|}$ and A^\dagger is the pseudoinverse. It is easy to see that $\kappa(A) = \frac{\sigma_{max}(A)}{\sigma_{min}(A)}$ that is the ratio of the maximal and minimal singular values of A .

The plot in the Figure 1 can be easily checked by calling the function “cond” in MatLab. The double descent pattern is apparently quite robust to choices of d and n , such that their ratio $\gamma = \frac{n}{d}$ is the same. The fact that the worse conditioning occurs when the inverse exists uniquely ($\gamma = 1$) seems at first surprising. This observation is new, as far as we know, though it is so simple that it must have been realized by many. The proof is also simple because of a relatively recent characterization of the eigenvalues of random matrices [2]. In fact, consider the n, d random matrix A . We characterize its condition number by using the Marchenko–Pastur law, which describes the asymptotic behavior of singular values of large rectangular random matrices. We

assume that the entries of A are independent, identically distributed random variables with mean 0 and variance σ^2 . We consider the limit for $n \rightarrow \infty$ with $\frac{n}{d} \rightarrow \gamma$. Marchenko–Pastur claims that for $\gamma < 1$ the smallest and the largest singular values of $\frac{1}{d}AA^T$ are, respectively $(1 - \sqrt{\gamma})^2$ and $(1 + \sqrt{\gamma})^2$. For $\gamma > 1$ the largest and the smallest eigenvalues of $\frac{1}{n}A^T A$ are $(1 + \sqrt{\gamma^{-1}})^2$ and $(1 - \sqrt{\gamma^{-1}})^2$. When $\gamma = 2$, and the entries are i.i.d. sub-Gaussian, the maximal singular value is concentrated around 2, but the minimal one is $\min\{n^{-1}, d^{-1}\}(\max\{\sqrt{n} - \sqrt{d-1}, \sqrt{d} - \sqrt{n-1}\})^2$, as was observed in [3].

For the system of linear equations $Ax = b$, the implication is that is better to have more variables than data: the condition number associated with the minimum norm solution $x = A^\dagger b$ is usually much better – that is closer to 1 – than the condition number of a well-determined system with $n = d$, if the matrix A is random.

There are interesting implications for machine learning. The most obvious is that kernel methods (see Box4), which are a popular workhorse in machine learning, *do not require regularization in order to be well-conditioned*, if the kernel matrices are based on high dimensional i.i.d data, especially when $\gamma < 1$. This claim follows from very recent results on kernels. The simplest form of the kernel matrix $K(x_j, x_i)$ is $K = XX^T$. One can think of the matrix K as given by $K(x_j, x_i) = \Phi(x_j)^T \Phi(x_i)$ since $K(x, y) = \sum_i^\infty \lambda_i \phi_i(x) \phi_i(y)$ because of Mercer theorem. We consider random matrices whose entries are $K(x_i^T x_j)$ or $K(\|x_i - x_j\|^2)$ with i.i.d. vectors x_i in \mathbb{R}^p with normalized distribution. Assuming that f is sufficiently smooth and the distribution of x_i 's is sufficiently nice, El Karoui [4] showed that the spectral distributions of kernel dot-product matrices $K(x_i, x_j) = f(XX^T)$ behave as if f is linear in the Marchenko–Pastur limit. In fact, El Karoui showed that under mild conditions, the kernel matrix is asymptotically equivalent to a linear combination of XX^T , the all-1's matrix, and the identity, and hence the limiting spectrum is Marcenko-Pastur. As a consequence, the claims about the condition number of a random matrix A also apply to kernel matrices with random data, see Figure 2.

In addition, the behavior of the condition number of K^\dagger provides a – perhaps oversimplified but clear – *explanation for the double descent* behavior of the test error by linear and kernel interpolants, which has recently attracted much attention [5, 6, 7, 8, 9, 10, 11].

