

# Gaussian RBF Centered Kernel Alignment (CKA) in the Large-Bandwidth Limit

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**Abstract**—Centered kernel alignment (CKA), also known as centered kernel-target alignment, is useful as a similarity measure between kernels and as a kernel-based similarity measure between feature representations. We prove that CKA based on a Gaussian RBF kernel converges to linear CKA in the large-bandwidth limit. The result relies on mean-centering of the feature maps and on a Hilbert-Schmidt Independence Criterion (HSIC) identity. We show that convergence onset is sensitive to the geometry of the feature representations, and that a notion of representation eccentricity,  $\rho$ , constrains the bandwidth range for which Gaussian CKA can differ noticeably from linear CKA. Our experimental results suggest that Gaussian bandwidths less than  $\rho$  should be selected in order to enable nonlinear modeling.

**Index Terms**—Nonlinear kernels, neural networks, representations, similarity.

## 1 INTRODUCTION

CENTERED Kernel Alignment (CKA) was first proposed as a measure of similarity between kernels in the context of kernel learning [1], [2], building on prior work on (non-centered) kernel-target alignment [3]. Versions for functional data of CKA and the associated Hilbert-Schmidt Independence Criterion (HSIC) were proposed later [4]. CKA has been used for multiple kernel learning (e.g., [5], [6]). CKA also enables measuring similarity between two feature representations of a set of data examples (e.g., two sets of neural network activation vectors), by comparing kernel-based similarity matrices (Gram matrices) of these representations [7]. Used in the latter manner, CKA and alternatives such as canonical correlation analysis (CCA) and orthogonal Procrustes distance [8] can provide insight into the relationship between architectural features of a network such as width and depth, and the network’s learned representations [7], [9]. CKA has been used to assess representation similarity in cross-lingual language models [10] and recurrent neural network dynamics [11], to identify potential drug side-effects [12], to differentiate among brain activity patterns [13], and to gauge the representational effects of watermarking [14], among others.

Any positive-definite symmetric kernel can be used as the base kernel for CKA, including linear, polynomial, and Gaussian radial basis function (RBF) kernels. Gaussian RBF kernels are of special interest due to their universality properties [15], which can lead to superior modeling of arbitrary nonlinearities. Understanding the behavior of CKA with Gaussian kernels is, therefore, relevant to its use as a representational similarity metric. Some prior work [7] reports finding little difference empirically between CKA similarity values based on Gaussian and linear kernels. In contrast, hyperparameter tuning experiments for [16] suggest that a noticeable difference can occur between CKA values for Gaussian and linear kernels, but also that the difference becomes negligible as Gaussian bandwidth

grows. We establish the latter phenomenon theoretically in the present paper, proving that Gaussian CKA converges to linear CKA as bandwidth approaches infinity, for all representations. We describe the convergence rate, as well.

We are not aware of published results on the large-bandwidth asymptotics of Gaussian CKA. A limit result for Gaussian kernel SVM classification appeared in [17], but rests on an analysis of the dual maximum-margin optimization problem that does not translate directly to kernel CKA.

While we find that approximation of Gaussian RBF CKA by linear CKA for large bandwidths becomes apparent by elementary means, the result relies on centering of the feature maps (and on Hilbert-Schmidt Independence Criterion properties that we also prove). Indeed, we show that a similar result fails for the non-centered kernel-target alignment of [3]. We also show that a geometric measure of representation eccentricity controls convergence of Gaussian to linear CKA, and bounds the range of bandwidths for which Gaussian and linear CKA differ for a given representation. This can be helpful in data-adaptive Gaussian bandwidth selection.

## 2 BACKGROUND AND NOTATION

Our perspective is that of measuring similarity between two feature representations of the same set of data examples. We briefly review the basic ingredients and notation related to kernel similarity and CKA below (see [7], [2]).

### 2.1 Feature representations

$X \in \mathbb{R}^{N \times p}$  and  $Y \in \mathbb{R}^{N \times q}$  will denote matrices of  $p$ -dimensional (resp.,  $q$ -dimensional) feature vectors for the same set of  $N$  data examples. Each row of  $X$  or  $Y$  consists of the feature vector for one of these examples. We use subindices to indicate the rows of  $X$  and  $Y$  (e.g.,  $x_i, y_i$ ).

### 2.2 Kernel similarity

Linear similarity between feature encodings  $X, Y$  can be expressed as similarity of their “similarity structures” (within-encoding dot product matrices)  $XX^T, YY^T$  [7]:

$$\|Y^T X\|_F^2 = \text{tr}(XX^T YY^T), \quad (1)$$

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where  $\| \cdot \|_F$  is the Frobenius norm and  $tr$  is the trace function. The left-hand side reflects similarity of the feature representations; the right-hand side reflects similarity of their respective self-similarity matrices.

CKA (defined in section 2.3) corresponds to a normalized version of Eq. 1, extended to kernel similarity by replacing  $XX^T$  and  $YY^T$  by Gram matrices  $\bar{K}(X) = (\bar{k}(x_i, x_j))_{i,j}$  and  $\bar{L}(Y) = (\bar{l}(y_i, y_j))_{i,j}$  for two positive semi-definite symmetric kernel functions,  $k$  and  $l$ . The bars indicate that columns have been mean-centered [18], [2]; see section 2.5.

Gram matrix entries can be viewed as inner products of the embedded images of the data examples in a high-dimensional reproducing kernel Hilbert space (RKHS) [19]. Thus, kernels allow modeling aspects of representations not easily accessible to the linear version.

### 2.3 HSIC and CKA

The kernel similarity perspective applied to Eq. 1 yields the Hilbert-Schmidt Independence Criterion (HSIC) [18] shown in Eq. 2, where  $N$  denotes the number of data examples, and the dependence on  $X$  and  $Y$  has been hidden for economy of notation. Mean-centering of the Gram matrices is assumed to have been carried out as described in section 2.5, below.

$$\text{HSIC}(K, L) = \frac{1}{(N-1)^2} \text{tr}(\bar{K} \bar{L}) \quad (2)$$

CKA (Eq. 3) is a normalized version of HSIC. It takes values in the interval  $[0, 1]$  if the kernel is positive semi-definite; see [2]. While this does not apply directly to CKA based on the Euclidean pseudo-kernel of Eq. 4, below, our Corollary 1 shows that CKA takes values in  $[0, 1]$  in that case, also.

$$\text{CKA}(K, L) = \frac{\text{HSIC}(K, L)}{\sqrt{\text{HSIC}(K, K) \text{HSIC}(L, L)}} \quad (3)$$

### 2.4 Kernels and Gram matrices

We consider Gram matrices  $K = (k(x_i, x_j))_{i,j}$  and  $L = (l(y_i, y_j))_{i,j}$ , where  $k(u, v)$  and  $l(u, v)$  denote positive semi-definite (p.d.) symmetric kernel functions. We focus on linear and Gaussian RBF kernels; a Euclidean pseudo-kernel (which is only conditionally p.d. [19]; see Theorem 6 of [20]) also proves to be useful. See Eq. 4, where  $\cdot$  is dot product and  $\| \cdot \|$  is Euclidean norm. Gram matrices have size  $N \times N$ , regardless of the dimensionality of the feature representation.

Linear	$K_{\text{lin}} = (x_i \cdot x_j)_{i,j}$
Gaussian, bandwidth $\sigma$	$K_{G(\sigma)} = \left( e^{-\frac{ x_i - x_j ^2}{2\sigma^2}} \right)_{i,j}$
(4)	
Euclidean (conditionally p.d.)	$K_E = \left( -\frac{ x_i - x_j ^2}{2} \right)_{i,j}$

*Note on scaling of distances in Gaussian Gram matrices:* Following the heuristic of [21] (also [7]), we use  $\sigma_X = d_X \sigma$  instead of  $\sigma$  in Eq. 4 when computing the Gaussian Gram matrix  $K_{G(\sigma)}(X)$ , where  $d_X$  is the median distance between rows of  $X$ . This ensures invariance of Gaussian HSIC under isotropic scaling [7], making  $\sigma$  itself “nondimensional”. The value  $\sigma = 2$ , for instance, denotes an actual bandwidth  $\sigma_X = 2d_X$  of twice the median distance between examples.

### 2.5 Mean-centering

Mean-centering the Gram matrices in Eq. 2 and Eq. 3 is crucial both for kernel learning [2] and for the results in this paper. Mean-centering of the Gram matrices corresponds to centering the embedded features in the RKHS, as considered in early work on kernel PCA [22].

We default to column mean-centering, that is, we ensure that each column has mean zero. Thus, we multiply by the centering matrix,  $H$ , on the left as in Eq. 5a (where  $I_N$  is the  $N \times N$  identity matrix and  $\mathbf{1}\mathbf{1}^T$  is an  $N \times N$  matrix of ones), with individual entries as in Eq. 5b. For row mean-centering,  $H$  would multiply from the right and the  $k$  summation would range over columns instead of rows.

$$\bar{K} = HK, \text{ where } H = I_N - \frac{1}{N} \mathbf{1}\mathbf{1}^T \quad (5a)$$

$$\bar{K}_{i,j} = K_{i,j} - \frac{1}{N} \sum_{k=1}^N K_{k,j} \quad (5b)$$

Our results hold for mean-centering of either rows or columns, and for simultaneous centering of both. The latter case [2] involves multiplication by  $H$  on both sides in Eq. 5a; two terms are added to the right in Eq. 5b, corresponding to subtracting  $1/N$  times the column-sum of the current Eq. 5b.

### 3 CONVERGENCE PROOF AND DERIVATION OF A BANDWIDTH-SELECTION HEURISTIC

We prove convergence of Gaussian CKA to linear CKA for large bandwidths in section 3.1, and provide a data-dependent criterion that bounds the range of Gaussian bandwidths for which nonlinear behavior occurs, in Section 3.2.

#### 3.1 Linear CKA approximation of Gaussian RBF CKA

Our main result is Theorem 1. We focus on the case in which only one of the two Gram matrix parameters uses a Gaussian RBF kernel with bandwidth  $\sigma \rightarrow \infty$ , as doing so leads to cleaner proofs; the other,  $L$ , is assumed to be any fixed, positive-definite symmetric kernel. The result holds equally if both Gram matrices are Gaussian with bandwidths approaching infinity (see Appendix in Supplemental Material).

**Theorem 1.** *CKA( $K_{G(\sigma)}$ ,  $L$ ) = CKA( $K_{\text{lin}}$ ,  $L$ ) +  $O(\frac{1}{\sigma^2})$  as  $\sigma \rightarrow \infty$ . In particular, CKA( $K_{G(\sigma)}$ ,  $L$ ) converges to CKA( $K_{\text{lin}}$ ,  $L$ ) as  $\sigma \rightarrow \infty$ . The result also holds if both kernels are Gaussian RBF kernels; in that case, the limit as both bandwidths approach infinity is CKA( $K_{\text{lin}}$ ,  $L_{\text{lin}}$ ) (i.e., it is CKA( $K_{\text{lin}}(X)$ ,  $K_{\text{lin}}(Y)$ )).*

We prove Theorem 1 by showing first, in Lemma 1, that Gaussian CKA converges to Euclidean CKA as  $\sigma \rightarrow \infty$ , and then, as a Corollary to the HSIC identity of Lemma 2, that Euclidean CKA and linear CKA are identical.

*Note:* Our results rely on mean-centering of features in Eqs. 2, 3. Indeed, the analog of Theorem 1 does not hold if, as in [3], features are not centered. This is easy to see by direct calculation for the case in which  $X$  is the  $2 \times 2$  identity and  $Y$  is a  $2 \times 2$  of ones except for a single off-diagonal 0. Linear CKA equals  $3/\sqrt{14}$  in that case, while Gaussian CKA is 1 for all  $\sigma$ , as  $X$  and  $Y$  have identical distance matrices after scaling by the median distances  $d_X, d_Y$  as described in the note in section 2.4. Details are provided in the Appendix. Lemma 2 would likewise fail without mean-centering.

**Lemma 1.**  $CKA(K_{G(\sigma)}, L) = CKA(K_E, L) + O\left(\frac{1}{\sigma^2}\right)$  as  $\sigma \rightarrow \infty$ , for any positive-definite kernel,  $L$ .

The proof of Lemma 1 also includes a large-bandwidth asymptotic result for Gaussian HSIC, in Eq. 10.

*Proof of Lemma 1:* Let  $\alpha_{i,j} = |x_i - x_j|$ . Also, let  $\sigma_X = d_X \sigma$ , where  $d_X$  is the median pairwise distance between feature vectors in  $X$ . Then, by Eq. 4 and Eq. 5b, the centered Gram matrix  $\overline{K_{G(\sigma)}}$  has the entries shown in Eq. 6. Mean-centering is an indispensable ingredient, as we will see.

$$\overline{K_{G(\sigma)}}_{i,j} = e^{-\frac{\alpha_{i,j}^2}{2\sigma_X^2}} - \frac{1}{N} \sum_{k=1}^N e^{-\frac{\alpha_{k,j}^2}{2\sigma_X^2}} \quad (6)$$

The argument uses the first-order series expansion of the exponential function at the origin (Eq. 7).

$$e^{-u} = 1 - u + O(u^2) \quad \text{as } u \rightarrow 0 \quad (7)$$

Applying Eq. 7 to the exponential terms of Eq. 6 as  $\sigma \rightarrow \infty$ , the importance of mean-centering becomes apparent. Due to subtraction of the sum for the column mean in Eq. 6, the constant 1 terms in Eq. 7 cancel, leaving only the centered Euclidean Gram matrix entries and higher-order terms:

$$\overline{K_{G(\sigma)}}_{i,j} = -\frac{\alpha_{i,j}^2}{2\sigma_X^2} + \frac{1}{N} \sum_{k=1}^N \frac{\alpha_{k,j}^2}{2\sigma_X^2} + O\left(\frac{1}{\sigma^4}\right) \quad (8)$$

The  $O\left(\frac{1}{\sigma^4}\right)$  residual persists in the HSIC expression of Eq. 2:

$$\begin{aligned} (N-1)^2 \text{HSIC}(K_{G(\sigma)}, L) &= \text{tr}(\overline{K_{G(\sigma)}} \overline{L}) \\ &= \sum_{i=1}^N \sum_{j=1}^N \left( -\frac{\alpha_{i,j}^2}{2\sigma_X^2} + \frac{1}{N} \sum_{k=1}^N \frac{\alpha_{k,j}^2}{2\sigma_X^2} \right) \overline{L}_{j,i} + O\left(\frac{1}{\sigma^4}\right) \end{aligned} \quad (9)$$

Multiplying by  $\sigma_X^2/(N-1)^2$ , we obtain the connection in Eq. 10 between  $\text{HSIC}(K_{G(\sigma)}, L)$  and  $\text{HSIC}(K_E, L)$ :

$$\sigma_X^2 \text{HSIC}(K_{G(\sigma)}, L) = \text{HSIC}(K_E, L) + O\left(\frac{1}{\sigma^2}\right) \quad (10)$$

An identity analogous to Eq. 10 relates the CKA denominator term  $\text{HSIC}(K_{G(\sigma)}, K_{G(\sigma)})$  to its Euclidean version. In the latter case, the HSIC expression involves products of two Gaussian Gram matrix entries of the sort in Eq. 8. The resulting higher-order error terms are  $O\left(\frac{1}{\sigma^6}\right)$ , because they arise from a product of the  $O\left(\frac{1}{\sigma^4}\right)$  error term from one Gram matrix entry by the  $O\left(\frac{1}{\sigma^2}\right)$  leading term in the other; multiplication by  $\sigma_X^4$  (or by  $\sigma_X^2$  after taking the square root of  $\text{HSIC}(K_{G(\sigma)}, K_{G(\sigma)})$ ) again yields a  $O\left(\frac{1}{\sigma^2}\right)$  residual.

Lemma 1 follows by dividing the HSIC term of Eq. 10 by its analog in the denominator, to form CKA as in Eq. 3:

$$\begin{aligned} CKA(K_{G(\sigma)}, L) &= \frac{\text{HSIC}(K_{G(\sigma)}, L)}{\sqrt{\text{HSIC}(K_{G(\sigma)}, K_{G(\sigma)}) \text{HSIC}(L, L)}} \\ &= CKA(K_E, L) + O\left(\frac{1}{\sigma^2}\right) \end{aligned} \quad (11)$$

The case of two Gaussian kernels with bandwidths approaching  $\infty$  (whether equal to one another or not) follows by considering one kernel argument at a time, freezing the bandwidth of the other, and using the scalar triangle inequality. Details appear in the Appendix.  $\square$

**Lemma 2.**  $\text{HSIC}(K_E, L) = \text{HSIC}(K_{\text{lin}}, L)$ , for any  $L$ .

*Proof:* First, we show that the column-centered Gram matrix entries  $\overline{K_{Ei,j}}$  can be written as  $\overline{K_{\text{lin}i,j}} + \delta_i$ , where the  $\delta_i$  term depends only on the row,  $i$ , not the column,  $j$ :

$$\begin{aligned} \overline{K_{Ei,j}} &= -\frac{|x_i - x_j|^2}{2} + \frac{1}{N} \sum_{k=1}^N \frac{|x_k - x_j|^2}{2} \\ &= -\frac{|x_i|^2}{2} - \frac{|x_j|^2}{2} + x_i \cdot x_j + \frac{1}{N} \sum_{k=1}^N \frac{|x_k|^2}{2} + \frac{1}{N} \sum_{k=1}^N \frac{|x_j|^2}{2} - \frac{1}{N} \sum_{k=1}^N x_k \cdot x_j \\ &= \left( x_i \cdot x_j - \frac{1}{N} \sum_{k=1}^N x_k \cdot x_j \right) - \frac{|x_i|^2}{2} + \frac{1}{N} \sum_{k=1}^N \frac{|x_k|^2}{2} \end{aligned}$$

The quantity in parentheses is  $\overline{K_{\text{lin}i,j}}$ , and the remaining term  $\delta_i = -\frac{|x_i|^2}{2} + \frac{1}{N} \sum_{k=1}^N \frac{|x_k|^2}{2}$  depends only on  $i$ , as stated. We can now relate the corresponding HSIC expressions:

$$\begin{aligned} \text{HSIC}(K_E, L) &= \text{tr}(\overline{K_E} \overline{L}) \\ &= \sum_{i=1}^N \sum_{j=1}^N (\overline{K_{\text{lin}i,j}} + \delta_i) \overline{L}_{j,i} \\ &= \sum_{i=1}^N \sum_{j=1}^N \overline{K_{\text{lin}i,j}} \overline{L}_{j,i} + \sum_{i=1}^N \sum_{j=1}^N \delta_i \overline{L}_{j,i} \\ &= \text{HSIC}(K_{\text{lin}}, L) + \sum_{i=1}^N \delta_i \sum_{j=1}^N \overline{L}_{j,i} \end{aligned}$$

Since the columns of  $\overline{L}$  have mean zero, the sum on the right is zero. If row-centering is used instead of column-centering, the conclusion follows by first expressing the entries of the Euclidean Gram matrix as the linear Gram matrix entries plus a term that depends only on the column.  $\square$

**Corollary 1.**  $CKA(K_E, L) = CKA(K_{\text{lin}}, L)$  for any  $L$ .

Theorem 1 follows from Lemma 1 and Corollary 1.

### 3.2 Bounding the nonlinear Gaussian bandwidth range

A bound on the  $O\left(\frac{1}{\sigma^2}\right)$  term in Theorem 1 follows along similar lines to the proof of Lemma 1, by examining in detail how the residual grows as the CKA terms are assembled. Theorem 2 shows how the relative magnitude of the residual reflects the representation-specific relative range of variation of pairwise distances between data examples in feature space, as captured by the *representation eccentricity*,  $\rho$ , of Eq. 12.