From the point of view of the foundations (see Box5) of learning theory, this observation implies that complexity control is important not only in the “classical” regime of fixed hypothesis space and $n \rightarrow \infty$ but also in the “modern” high dimensional regime of $\frac{n}{d} \rightarrow \infty$, in which the minimum norm pseudoinverse plays a key role. In both cases, well-posedness that is existence, uniqueness and especially stability of the solution, are the key requirement for predictivity. Stability, defined as CV_{loo} , reduces to the condition number of K^\dagger for kernel methods both in the “classical” and in the “modern” regime. Stability is usually guaranteed during optimization, that is learning from examples, by complexity control under the form of vanishing regularization (as in the definition of the pseudoinverse or as implicitly provided by iterative gradient descent [12]).

It is quite possible that a similar argument may explain the behavior of overparametrized deep neural networks. It has been shown recently [13, 14, 15] that with the exponential loss, gradient descent induces a dynamics of the weight matrix for each layer of the network that

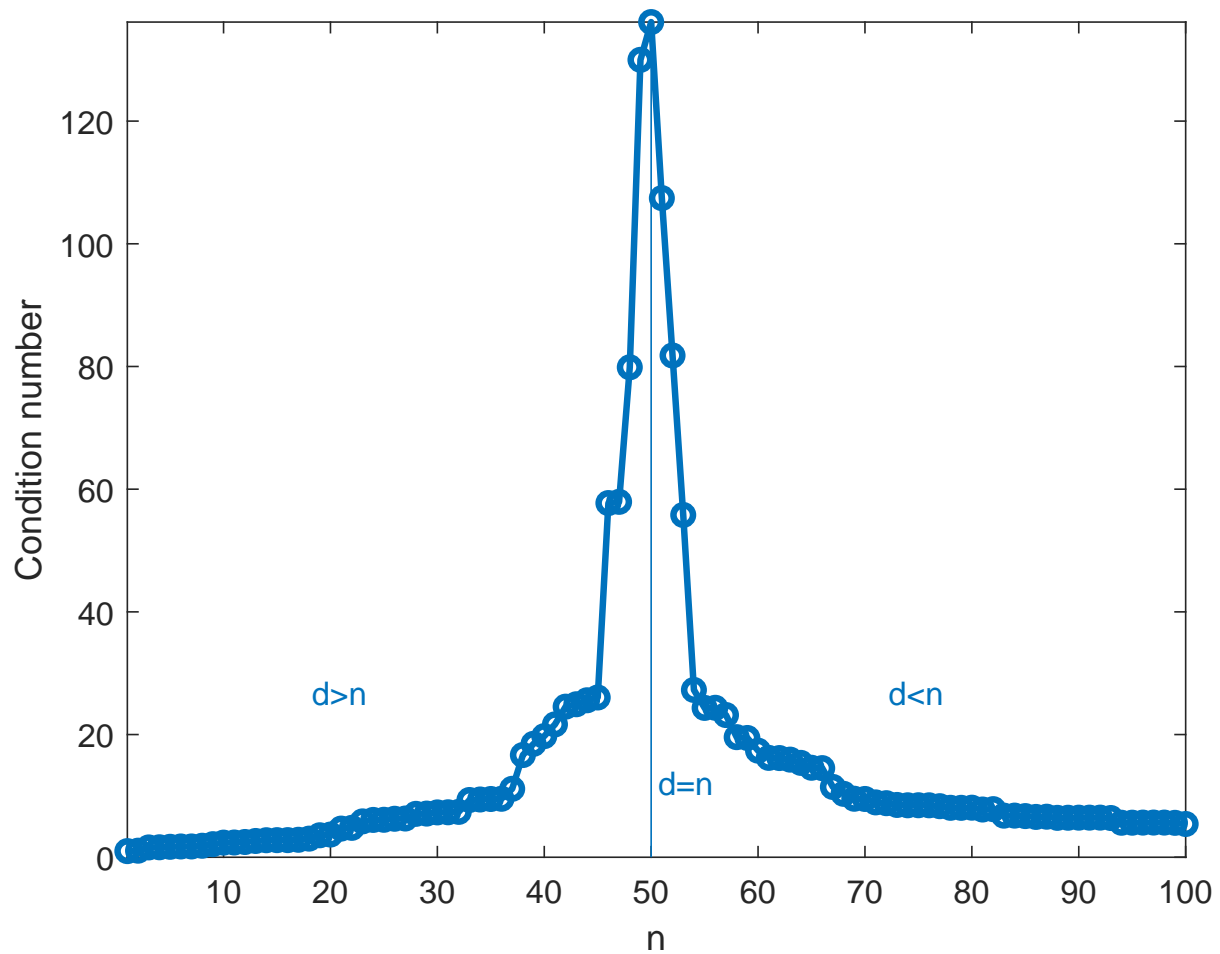


Figure 1: Typical double descent of the condition number (y axis) of a random data matrix distributed as $\mathcal{N}(0, 1)$: the condition number is worse when $n = d$, better if $n > d$ (on the right of $n = d$) and also better if $n < d$ (on the left of $n = d$).