**Theorem 2.** *The residual in Lemma 1 is bounded by  $C\left(\frac{\rho}{\sigma}\right)^2$  when  $\frac{\rho}{\sigma} \leq 2$ , where  $C$  is a finite constant that does not depend on the representations  $X, Y$ , and  $\rho$  is the representation eccentricity defined in terms of the ratios of representation diameters to median distances in Eq. 12.*

$$\rho = \max\left(\frac{\text{diam}(X)}{d_X}, \frac{\text{diam}(Y)}{d_Y}\right) \quad (12)$$

Observations on the statement of Theorem 2:

1.  $\rho$  depends only on pairwise distances, and  $\rho \geq 1$ , with equality only if all pairwise distances are equal in each of  $X, Y$ .

2. The condition  $\frac{\rho}{\sigma} \leq 2$  goes beyond the statement that the result applies to the large- $\sigma$  limit, by providing a data-sensitive measure of what constitutes a “large” value of  $\sigma$ .

3. We include both  $X$  and  $Y$  in Eq. 12 to cover the case in which  $L$  is also Gaussian with bandwidth  $\rightarrow \infty$  (Appendix A.2).

*Proof of Theorem 2:* The power series for  $e^{-u}$  in Eq. 7 is alternating if  $u > 0$ , with decreasing terms after the second if  $u \leq 2$ ; the  $O(u^2)$  error term in Eq. 7 is then no larger than  $u^2/2$ . The residual is controlled by the magnitude of  $u$ . As  $u \rightarrow 0$ , the  $O(u^2)$  residual becomes negligible relative to the leading linear term. We examine the details in Eq. 8 in this light. The role of  $u$  is played by each term  $\frac{\alpha_{k,j}^2}{2\sigma_X^2}$  (including  $\frac{\alpha_{i,j}^2}{2\sigma_X^2}$ ). Expanding Eq. 6 term by term, we obtain Eq. 13 after grouping second-order (in  $u$ ) parts at far right.

$$\overline{K_{G(\sigma)}_{i,j}} \approx -\frac{\alpha_{i,j}^2}{2\sigma_X^2} + \frac{1}{N} \sum_{k=1}^N \frac{\alpha_{k,j}^2}{2\sigma_X^2} + \frac{1}{2} \frac{\alpha_{i,j}^4}{4\sigma_X^4} - \frac{1}{N} \sum_{k=1}^N \frac{1}{2} \frac{\alpha_{k,j}^4}{4\sigma_X^4} \quad (13)$$

Higher-order terms are not shown, for space reasons. The first and third terms on the right of Eq. 13 are the beginning of the power series for  $e^{-\frac{\alpha_{i,j}^2}{2\sigma_X^2}}$ , while the second and fourth correspond to the centering sum at the far right of Eq. 6. As explained above, the third and fourth terms bound the respective residuals, including omitted higher-order terms.

Since  $\alpha_{k,j} = |x_k - x_j|$  and  $\sigma_X = d_X \sigma$  as described at the beginning of the proof of Lemma 1, each  $u = \frac{\alpha_{k,j}^2}{2\sigma_X^2}$  satisfies

$$u \leq \frac{\text{diam}(X)^2}{2d_X^2 \sigma^2} \leq \frac{\rho^2}{2\sigma^2}, \quad (14)$$

where the ‘‘representation eccentricity’’,  $\rho$ , is as in Eq. 12.

The bound in Eq. 14 is uniform across all terms in Eq. 13, and it depends on the ratio  $\sigma/\rho$ , rather than on  $\sigma$  alone. We ensure  $u \leq 2$ , and therefore that the  $O(u^2)$  residual in the alternating power series of Eq. 7 will be bounded by  $\frac{u^2}{2}$ , by imposing the large- $\sigma$  condition in Eq. 15.

$$\frac{\rho}{\sigma} \leq 2 \quad (15)$$

Since  $u \leq \frac{\rho^2}{2\sigma^2}$  for each term  $u = \frac{\alpha_{k,j}^2}{2\sigma_X^2}$  in Eq. 13, the corresponding residual is at most  $\frac{u^2}{2} \leq \frac{1}{4} \left(\frac{\rho}{\sigma}\right)^4$ ; therefore, the mean of such terms at far right in Eq. 13, and the difference between the remaining positive second-order term and that mean, are also  $\leq \frac{1}{4} \left(\frac{\rho}{\sigma}\right)^4$  in absolute value, so we obtain an explicit bound on the  $O\left(\frac{1}{\sigma^4}\right)$  residual of Eq. 8, in Eq. 16.

$$\left| \frac{1}{2} \frac{\alpha_{i,j}^4}{4\sigma_X^4} - \frac{1}{N} \sum_{k=1}^N \frac{1}{2} \frac{\alpha_{k,j}^4}{4\sigma_X^4} \right| \leq \frac{1}{4} \left(\frac{\rho}{\sigma}\right)^4 \quad (16)$$

Next, we note that since HSIC (Eq. 2) is bilinear, CKA (Eq. 3) is invariant under uniform scaling of either Gram matrix  $K$  or  $L$ . We assume without loss of generality that  $L$  is bounded by 1 in absolute value.

Therefore, aggregating the  $N^2$  residual terms scaled by  $\overline{L}_{j,i}$  in Eq. 9 only multiplies the constant  $1/4$  on the right of Eq. 16 by a finite, representation-independent factor. Scaling by  $\sigma_X^2 = d_X^2 \sigma^2$  in Eq. 10 changes the  $\left(\frac{\rho}{\sigma}\right)^4$  core of the residual to  $d_X^2 \rho^2 \left(\frac{\rho}{\sigma}\right)^2$ ; the additional  $d_X^2 \rho^2$  factor can be ignored because of exact cancelation with the denominator.

We argue similarly about the analogous residuals in the denominator term  $\text{HSIC}(K_{G(\sigma)}(X), K_{G(\sigma)}(X))$  in Lemma 1,

which is the sum of the squares of the  $\overline{K_{G(\sigma)}_{i,j}}$  from Eq. 13. By Eq. 14, the leading term in Eq. 13 satisfies Eq. 17.

$$\left| -\frac{\alpha_{i,j}^2}{2\sigma_X^2} + \frac{1}{N} \sum_{k=1}^N \frac{\alpha_{k,j}^2}{2\sigma_X^2} \right| \leq \frac{\rho^2}{2\sigma^2} \quad (17)$$

We also have the bound on the Eq. 13 residual, in Eq. 16. From Eq. 13, the residual of the square  $\overline{K_{G(\sigma)}_{i,j}}^2$  is, therefore, at most twice the product  $\frac{\rho^2}{2\sigma^2} \frac{1}{4} \left(\frac{\rho}{\sigma}\right)^4$ , hence at most  $\frac{1}{4} \left(\frac{\rho}{\sigma}\right)^6$ , plus a  $O\left(\frac{1}{\sigma^8}\right)$  term that can be accommodated by slightly increasing the multiplicative constant in front of  $\left(\frac{\rho}{\sigma}\right)^4$ ; only a bounded  $\frac{1}{\sigma}$  range needs to be considered, as in Eq. 15.

Taking square roots and multiplying by the  $\text{HSIC}(L, L)$  factor in the denominator scales the residual by a finite representation-independent factor due to the bound of 1 on  $L$ , as in the above discussion for the numerator.

Including  $X$  and  $Y$  in Eq. 12 extends the above arguments to the case of two Gaussian kernels of bandwidths  $\rightarrow \infty$ .

Express the CKA quotient in the form  $R(1+a)/(1+b) = (1+a) \sum_{k=0}^{\infty} (-1)^k b^k$ , where  $R$  is the ratio of the leading terms in numerator and denominator (which equals  $\text{CKA}(K_{\text{lin}}, L)$  by Theorem 1) and  $a, b$  are relative residuals in the numerator and denominator. We see that the net CKA relative residual is approximately the difference  $a - b$  of the relative residuals. The preceding paragraphs imply that both  $a$  and  $b$  are bounded by a finite representation-independent constant times  $\left(\frac{\rho}{\sigma}\right)^2$ . Since CKA takes values in the bounded interval  $[0, 1]$ , it follows that the  $O\left(\frac{1}{\sigma^2}\right)$  absolute residual in Eq. 11 is likewise bounded by such a constant times  $\left(\frac{\rho}{\sigma}\right)^2$ . This completes the proof of Theorem 2.  $\square$

*Notes:* Theorem 2 implies that Gaussian RBF CKA approximately equals Euclidean CKA for bandwidths  $\sigma \gg \rho$ . For lower-dimensional representations  $X, Y$ , the representation eccentricity,  $\rho$ , provides a data-sensitive approximate threshold between nonlinear and linear regimes of Gaussian CKA. If feature dimensionality is high, concentration of Euclidean distance [23] will make  $\rho \approx 1$ ; hence, for high-dimensional representations, Gaussian CKA will behave linearly if  $\sigma \gg 1$ .

One might expect higher values of  $\rho$  for multimodal distributions, for example, or in the presence of outliers, as larger representation diameters can occur in these cases relative to median distance. Theorem 2 suggests that nonlinear behavior of Gaussian CKA may be more noticeable at a given bandwidth,  $\sigma$ , for such data.

## 4 EXPERIMENTAL ILLUSTRATION

In this section we describe the results of a limited number of experiments that compare CKA similarity of neural feature representations based on Gaussian kernels of different bandwidths, with linear CKA similarity. For simplicity, we restrict attention to the case in which both of the kernels  $K, L$  in Eq. 3 are of the same type, either Gaussian RBF kernels of equal bandwidth, or standard linear kernels. Software for these experiments is available from the author upon request.

*Notation:* In this section, we write  $\text{CKA}_{G(\sigma)}$  as shorthand for  $\text{CKA}(K_{G(\sigma)}, K_{G(\sigma)})$ . Likewise, we abbreviate  $\text{CKA}(K_{\text{lin}}, L_{\text{lin}})$  (i.e.,  $\text{CKA}(K_{\text{lin}}(X), K_{\text{lin}}(Y))$ ) as  $\text{CKA}_{\text{lin}}$ .

## 4.1 Experimental setup

*Data sets:* We used sample OpenML data sets [24] (CC BY 4.0 license, <https://creativecommons.org/licenses/by/4.0/>) for classification (splice, tic-tac-toe, wdbc, optdigits, wine, dna) and regression (cpu, boston, Diabetes(scikit-learn), stock, balloon, cloud); for data sets with multiple versions, we used version 1. These data sets were selected based on two considerations only: smaller size, in order to eliminate the need for GPU acceleration and reduce environmental impact; and an absence of missing values, to simplify the development of internal feature representations for the CKA computations. Data set sizes are given in Table 1.

*Neural feature representations:* Fully-connected neural networks (NN) with two hidden layers were used. Feature encodings  $X, Y$  were the sets of activation vectors of the first and second hidden layers, respectively. Alternative NN widths,  $w = 16, 32, 64, 128, 256, 512, 1024$  were tested, with  $w$  and  $\frac{w}{4}$  hidden nodes in the first and second hidden layers. A configuration with three hidden layers, of sizes 128, 32, 8, was also tested, for which  $X, Y$  were the activation vectors from layers 1 and 3.

*Implementation:* NN were trained using the `MLPClassifier` and `MLPRegressor` classes in `scikit-learn` [25], with cross-entropy or quadratic loss for classification and regression, respectively, ReLU activation functions, Glorot-He pseudorandom initialization [26], [27], Adam optimizer [28], learning rate of 0.001, and a maximum of 2000 training iterations. CKA was implemented in Python (<https://docs.python.org/3/license.html>), using NumPy [29] (<https://numpy.org/doc/stable/license.html>) and Matplotlib [30] (PSF license, <https://docs.python.org/3/license.html>). Experiments were performed on a workstation with an Intel i9-7920X (12 core) processor and 128GB RAM, under Ubuntu 18.04.5 LTS (GNU public license).

*Experiments:* 50 runs were performed for each pair  $(D, w)$  of a data set  $D$  and NN width  $w$ . In each run, a new NN model was trained on the full data set, starting from fresh pseudorandom initial parameter values. A training run was repeated if the resulting in-sample accuracy was below 0.8 (classification) or if in-sample coefficient of determination was below 0.5 (regression), but not if the optimization had not converged within the allowed number of iterations. After the network had been trained in a given run,  $CKA_{lin}$  was computed once, and  $CKA_{G(\sigma)}$  was computed for each bandwidth  $\sigma = 2^p$ ,  $p = -4, -3, \dots, 8$ , for a total of 50  $CKA_{lin}$  and 650  $CKA_{G(\sigma)}$  evaluations per  $(D, w)$  pair.

*Compute time:* Compute time for the results presented in the paper was approximately 32 hours, much of it on the  $8 \cdot 12 \cdot (50 + 650) = 67200$  CKA evaluations needed across the 8 network widths (including the 128-32-8 three-hidden-layer configuration) and the 12 data sets. Additional runs for validation required another 12 hours. Several shorter preliminary runs were carried out for debugging and initial selection of the NN hyperparameters; configurations and threshold values were selected empirically in order to ensure a successful end to training after no more than a handful of runs in nearly all cases. Total compute time across all runs is estimated to have been 50 hours.

*Evaluation metrics:* CKA means and standard errors (SE = standard deviation divided by  $\sqrt{50}$ ), and medians and

standard error equivalents (SE = inter-quartile range divided by  $\sqrt{50}$ ) of the ratio  $\rho$  of Eq. 12 were computed across runs. We measured the magnitude of the discrepancy between  $CKA_{G(\sigma)}$  and  $CKA_{lin}$  by the base-2 logarithm of the relative difference between the two measures as in Eq. 18.

$$\log_2 \text{ rel. CKA difference} = \log_2 \left( \frac{|CKA_{G(\sigma)} - CKA_{lin}|}{CKA_{lin}} \right) \quad (18)$$

Theorem 1 implies that, for large  $\sigma$ , the logarithmic relative difference of Eq. 18 should decrease along a straight line of slope  $-2$  as a function of  $\log_2 \sigma$ , reflecting a  $O(1/\sigma^2)$  dependence. Accordingly, for each data set, we determined a  $1/\sigma^2$  asymptote by extrapolating backward from the largest tested bandwidth value,  $\sigma = 2^8$ . If  $\sigma < 2^8$ , the predicted  $\log_2$  relative difference along the  $1/\sigma^2$  asymptote is as in Eq. 19, where  $r_8$  is the observed relative difference at  $\sigma = 2^8$ .

$$\text{predicted } \log_2(\text{rel. CKA diff. at } \sigma) = \log_2 r_8 - 2(\log_2 \sigma - 8) \quad (19)$$

We determined a  $1/\sigma^2$  convergence onset bandwidth,  $\sigma_0^*$  (Eq. 20), as the minimum bandwidth above which the observed  $\log_2$  relative difference between Gaussian and linear CKA differs by less than 0.25 from its predicted value in Eq. 19, uniformly along that data set's  $1/\sigma^2$  asymptote.

$$\sigma_0^* = \min\{\sigma_0 \mid \log \text{ rel. diff.}(\sigma) < 0.25 \text{ for all } \sigma \geq \sigma_0\} \quad (20)$$

Threshold values other than 0.25 in Eq. 20 (1, 0.5, 0.1), corresponding to different tolerances for the log relative difference, yielded similar results in most cases in terms of the resulting relative  $\sigma_0^*$  ranks of the different data sets.

## 4.2 Discussion of experimental results

The results show a range of geometric characteristics of learned feature representations across data sets, seen as differences in the representation eccentricity,  $\rho$ , defined in Eq. 12. Geometry is stable for a given data set, as indicated by a small standard deviation for  $\rho$ , with some dependence on network size. See Table 2 for the case of regression; the Appendix includes the information for classification.

We observe generally lower values of  $\rho$  (Eq. 12) for wider networks in Table 2. This is consistent with expectations, as concentration of Euclidean distance in high dimensions [23] will bring the ratio of maximum to median distance between feature vectors closer to 1 as network width grows. The balloon data set is the only one for which  $\rho$  increases with network width. That data set contains a small group of examples with lower values of the two attributes than the rest (indices 332, 706, 969, 1025, 1041, 1399, 1453, 1510). Those examples are increasingly distant from the majority (in units of median distance) in the deeper (second or third) hidden layer representations as width increases, driving the increase in  $\rho$ ; the ratio of maximum to median distance in the first hidden layer representation does not exhibit similar growth.

Dimensionality of the raw data sets (Table 1) appears to filter into the learned neural representations, as well. For a fixed network width, the correlation between raw data dimensionality and  $\rho$  is unambiguously negative, between  $-0.38$  and  $-0.33$  for classification, and between  $-0.8$  and  $-0.85$  for regression, even though representation dimensionality is fixed by network width.

TABLE 1  
 Sizes of the data sets considered in the experimental evaluation.

data set	Classification		data set	Regression	
	examples	attributes		examples	attributes
splice	3190	60	cpu	209	7
tic-tac-toe	958	9	boston	506	13
wdbc	569	30	Diabetes(scikit-learn)	442	10
optdigits	5620	64	stock	950	9
wine	178	13	balloon	2001	1
dna	3186	180	cloud	108	5

TABLE 2  
 Median ratios,  $\rho = \max(\text{diam}(X)/d_X, \text{diam}(Y)/d_Y)$ , and  $\pm 2$  standard error equivalent confidence intervals, of maximum to median distance between features.  $w$  is NN width. Regression.

$w$	cpu	boston	Diab(skl)	stock	balloon	cloud
16	10.63 $\pm$ 0.53	5.08 $\pm$ 0.54	4.87 $\pm$ 0.01	3.09 $\pm$ 0.28	14.62 $\pm$ 0.88	6.59 $\pm$ 0.45
32	9.60 $\pm$ 0.58	3.87 $\pm$ 0.23	4.86 $\pm$ 0.01	2.68 $\pm$ 0.14	15.64 $\pm$ 0.83	5.76 $\pm$ 0.38
64	9.23 $\pm$ 0.29	3.57 $\pm$ 0.29	4.86 $\pm$ 0.01	2.62 $\pm$ 0.12	16.25 $\pm$ 0.90	5.99 $\pm$ 0.26
128	9.15 $\pm$ 0.20	3.61 $\pm$ 0.11	4.85 $\pm$ 0.01	2.50 $\pm$ 0.05	18.49 $\pm$ 0.86	5.84 $\pm$ 0.19
256	9.19 $\pm$ 0.16	3.40 $\pm$ 0.07	4.84 $\pm$ 0.01	2.48 $\pm$ 0.05	20.70 $\pm$ 0.88	6.05 $\pm$ 0.10
512	8.91 $\pm$ 0.12	3.38 $\pm$ 0.04	4.84 $\pm$ 0.01	2.44 $\pm$ 0.04	22.65 $\pm$ 0.72	6.20 $\pm$ 0.12
1024	8.82 $\pm$ 0.11	3.42 $\pm$ 0.03	4.82 $\pm$ 0.04	2.43 $\pm$ 0.02	25.18 $\pm$ 1.14	6.16 $\pm$ 0.19
128-32-8	9.96 $\pm$ 0.54	3.91 $\pm$ 0.24	4.83 $\pm$ 0.01	3.11 $\pm$ 0.25	22.71 $\pm$ 2.97	7.30 $\pm$ 0.23

Noticeable differences between Gaussian and linear CKA occur for small bandwidths: Mean relative difference values between  $CKA_{G(\sigma)}$  and  $CKA_{lin}$  greater than 0.2 ( $\log_2$  values greater than  $-2.3$ ), are observed for several data sets when  $\sigma \leq 0.25$  (when  $\log_2 \sigma \leq -2$ ) in the case of classification; in fact, relative CKA difference values greater than 0.7 ( $\log_2$  rel. CKA diff.  $> -0.5$ , values in the Appendix) are observed for the dna data set when network width  $w$  is 128 or greater. This shows that noticeably nonlinear behavior of Gaussian CKA is quite possible for small bandwidth values. For some classification data sets, however (wdbc, wine), and most regression data sets, the relative CKA difference remains comparatively small for all bandwidths.