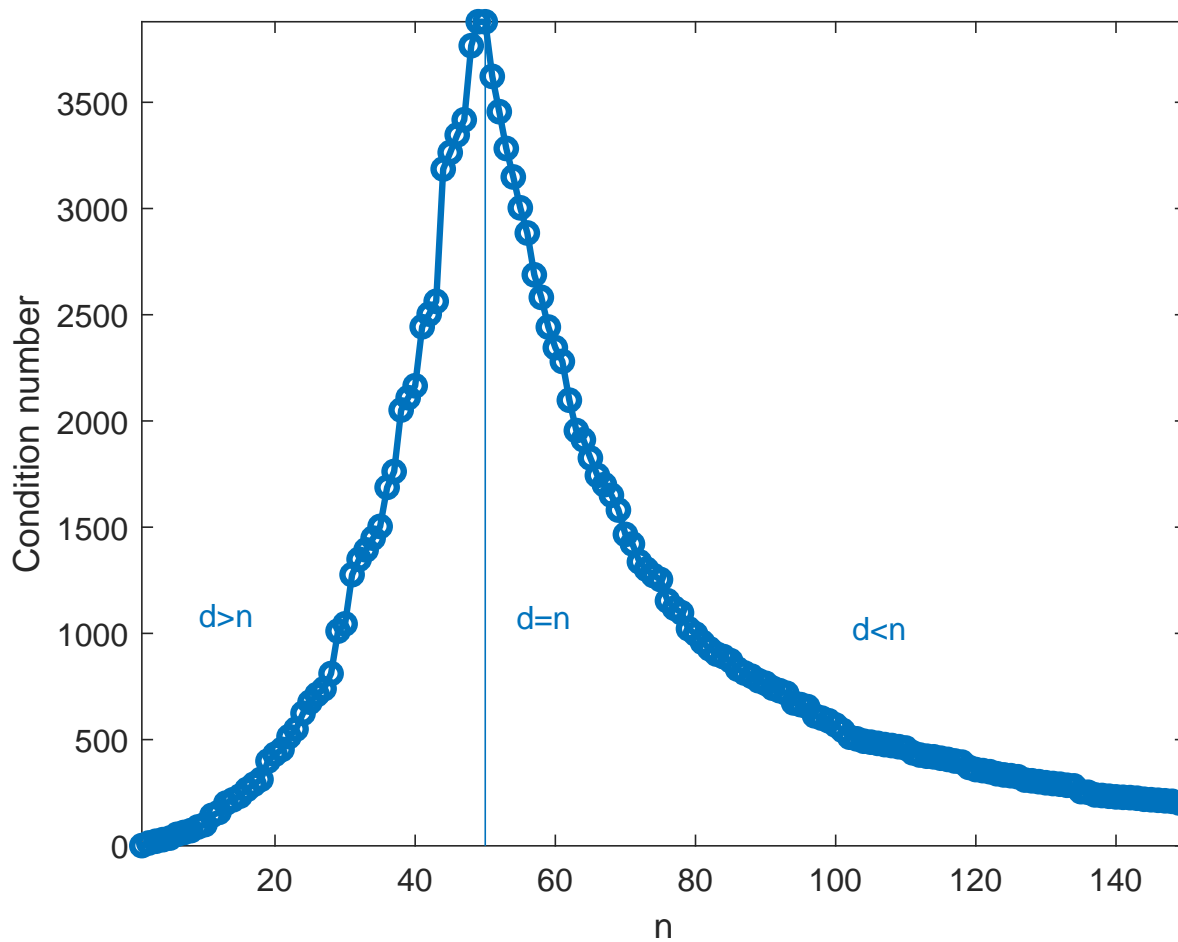


Figure 2: Typical double descent of the condition number (y axis) of a radial basis function kernel $K(x, x') = \exp\left(-\frac{\|x-x'\|^2}{2\sigma^2}\right)$ built from a random data matrix distributed as $\mathcal{N}(0, 1)$: as in the linear case, the condition number is worse when $n = d$, better if $n > d$ (on the right of $n = d$) and also better if $n < d$ (on the left of $n = d$). The parameter σ was chosen to be 5.

converges, because of a hidden vanishing regularization term, to a minimum norm solution analog to the pseudoinverse.

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Author Contribution All developed the basic theory.

Boxes

Box4: ERM and Kernel Machines

Consider “learning the function f from data $S = (x_1, y_1; x_2, y_2, \dots, x_n, y_n)$ by computing

$$\min_{f \in B_R} \frac{1}{n} \sum_{i=1}^n (f(\mathbf{x}_i) - y_i)^2. \quad (1)$$

We assume that $f(\mathbf{x}) = \sum_{i=1}^n c_i K(\mathbf{x}_i, \mathbf{x})$ and that f is in the ball B_R of radius R in \mathcal{H} (eg $\|f\|_K \leq R$). Then $\mathcal{H} = \overline{I_K(B_R)}$ is compact – where $I_K : \mathcal{H}_K \hookrightarrow C(X)$ is the inclusion and $C(X)$ is the space of continuous functions with the sup norm [16]. In this case the minimizer of the generalization error $I[f]$ is well-posed. Minimization of the empirical risk (Equation (1)) is also well-posed: it provides a set of linear equations to compute the coefficients \mathbf{c} of the solution f as

$$K\mathbf{c} = \mathbf{y} \quad (2)$$