Gaussian CKA converges to linear CKA like  $1/\sigma^2$ : Fig. 1 shows confidence intervals for the means, of radius two standard errors, of the observed  $\log_2$  relative difference between  $CKA_{G(\sigma)}$  and  $CKA_{lin}$  as a function of Gaussian bandwidth,  $\sigma$  (Eq. 18). Convergence at the rate  $1/\sigma^2$  for  $\sigma \gg 1$  is observed (log-log slope of  $-2$  in Fig. 1), as described in Theorem 1. Results are stable across the range of neural network configurations tested. Standard error of the relative CKA difference is observed to decrease as network width increases (e.g., Fig. 2), suggesting that wider networks are less sensitive to variations in initial parameter values.

The Diabetes(scikit-learn) data set stands out for having, by far, the smallest mean relative CKA difference among data sets tested, across much of the  $\sigma$  range. The neural feature maps  $X$  and  $Y$  for that data set have nearly proportional linear Gram matrices  $K_{lin}$  and  $L_{lin}$ , hence the linear CKA value is very close to 1. Because the matrix of squared inter-example distances depends linearly on the linear Gram matrix, the Gaussian CKA value is also very close to 1.

The representation eccentricity  $\rho$  (Eq. 12) is reflected in convergence onset: Our experimental results suggest that noticeably nonlinear behavior of Gaussian CKA occurs almost exclusively for bandwidths  $\sigma < \rho$ : for all data sets

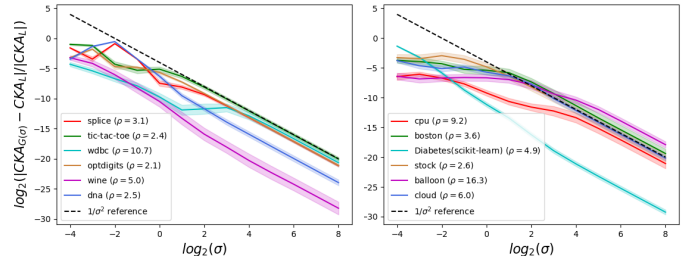


Fig. 1. Relative difference between Gaussian and linear CKA for neural feature representations of classification (left) and regression (right) data sets. Neural network width is  $w = 64$ . Shading extends two standard errors from the mean. Dotted reference line of slope  $-2$  indicates  $1/\sigma^2$  relationship. Gaussian CKA (bandwidth  $\sigma$ ) converges to linear CKA like  $1/\sigma^2$  as  $\sigma \rightarrow \infty$ , for all network widths. Onset of  $1/\sigma^2$  convergence is delayed for representations of high eccentricity,  $\rho$  (Table 3).

tested, the observed mean  $\log_2$  relative difference between linear and Gaussian CKA is less than 0.01 when  $\sigma > \rho$ , where  $\rho$  is the ratio of maximum to median distance between feature vectors (Eq. 12). This confirms our finding in section 3.2 that  $CKA_{G(\sigma)}$  differs little from  $CKA_{lin}$  if  $\sigma \gg \rho$ . The results further suggest that the threshold between nonlinear and linear regimes of Gaussian CKA is not substantially less than  $\rho$ : while mean relative CKA difference for  $\sigma \geq 1$  peaked under 0.1 for two-hidden-layer neural representations, across all data sets tested, relative difference values less than 0.1 occur for the tic-tac-toe data set in the three-layer 128-32-8 representation only when  $\sigma \geq 4$ ; the lower end of this bandwidth range is quite close to the median  $\rho$  value of 4.2 for that representation (which differs from the width-64 two-layer representation in Figs. 1, 2).

Fig. 3 shows a noticeable positive correlation between  $\rho$  and convergence onset bandwidth,  $\sigma_0^*$  (Eq. 20), across all data sets and network widths; correlation is 0.85 to two digits.

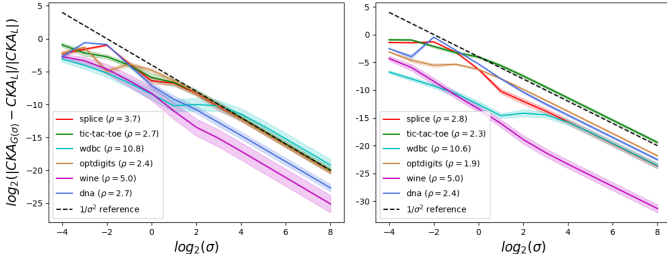


Fig. 2. Relative difference between Gaussian and linear CKA for neural feature representations associated with networks of different widths  $w = 32$  (left) and  $w = 256$  (right). Classification data sets. Shading extends two standard errors from the mean.  $1/\sigma^2$  convergence is observed in both cases, as well as for all tested widths not shown. Wider networks are less sensitive to initial parameter values, as evidenced by lower standard error of the CKA relative difference; values appear in the Appendix.

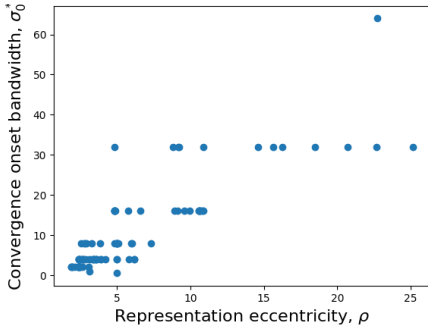


Fig. 3. Eccentricity vs. convergence onset. Classification and regression.

We find additional support for the view that  $\rho$  approximates the boundary between nonlinear and linear regimes of Gaussian CKA in the fact that  $\sigma_0^*$  is largest for the data sets of largest  $\rho$ : median  $\log_2 \sigma_0^* = 5, 4, 4$  for balloon ( $\rho \approx 16$ ), wdbc ( $\rho \approx 11$ ), cpu ( $\rho \approx 9$ ), respectively ( $\sigma_0^*$  and  $\rho$  values differ slightly among network widths and depths, but data sets of largest  $\rho$  are the same). See Table 3. Diabetes(scikit-learn) ties for third with  $\log_2 \sigma_0^* = 4$ ; median  $\log_2 \sigma_0^* < 4$  for all other data sets tested.

Our experimental results as a whole confirm  $1/\sigma^2$  convergence of  $CKA_{G(\sigma)}$  to  $CKA_{lin}$  as  $\sigma \rightarrow \infty$  (Theorem 1, 2), and support the use of the representation eccentricity,  $\rho$  (Eq. 12), as a useful heuristic upper bound on the range of bandwidths for which Gaussian CKA can display nonlinear behavior.

## 5 CONCLUSIONS

This paper considered the large-bandwidth asymptotics of CKA using Gaussian RBF kernels. We proved that mean-centering of the feature maps ensures that Gaussian RBF CKA converges to linear CKA in the large bandwidth limit, with an  $O(1/\sigma^2)$  asymptotic relative difference; we also proved related results for HSIC. We showed that an analogous result fails for the non-centered kernel alignment measure of [3].

Furthermore, we showed that the geometry of the feature representations impacts the bandwidth range for which Gaussian CKA can behave nonlinearly, by proving that the nonlinear residual is of order  $O((\rho/\sigma)^2)$ , where  $\rho$  is the representation eccentricity ratio,  $\rho$ , of maximum to median distance between feature vectors. Our experimental results

suggest that bandwidth values  $\sigma < \rho$  can lead to noticeably nonlinear behavior of Gaussian CKA, whereas bandwidths  $\sigma \geq \rho$  will yield essentially linear behavior. In order to enable nonlinear modeling, the bandwidth should, therefore, be selected in the interval  $(0, \rho)$ .

## 6 FUTURE WORK

Representation eccentricity,  $\rho$ , correlates well with the bandwidth at which Gaussian CKA transitions between nonlinear and linear regimes, and our theoretical results establish convergence of Gaussian to linear CKA for large bandwidths. One direction for future work is to seek additional representation characteristics that, in conjunction with eccentricity, can better gauge the order of magnitude of the Gaussian-linear CKA difference for a given representation. Such work could provide further guidance in selecting between Gaussian and linear CKA kernels in specific applications.

Robust versions of the representation eccentricity can also be explored, in which maximum and median distance are replaced by other quantile pairs of the distance distribution.

## DECLARATIONS

This work did not involve human subjects. Data sets do not include any personally identifiable information or offensive content. The author has no conflicts of interest to report.

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TABLE 3  
Log bandwidth,  $\log_2 \sigma_0^*$ , of  $1/\sigma^2$  convergence onset.  $w$  denotes network width.

$w$	Classification						Regression					
	splice	t-t-t	wdbc	optd	wine	dna	cpu	bost	diab	stock	balln	cloud
16	2	2	5	2	-1	2	4	3	4	1	5	4
32	2	2	4	1	3	2	4	3	4	1	5	4
64	2	2	4	1	3	3	5	2	4	2	5	3
128	3	1	4	1	2	2	4	2	4	1	5	2
256	3	1	4	1	3	2	5	2	4	1	5	3
512	3	1	4	1	3	2	4	2	4	1	5	2
1024	2	1	4	1	3	2	5	2	5	1	5	2
128-32-8	3	2	4	1	2	2	4	2	3	0	6	3

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## APPENDIX A

### SUPPLEMENTARY INFORMATION FOR THE PAPER Gaussian RBF CKA in the large bandwidth limit

#### A.1 Details of the counterexample for non-centered kernel alignment in section 3.1

Theorem 1 hinges on the assumption that the Gram matrices are mean-centered. We show here that an analogous convergence result does not hold for the non-centered kernel alignment of [3], by considering the feature matrices below.

$$X = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad Y = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}$$

In order to compute  $\text{CKA}(K_{G(\sigma)}, L_{G(\sigma)})$ , we first compute, for each of the feature matrices  $X$  and  $Y$ , the corresponding matrix of distances between pairs of feature vectors (rows):

$$D(X) = \begin{bmatrix} 0 & \sqrt{2} \\ \sqrt{2} & 0 \end{bmatrix} \quad D(Y) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$D(X)$  and  $D(Y)$  are scalings of one another. Given a bandwidth,  $\sigma$ , we interpret  $\sigma$  as expressed in units of median distance, as in the note in section 2.4. If diagonal zeros are included in the median computation, then  $\sigma_X = d_X \sigma = \frac{\sigma}{\sqrt{2}}$

in the non-centered Gaussian entries  $e^{-\frac{|x_i - x_j|^2}{2\sigma_X^2}}$  of  $K_{G(\sigma)}$ , and  $\sigma_Y = d_Y \sigma = \frac{\sigma}{2}$  in the entries  $e^{-\frac{|y_i - y_j|^2}{2\sigma_Y^2}}$  of  $L_{G(\sigma)}$ . The non-centered matrices  $K_{G(\sigma)}(X)$  and  $L_{G(\sigma)}(Y)$  are identical:

$$K_{G(\sigma)}(X) = \begin{bmatrix} 1 & e^{-\frac{2}{\sigma^2}} \\ e^{-\frac{2}{\sigma^2}} & 1 \end{bmatrix} = L_{G(\sigma)}(Y)$$

Thus, numerator and denominator of the non-centered CKA expression are also equal, so Gaussian CKA has the value 1:

$$\begin{aligned} \text{CKA}(K_{G(\sigma)}, L_{G(\sigma)}) &= \frac{\text{tr}(K_{G(\sigma)} L_{G(\sigma)})}{\sqrt{\text{tr}(K_{G(\sigma)} K_{G(\sigma)}) \text{tr}(L_{G(\sigma)} L_{G(\sigma)})}} \\ &= \frac{(1 + e^{-\frac{2}{\sigma^2}})^2}{\sqrt{(1 + e^{-\frac{2}{\sigma^2}})^2 (1 + e^{-\frac{2}{\sigma^2}})^2}} = 1 \end{aligned} \quad (21)$$

Different intermediate numerical values occur if diagonal zeros in  $D(X)$  and  $D(Y)$  are excluded from the median computation, but the final result in Eq. 21 is the same.

Now consider a linear kernel. First, compute the Gram matrices of pairwise dot products between rows:

$$K_{\text{lin}}(X) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad L_{\text{lin}}(Y) = \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix}$$

We find non-centered linear CKA straight from the definition:

$$\begin{aligned} \text{CKA}(K_{\text{lin}}, L_{\text{lin}}) &= \frac{\text{tr}(K_{\text{lin}} L_{\text{lin}})}{\sqrt{\text{tr}(K_{\text{lin}} K_{\text{lin}}) \text{tr}(L_{\text{lin}} L_{\text{lin}})}} \\ &= \frac{1 + 2}{\sqrt{(1 + 1)(2 + 5)}} = \frac{3}{\sqrt{14}} \end{aligned} \quad (22)$$

Eqs. 21 and 22 show that, without centering, Gaussian and linear CKA remain at a fixed positive distance from one another in this example for all bandwidths  $\sigma$ . This proves that an analog of Theorem 1 fails for non-centered CKA. For these same  $X, Y$ , also note  $\text{HSIC}(K_E, L_{\text{lin}}) \neq \text{HSIC}(K_{\text{lin}}, L_{\text{lin}})$ , so the analog of Lemma 2 also fails without mean-centering.

#### A.2 Proof of Theorem 1 in case of two Gaussian kernels

The proofs in the paper focus on the case in which one kernel is Gaussian with bandwidth  $\sigma \rightarrow \infty$  and the other is a fixed kernel,  $L$ . We show here how, as indicated at the end of the proof of Lemma 1, the case of two Gaussian kernels with large bandwidths follows by a triangle inequality argument. We will abbreviate  $\text{CKA}(K, L)$  as  $C(K, L)$ ; note that the feature representations in  $K, L$  are  $X, Y$ , respectively.

First, we address Lemma 1 in the case of two Gaussian kernels. Begin by decomposing the target difference between Gaussian and Euclidean CKA as follows:

$$\begin{aligned} C(K_{G(\sigma_1)}, L_{G(\sigma_2)}) - C(K_E, L_E) &= \\ C(K_{G(\sigma_1)}, L_{G(\sigma_2)}) - C(K_E, L_{G(\sigma_2)}) + C(K_E, L_{G(\sigma_2)}) - C(K_E, L_E) \end{aligned}$$

Given any desired tolerance,  $\epsilon > 0$ , the single-Gaussian case of Lemma 1 as proved in the main text (together with symmetry of CKA in its two arguments) shows that there exists a bandwidth  $\underline{\sigma}_2$ , such that the difference term at far right, above, is less than  $\epsilon/2$  in absolute value whenever  $\sigma_2 > \underline{\sigma}_2$ .

Having fixed the bandwidth  $\underline{\sigma}_2$ , there similarly exists a bandwidth  $\underline{\sigma}_1$  such that the absolute value of the first difference term on the right-hand side above is less than  $\epsilon/2$  whenever  $\sigma_1 > \underline{\sigma}_1$ . By the scalar triangle inequality, it now follows that the absolute value of the target difference on the left-hand side above is smaller than  $\epsilon$  whenever both  $\sigma_1 > \underline{\sigma}_1$  and  $\sigma_2 > \underline{\sigma}_2$ .

This argument proves Lemma 1 in the case of two Gaussian kernels: as  $\sigma_1, \sigma_2 \rightarrow \infty$ ,

$$C(K_{G(\sigma_1)}, L_{G(\sigma_2)}) = C(K_E, L_E) + O\left(\frac{1}{\min(\sigma_1, \sigma_2)^2}\right) \quad (23)$$

Lemma 2 and its Corollary hold for any kernel  $L$ , including the Euclidean pseudo-kernel,  $L_E$ :

$$C(K_E, L_E) = C(K_{\text{lin}}, L_{\text{lin}}) \quad (24)$$

Theorem 1 for two Gaussian kernels follows from Eqs. 23, 24. The  $\min(\sigma_1, \sigma_2)$  term in Eq. 23 motivates the form of  $\rho$  in Eq. 12, via the reasoning behind Eq. 14.

#### A.3 CKA difference for three-layer NN architecture

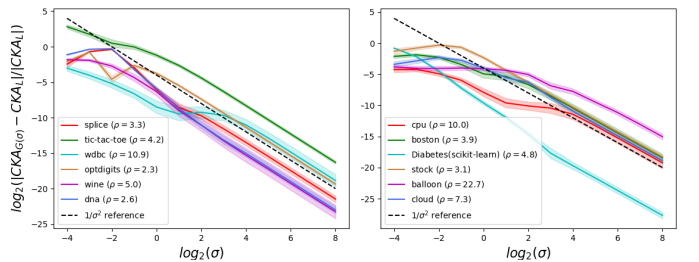


Fig. 4. Relative difference between Gaussian and linear CKA for neural feature representations of classification (left) and regression (right) data sets. Three-layer 128-32-8 neural network configuration. Shading extends two standard errors from the mean. Dotted reference line of slope  $-2$  indicates  $1/\sigma^2$  relationship. Gaussian CKA (bandwidth  $\sigma$ ) is observed to converge to linear CKA like  $1/\sigma^2$  as  $\sigma \rightarrow \infty$ . Onset of  $1/\sigma^2$  convergence is delayed for data sets of large  $\rho$  (see text).

**A.4 Results tables for section 4.2 experiments**

**TABLE 4**  
Mean rel. difference  $\log_2(|CKA_{G(\sigma)} - CKA_{lin}|/CKA_{lin})$ .  
NN width  $w = 16$ . Classification.

$\log_2 \sigma$	splice	tic-tac-toe	wdbc	optdigits	wine	dna
-4	-1.28	-1.34	-2.25	-0.83	-2.21	-0.80
-3	-0.54	-2.04	-3.03	-1.75	-2.54	-0.40
-2	-1.29	-2.12	-4.08	-3.66	-3.58	-1.51
-1	-3.99	-3.12	-5.46	-2.92	-4.85	-4.64
0	-5.52	-4.29	-6.70	-3.70	-6.87	-6.21
1	-5.78	-5.41	-8.33	-4.97	-8.81	-6.84
2	-7.30	-6.88	-8.12	-6.70	-11.00	-8.50
3	-9.19	-8.70	-8.96	-8.63	-12.83	-10.42
4	-11.17	-10.66	-9.97	-10.61	-14.82	-12.39
5	-13.16	-12.64	-11.70	-12.61	-16.83	-14.39
6	-15.16	-14.64	-13.64	-14.61	-18.84	-16.39
7	-17.16	-16.64	-15.63	-16.61	-20.84	-18.39
8	-19.16	-18.64	-17.62	-18.61	-22.84	-20.39

**TABLE 5**  
Mean rel. difference  $\log_2(|CKA_{G(\sigma)} - CKA_{lin}|/CKA_{lin})$ .  
NN width  $w = 32$ . Classification.

$\log_2 \sigma$	splice	tic-tac-toe	wdbc	optdigits	wine	dna
-4	-2.29	-0.94	-3.08	-2.27	-2.73	-2.77
-3	-1.60	-2.18	-4.05	-1.28	-3.35	-0.60
-2	-0.99	-2.74	-5.23	-4.98	-4.62	-0.89
-1	-3.83	-4.04	-6.72	-3.87	-6.39	-4.01
0	-6.39	-5.88	-8.43	-4.80	-8.30	-7.12
1	-6.78	-6.68	-10.19	-6.37	-10.99	-9.20
2	-8.30	-8.17	-10.01	-8.24	-13.46	-10.80
3	-10.35	-10.05	-10.20	-10.20	-15.15	-12.75
4	-12.19	-12.03	-11.45	-12.19	-17.1	-14.71
5	-14.18	-14.02	-13.27	-14.19	-19.1	-16.69
6	-16.17	-16.02	-15.22	-16.19	-21.11	-18.69
7	-18.17	-18.02	-17.21	-18.19	-23.11	-20.69
8	-20.17	-20.02	-19.21	-20.19	-25.11	-22.69

**TABLE 6**  
Mean rel. difference  $\log_2(|CKA_{G(\sigma)} - CKA_{lin}|/CKA_{lin})$ .  
NN width  $w = 64$ . Classification.