where $\mathbf{y} = (y_1, \dots, y_n)$ and $(K)_{i,j} = K(\mathbf{x}_i, \mathbf{x}_j)$. Notice that this last set of linear equations is well-posed even without the constraint $\|f\|_K \leq R$: if K is symmetric and positive definite and the x_i are distinct the K^{-1} exists and $\|f\|_K^2$ is automatically bounded, with a bound that increase with n . For any fixed n the condition number of K is finite. A regularized form of ERM is

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n (f(\mathbf{x}_i) - y_i)^2 + \lambda \|f\|_K^2, \quad (3)$$

which gives the following set of equations for \mathbf{c} (with $\lambda \geq 0$)

$$(K + n\lambda I)\mathbf{c} = \mathbf{y}, \quad (4)$$

which for $\lambda = 0$ reduces to Equation (2). In both cases, stability of the empirical risk minimizer provided by Equation (3) can be characterized using the classical notion of *condition number* of the problem. The change in the solution f due to a variation in the data \mathbf{y} can be bounded as $\frac{\|\Delta f\|}{\|f\|} \leq \|K + n\lambda I\| \|(K + n\lambda I)^{-1}\| \frac{\|\Delta \mathbf{y}\|}{\|\mathbf{y}\|}$ where the condition number $\|K + n\lambda I\| \|(K + n\lambda I)^{-1}\|$ is controlled by $n\lambda$. A large value of $n\lambda$ gives condition numbers close to 1, whereas ill-conditioning may result if $\lambda = 0$ and the ratio of the largest to the smallest eigenvalue of K is large. Though this is the classical argument, it is now clear (because of recent results such as El Karoui [4]) that random K matrices are typically well-conditioned even for $\lambda = 0$ as described in Box 3. In other words, for i.i.d high-dimensional data,