$\log_2 \sigma$	splice	tic-tac-toe	wdbc	optdigits	wine	dna
-4	-1.57	-0.99	-4.30	-3.18	-3.21	-3.43
-3	-3.44	-1.18	-5.4	-1.78	-4.15	-1.32
-2	-0.86	-4.28	-6.69	-4.70	-6.03	-0.53
-1	-3.44	-5.30	-7.89	-4.81	-8.24	-3.42
0	-7.45	-5.12	-9.74	-5.67	-10.49	-6.29
1	-8.09	-6.32	-11.90	-7.25	-13.27	-9.53
2	-9.34	-8.12	-11.71	-9.14	-15.92	-11.70
3	-11.19	-10.06	-11.51	-11.12	-18.06	-13.91
4	-13.15	-12.05	-12.87	-13.11	-20.29	-15.93
5	-15.14	-14.05	-14.71	-15.11	-22.31	-17.96
6	-17.14	-16.05	-16.67	-17.11	-24.24	-19.96
7	-19.14	-18.05	-18.66	-19.11	-26.23	-21.97
8	-21.14	-20.05	-20.66	-21.11	-28.23	-23.97

**TABLE 7**  
Mean rel. difference  $\log_2(|CKA_{G(\sigma)} - CKA_{lin}|/CKA_{lin})$ .  
NN width  $w = 128$ . Classification.

$\log_2 \sigma$	splice	tic-tac-toe	wdbc	optdigits	wine	dna
-4	-1.53	-0.97	-5.84	-2.96	-3.82	-2.76
-3	-1.75	-1.04	-7.05	-3.04	-5.25	-3.80
-2	-1.03	-2.83	-8.33	-5.01	-7.65	-0.46
-1	-3.31	-4.17	-9.70	-5.24	-10.18	-3.13
0	-7.09	-4.49	-11.86	-6.08	-12.56	-5.65
1	-9.31	-5.94	-13.17	-7.72	-15.33	-8.56
2	-10.32	-7.80	-13.25	-9.63	-18.46	-11.12
3	-12.10	-9.76	-13.76	-11.61	-20.20	-13.27
4	-14.05	-11.75	-15.07	-13.60	-22.23	-15.45
5	-16.04	-13.75	-16.90	-15.60	-24.26	-17.33
6	-18.04	-15.75	-18.86	-17.60	-26.27	-19.32
7	-20.04	-17.75	-20.85	-19.60	-28.27	-21.32
8	-22.04	-19.75	-22.85	-21.60	-30.27	-23.32

**TABLE 8**  
Mean rel. difference  $\log_2(|CKA_{G(\sigma)} - CKA_{lin}|/CKA_{lin})$ .  
NN width  $w = 256$ . Classification.

$\log_2 \sigma$	splice	tic-tac-toe	wdbc	optdigits	wine	dna
-4	-1.43	-0.94	-6.75	-3.12	-4.30	-2.52
-3	-1.48	-0.97	-7.98	-4.65	-5.93	-3.99
-2	-1.31	-2.14	-9.24	-5.54	-8.42	-0.47
-1	-3.22	-3.25	-10.63	-5.35	-10.98	-2.88
0	-6.27	-4.05	-12.57	-6.28	-13.40	-5.30
1	-10.21	-5.59	-14.61	-7.94	-16.01	-7.96
2	-12.02	-7.46	-14.16	-9.85	-18.90	-10.36
3	-13.77	-9.43	-14.44	-11.83	-21.26	-12.50
4	-15.70	-11.42	-15.80	-13.82	-23.34	-14.52
5	-17.69	-13.42	-17.64	-15.82	-25.34	-16.52
6	-19.67	-15.42	-19.61	-17.82	-27.34	-18.52
7	-21.66	-17.42	-21.60	-19.82	-29.33	-20.52
8	-23.66	-19.42	-23.59	-21.82	-31.33	-22.53

**TABLE 9**  
Mean rel. difference  $\log_2(|CKA_{G(\sigma)} - CKA_{lin}|/CKA_{lin})$ .  
NN width  $w = 512$ . Classification.

$\log_2 \sigma$	splice	tic-tac-toe	wdbc	optdigits	wine	dna
-4	-1.34	-0.60	-7.68	-3.27	-5.05	-2.40
-3	-1.39	-0.63	-8.90	-5.91	-7.02	-3.27
-2	-1.16	-1.71	-10.17	-5.70	-9.59	-0.45
-1	-3.01	-2.81	-11.52	-5.51	-12.10	-2.68
0	-5.71	-3.69	-13.38	-6.48	-14.47	-5.09
1	-9.51	-5.23	-14.60	-8.15	-17.21	-7.63
2	-12.15	-7.10	-14.53	-10.06	-19.76	-9.91
3	-14.51	-9.06	-14.86	-12.04	-21.92	-12.00
4	-16.45	-11.05	-16.14	-14.04	-24.06	-14.02
5	-18.45	-13.05	-17.98	-16.03	-26.11	-16.02
6	-20.45	-15.05	-19.94	-18.03	-28.13	-18.03
7	-22.45	-17.05	-21.93	-20.03	-30.13	-20.03
8	-24.45	-19.05	-23.93	-22.03	-32.13	-22.03

TABLE 10  
Mean rel. difference  $\log_2(|CKA_{G(\sigma)} - CKA_{lin}|/CKA_{lin})$ .  
NN width  $w = 1024$ . Classification.

$\log_2 \sigma$	splice	tic-tac-toe	wdbc	optdigits	wine	dna
-4	-1.40	-0.67	-7.96	-3.29	-5.01	-2.44
-3	-1.57	-0.72	-9.40	-4.01	-6.95	-4.48
-2	-0.72	-1.97	-10.78	-4.81	-9.55	-0.38
-1	-2.73	-3.06	-11.84	-5.81	-12.18	-2.56
0	-5.28	-3.93	-13.24	-6.60	-14.67	-4.98
1	-8.57	-5.46	-13.84	-8.23	-17.52	-7.49
2	-11.26	-7.32	-13.95	-10.13	-20.21	-9.75
3	-13.32	-9.29	-14.43	-12.11	-22.60	-11.83
4	-15.36	-11.28	-15.89	-14.10	-24.46	-13.85
5	-17.37	-13.28	-17.73	-16.10	-26.47	-15.86
6	-19.37	-15.28	-19.70	-18.10	-28.48	-17.86
7	-21.37	-17.28	-21.69	-20.10	-30.48	-19.86
8	-23.37	-19.28	-23.69	-22.10	-32.49	-21.86

TABLE 13  
Mean rel. difference  $\log_2(|CKA_{G(\sigma)} - CKA_{lin}|/CKA_{lin})$ .  
NN width  $w = 32$ . Regression.

$\log_2 \sigma$	cpu	boston	Diab(skl)	stock	balloon	cloud
-4	-4.60	-2.91	-1.63	-2.90	-7.09	-3.94
-3	-4.67	-2.84	-3.43	-2.89	-7.61	-4.59
-2	-5.43	-3.57	-5.88	-2.47	-7.47	-3.74
-1	-6.77	-4.74	-8.64	-2.82	-7.50	-3.62
0	-7.95	-4.92	-11.10	-4.25	-7.71	-4.48
1	-9.01	-5.67	-13.36	-6.00	-8.17	-5.53
2	-10.07	-7.08	-16.02	-7.78	-8.49	-7.37
3	-10.37	-8.95	-18.57	-9.75	-9.84	-9.76
4	-11.42	-10.88	-20.81	-11.77	-10.58	-11.83
5	-13.24	-12.87	-22.88	-13.80	-12.05	-13.88
6	-15.21	-14.87	-24.90	-15.82	-13.95	-15.88
7	-17.20	-16.87	-26.90	-17.83	-15.99	-17.88
8	-19.20	-18.87	-28.90	-19.84	-17.94	-19.88

TABLE 11  
Mean rel. difference  $\log_2(|CKA_{G(\sigma)} - CKA_{lin}|/CKA_{lin})$ .  
Three-layer 128-32-8 NN. Classification.

$\log_2 \sigma$	splice	tic-tac-toe	wdbc	optdigits	wine	dna
-4	-2.46	2.82	-3.03	-2.1	-1.82	-1.13
-3	-0.68	1.76	-4.02	-0.76	-1.91	-0.36
-2	-0.38	0.50	-5.2	-4.57	-2.72	-0.29
-1	-2.94	-0.03	-6.63	-2.64	-4.34	-3.21
0	-6.07	-1.20	-8.5	-3.76	-6.33	-5.92
1	-8.57	-2.64	-9.48	-5.46	-8.96	-8.69
2	-9.72	-4.40	-9.24	-7.38	-11.05	-11.03
3	-11.57	-6.32	-9.68	-9.36	-13.27	-13.14
4	-13.49	-8.31	-11.03	-11.35	-15.29	-15.03
5	-15.47	-10.30	-12.87	-13.35	-17.26	-17.01
6	-17.47	-12.30	-14.85	-15.35	-19.26	-19.00
7	-19.47	-14.30	-16.85	-17.35	-21.26	-21.00
8	-21.46	-16.30	-18.85	-19.35	-23.26	-23.00

TABLE 14  
Mean rel. difference  $\log_2(|CKA_{G(\sigma)} - CKA_{lin}|/CKA_{lin})$ .  
NN width  $w = 64$ . Regression.

$\log_2 \sigma$	cpu	boston	Diab(skl)	stock	balloon	cloud
-4	-6.48	-3.74	-1.34	-3.27	-6.41	-3.78
-3	-6.06	-3.94	-3.23	-3.45	-6.85	-4.63
-2	-6.71	-4.30	-5.85	-2.95	-6.70	-5.10
-1	-7.69	-5.24	-8.71	-3.56	-6.62	-4.85
0	-9.22	-5.40	-11.15	-4.83	-6.66	-5.72
1	-10.64	-5.81	-13.42	-6.37	-6.96	-6.34
2	-11.59	-7.36	-16.22	-8.22	-7.81	-7.71
3	-12.25	-9.30	-18.91	-10.14	-9.37	-10.15
4	-13.37	-11.34	-21.14	-12.13	-10.42	-12.16
5	-15.17	-13.41	-23.21	-14.12	-11.99	-14.17
6	-17.09	-15.40	-25.23	-16.12	-13.92	-16.17
7	-19.08	-17.39	-27.24	-18.12	-15.91	-18.16
8	-21.07	-19.39	-29.24	-20.12	-17.90	-20.16

TABLE 12  
Mean rel. difference  $\log_2(|CKA_{G(\sigma)} - CKA_{lin}|/CKA_{lin})$ .  
NN width  $w = 16$ . Regression.

$\log_2 \sigma$	cpu	boston	Diab(skl)	stock	balloon	cloud
-4	-3.28	-2.15	-2.11	-2.76	-8.00	-3.19
-3	-3.38	-2.02	-3.95	-2.53	-8.26	-2.38
-2	-4.06	-2.56	-6.42	-2.25	-8.25	-2.16
-1	-5.25	-3.49	-9.22	-2.95	-8.58	-2.75
0	-6.73	-4.42	-11.72	-4.42	-9.08	-3.70
1	-8.14	-4.95	-14.04	-5.90	-9.26	-4.90
2	-9.67	-6.09	-16.74	-7.77	-9.63	-6.70
3	-9.78	-7.81	-19.29	-9.73	-10.23	-8.85
4	-10.63	-9.77	-21.56	-11.71	-11.50	-11.03
5	-12.57	-11.76	-23.69	-13.70	-12.94	-13.16
6	-14.42	-13.76	-25.70	-15.70	-14.81	-15.23
7	-16.40	-15.76	-27.70	-17.70	-16.75	-17.22
8	-18.39	-17.76	-29.70	-19.70	-18.73	-19.22

TABLE 15  
Mean rel. difference  $\log_2(|CKA_{G(\sigma)} - CKA_{lin}|/CKA_{lin})$ .  
NN width  $w = 128$ . Regression.

$\log_2 \sigma$	cpu	boston	Diab(skl)	stock	balloon	cloud
-4	-7.58	-4.12	-1.10	-3.42	-5.11	-3.80
-3	-7.11	-4.02	-2.94	-3.51	-5.31	-4.32
-2	-7.86	-4.92	-5.60	-3.11	-5.26	-5.37
-1	-8.80	-6.51	-8.49	-3.65	-5.23	-5.38
0	-10.61	-7.14	-10.94	-4.65	-5.26	-6.05
1	-11.41	-7.45	-13.18	-6.09	-5.46	-6.85
2	-12.66	-9.00	-16.06	-7.92	-5.96	-8.36
3	-12.60	-10.99	-18.78	-9.88	-7.47	-10.43
4	-13.70	-13.04	-21.18	-11.86	-8.63	-12.50
5	-15.50	-14.99	-23.36	-13.86	-10.28	-14.45
6	-17.47	-16.98	-25.38	-15.86	-12.22	-16.42
7	-19.46	-18.98	-27.37	-17.86	-14.21	-18.41
8	-21.46	-20.98	-29.37	-19.86	-16.20	-20.41

TABLE 16

Median ratios,  $\rho = \max(\text{diam}(X)/d_X, \text{diam}(Y)/d_Y)$ , with  $\pm 2$  standard error equivalent confidence intervals, of maximum to median distance between features.  $w$  is NN width. Classification.

$w$	splice	tic-tac-toe	wdbc	optdigits	wine	dna
16	3.91 $\pm$ 0.21	3.53 $\pm$ 0.30	10.88 $\pm$ 0.56	3.33 $\pm$ 0.29	5.00 $\pm$ 0.01	2.87 $\pm$ 0.08
32	3.67 $\pm$ 0.13	2.71 $\pm$ 0.14	10.82 $\pm$ 0.26	2.42 $\pm$ 0.08	5.00 $\pm$ 0.01	2.68 $\pm$ 0.06
64	3.14 $\pm$ 0.10	2.43 $\pm$ 0.10	10.74 $\pm$ 0.18	2.15 $\pm$ 0.04	5.01 $\pm$ 0.00	2.55 $\pm$ 0.04
128	2.95 $\pm$ 0.07	2.36 $\pm$ 0.05	10.64 $\pm$ 0.09	2.00 $\pm$ 0.05	5.00 $\pm$ 0.00	2.47 $\pm$ 0.03
256	2.83 $\pm$ 0.06	2.34 $\pm$ 0.07	10.57 $\pm$ 0.06	1.92 $\pm$ 0.03	5.00 $\pm$ 0.00	2.43 $\pm$ 0.02
512	2.76 $\pm$ 0.05	2.48 $\pm$ 0.06	10.57 $\pm$ 0.06	1.87 $\pm$ 0.03	5.00 $\pm$ 0.00	2.39 $\pm$ 0.02
1024	2.74 $\pm$ 0.05	2.45 $\pm$ 0.04	10.62 $\pm$ 0.06	1.89 $\pm$ 0.03	5.01 $\pm$ 0.00	2.39 $\pm$ 0.02
128-32-8	3.28 $\pm$ 0.12	4.23 $\pm$ 0.33	10.87 $\pm$ 0.26	2.34 $\pm$ 0.08	5.00 $\pm$ 0.00	2.55 $\pm$ 0.08

TABLE 17

Mean rel. difference  $\log_2(|\text{CKA}_{G(\sigma)} - \text{CKA}_{\text{lin}}|/\text{CKA}_{\text{lin}})$ .  
NN width  $w = 256$ . Regression.

$\log_2 \sigma$	cpu	boston	Diab(skl)	stock	balloon	cloud
-4	-8.24	-4.48	-0.90	-2.70	-4.23	-3.26
-3	-7.87	-4.47	-2.61	-2.74	-4.35	-3.56
-2	-8.71	-5.97	-5.28	-2.45	-4.33	-5.20
-1	-9.64	-7.36	-8.22	-2.94	-4.31	-6.21
0	-11.44	-7.40	-10.70	-4.17	-4.32	-6.63
1	-12.89	-7.67	-13.00	-5.66	-4.44	-7.99
2	-13.74	-9.13	-15.68	-7.51	-4.81	-8.36
3	-14.18	-10.99	-18.37	-9.46	-6.17	-10.52
4	-15.26	-12.96	-20.66	-11.45	-7.44	-12.68
5	-17.03	-14.95	-22.75	-13.45	-9.08	-14.69
6	-18.97	-16.95	-24.78	-15.45	-11.00	-16.69
7	-20.95	-18.95	-26.79	-17.45	-12.98	-18.69
8	-22.95	-20.95	-28.79	-19.45	-14.98	-20.69

TABLE 19

Mean rel. difference  $\log_2(|\text{CKA}_{G(\sigma)} - \text{CKA}_{\text{lin}}|/\text{CKA}_{\text{lin}})$ .  
NN width  $w = 1024$ . Regression.

$\log_2 \sigma$	cpu	boston	Diab(skl)	stock	balloon	cloud
-4	-6.87	-3.35	-0.67	-2.18	-3.26	-2.72
-3	-6.86	-3.19	-1.71	-2.22	-3.39	-3.11
-2	-7.90	-4.01	-3.64	-2.05	-3.35	-5.58
-1	-8.70	-6.49	-5.97	-2.46	-3.33	-5.28
0	-10.07	-7.61	-8.20	-3.61	-3.36	-6.10
1	-11.85	-7.65	-10.35	-5.15	-3.48	-7.13
2	-13.22	-8.89	-13.34	-7.01	-3.78	-7.77
3	-15.36	-10.72	-16.72	-8.98	-4.91	-9.62
4	-17.14	-12.68	-19.23	-10.97	-6.16	-11.53
5	-18.91	-14.67	-21.48	-12.97	-7.69	-13.53
6	-20.81	-16.66	-23.63	-14.97	-9.58	-15.53
7	-22.80	-18.66	-25.64	-16.97	-11.55	-17.53
8	-24.80	-20.66	-27.63	-18.97	-13.55	-19.53

TABLE 18

Mean rel. difference  $\log_2(|\text{CKA}_{G(\sigma)} - \text{CKA}_{\text{lin}}|/\text{CKA}_{\text{lin}})$ .  
NN width  $w = 512$ . Regression.

$\log_2 \sigma$	cpu	boston	Diab(skl)	stock	balloon	cloud
-4	-8.29	-3.78	-0.75	-2.35	-3.68	-2.91
-3	-8.12	-3.80	-2.10	-2.39	-3.81	-3.25
-2	-9.00	-5.10	-4.40	-2.20	-3.78	-5.28
-1	-9.90	-7.37	-7.15	-2.64	-3.76	-6.29
0	-11.48	-7.91	-9.61	-3.78	-3.79	-6.54
1	-13.07	-8.15	-11.85	-5.31	-3.91	-7.45
2	-13.93	-9.65	-14.89	-7.17	-4.24	-7.95
3	-15.26	-11.56	-18.07	-9.13	-5.56	-9.79
4	-16.44	-13.51	-20.29	-11.12	-6.86	-11.83
5	-18.24	-15.49	-22.44	-13.12	-8.35	-13.85
6	-20.22	-17.49	-24.47	-15.12	-10.25	-15.86
7	-22.23	-19.49	-26.52	-17.12	-12.22	-17.86
8	-24.23	-21.49	-28.50	-19.12	-14.22	-19.86

TABLE 20

Mean rel. difference  $\log_2(|\text{CKA}_{G(\sigma)} - \text{CKA}_{\text{lin}}|/\text{CKA}_{\text{lin}})$ .  
Three-layer 128-32-8 NN. Regression.

$\log_2 \sigma$	cpu	boston	Diab(skl)	stock	balloon	cloud
-4	-4.25	-2.12	-0.78	-1.29	-3.81	-3.40
-3	-4.20	-1.87	-2.17	-0.79	-4.05	-2.85
-2	-4.91	-2.27	-4.50	-0.31	-4.06	-2.29
-1	-5.96	-3.41	-7.20	-0.67	-3.99	-2.75
0	-7.90	-4.93	-9.61	-2.32	-4.10	-4.03
1	-9.61	-5.34	-11.94	-4.36	-4.36	-5.54
2	-10.09	-6.66	-14.60	-6.31	-5.03	-6.30
3	-10.43	-8.49	-17.68	-8.28	-6.84	-8.70
4	-11.44	-10.43	-19.71	-10.27	-7.76	-10.94
5	-13.27	-12.41	-21.68	-12.27	-9.48	-12.94
6	-15.25	-14.41	-23.69	-14.27	-11.16	-14.90
7	-17.25	-16.41	-25.69	-16.27	-13.06	-16.90
8	-19.25	-18.41	-27.69	-18.27	-15.04	-18.90