$$\frac{\|\Delta f\|}{\|f\|} \leq \|K\| \|(K)^\dagger\| \frac{\|\Delta \mathbf{y}\|}{\|\mathbf{y}\|}, \quad (5)$$

and the condition number $\kappa(K) = \|KI\| \|(KI)^\dagger\|$ is close to 1, especially for $\gamma \ll 1$ (see Box2).

Box5: Classical Learning Theory

In the classical setting, a key property of a learning algorithm is *generalization*: the empirical error must converge to the expected error when the number of examples n increases to infinity, while the class of functions \mathcal{H} , called the *hypothesis space*, is kept fixed. An algorithm that guarantees good generalization will predict well, if its empirical error on the training set is small. Empirical risk minimization (ERM) on \mathcal{H} represents perhaps the most natural class of learning algorithms: the algorithm selects a function $f \in \mathcal{H}$ that minimizes the empirical error – as measured on the training set.

One of the main achievements of the classical theory was a complete characterization of the necessary and sufficient conditions for generalization of ERM, and for its *consistency* (consistency requires asymptotic convergence of the expected risk to the minimum risk achievable by functions in \mathcal{H} ; for ERM generalization is equivalent to asymptotic consistency). It turns out that consistency of ERM is equivalent to a precise property of the hypothesis space: \mathcal{H} has to be a *uniform Glivenko-Cantelli (uGC)* class of functions.

Later work showed that an apparently separate requirement – the well-posedness of ERM – is in fact equivalent to consistency of ERM. Well-posedness usually means *existence, uniqueness and stability* of the solution. The critical condition is stability of the solution. Stability is equivalent to some notion of continuity of the learning map (induced by ERM) that maps training sets into the space of solutions, eg $L : Z^n \rightarrow \mathcal{H}$. In particular, it was proved [17, 18] that *CV_{loo} stability guarantees generalization and in the case of ERM is in fact equivalent to consistency*.

We recall the definition of *leave-one-out cross-validation (in short, CV_{loo}) stability*:

$$\forall i \in \{1, \dots, n\} \quad P_S \{|V(f_S, z_i) - V(f_{S^i}, z_i)| \leq \beta_{CV}\} \geq 1 - \delta_{CV}. \quad (6)$$

CV_{loo} stability measures the difference between the errors at a point z_i when it is in the training set or when it is not. The definition of CV_{loo} was introduced to deal with general situations in which \mathcal{H} may not have a norm. It is much simpler in the case in which \mathcal{H} is a RKHS. Then a condition number can be defined and then a good condition number implies good CV_{loo} stability. Both definitions capture the basic idea of stability of a well-posed problem: the function “learned” from a training set should, with high probability, change little in its pointwise predictions for a small change in the training set, such as deletion of one of the examples.

Notice that we can rewrite the definition as $CV_{loo}^r = \frac{1 + \mathbf{E}(V(f_{S^i}, z_i))}{1 + \mathbf{E}(V(f_S, z_i))}$ (and require it to converge to 1 for $n \rightarrow \infty$ to ensure generalization in the classical regime). This alternative definition of CV_{loo} stability makes it almost equivalent to the condition number, when this exists.

In the modern regime, in which both n and d (or a property of \mathcal{H} equivalent to d) grow to infinity, generalization is not expected. The classical approach – of asymptotic generalization and then consistency – cannot be used because there is no fixed hypothesis space. However, the requirement of well-posedness and stability remains. When it exists meaningfully, the condition number is then the obvious definition of stability for the “modern” regime. It is an obvious notion of stability and furthermore it provides a bound on the test error: CV_{loo}^r close to 1 bounds the test error wrt to perturbations, including deletion or substitution of one example.

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