An Introduction to Function Approximation for Machine Learning

Volker Tresp

Winter 2024-2025

Problem Setting

- In an actual application, the data scientist needs to decide which model to use (linear Perceptron, fixed basis functions, neural networks, kernels, ...?)
- How well is one doing in solving the actual problem with the data actually available; in the lecture on model selection, we learn about some empirical methods for analysing some of these issues
- But what can theory tell us about these issues? Why are, e.g., deep neural networks so successful?
- In this lecture we will be a bit informal since formal treatments require advanced mathematical frameworks and are beyond the scope of this lecture

Target Function Class

- Let $\mathcal{F}$ be the set of target functions
- What characterizes the functions that mother nature generates for a particular problem, e.g., image classification, and how can I characterize them?
- In a theoretical analysis one characterizes this class in some way, hopefully limiting the class to the one actually occurring in practice (neither larger nor smaller)
- Often one defines the target class by some degree of smoothness of the functions; another target class of functions are composable functions (see lecture on deep learning)

Target Function Class (cont'd)

- The modern view is that the target function class assumes a tiny space in the space of all functions and e.g., deep learning models, work so well because they match this class reasonably well
- Some claim that machine learning is impossible if the target function class is not restricted (*no-free-lunch theorem*)

Model Function Class

- What characterizes the model function class $\mathcal{M}$
- To simplify matter (mostly for notational simplicity), we assume a model function class can be described as

$$\mathcal{M} = \{f_{\mathbf{w}}(\cdot)\}_{\mathbf{w}}$$

i.e. functions which only vary in their parameters (but this is not essential)

Average Squared Distance Between Functions

- Consider the true function $f(\cdot)$ and an model $f_{\mathbf{w}}(\cdot)$. The average squared distance is

$$\|\mathbf{f} - f_{\mathbf{w}}(\cdot)\|_B^2 = \frac{1}{V_B} \int_B (f(\mathbf{x}) - f_{\mathbf{w}}(\mathbf{x}))^2 d\mathbf{x}$$

  Here V_B is the volume of the unit ball B in M dimensions

- This is simply the average squared Euclidean distance, applied to two functions

Expected Squared Distance Between Functions

- The expected squared distance between the two function is

$$\|\mathbf{f} - f_{\mathbf{w}}(\cdot)\|^2_{P(\mathbf{x})} = \int (f(\mathbf{x}) - f_{\mathbf{w}}(\mathbf{x}))^2 P(\mathbf{x}) d\mathbf{x}$$

- $P(\mathbf{x})$ is the probability distribution of the input data
- If $\mathbf{x}_i \sim P(\mathbf{x})$

$$\|\mathbf{f} - f_{\mathbf{w}}(\cdot)\|^2_{P(\mathbf{x})} \approx \frac{1}{N} \sum_{i=1}^{N} (f(\mathbf{x}_i) - f_{\mathbf{w}}(\mathbf{x}_i))^2$$

- In some cases the input data only occupy a small subspace (manifold) of the unit ball; some learning approaches are able to explore this

Distance between Functions

- We define ϵ_B to be the minimum Euclidean distance for the "most difficult" function from the function class

$$\epsilon_B = \min_{\mathbf{w}} \max_{\mathbf{f}} \|\mathbf{f} - \mathbf{f}_{\mathbf{w}}\|_B$$

$$\epsilon_{P(x)} = \min_{\mathbf{w}} \max_{\mathbf{f}} \|\mathbf{f} - \mathbf{f}_{\mathbf{w}}\|_{P(x)}$$

$\mathbf{f} \in \mathcal{F}$, $\mathbf{f}_{\mathbf{w}} \in \mathcal{M}$

Statistical Machine Learning

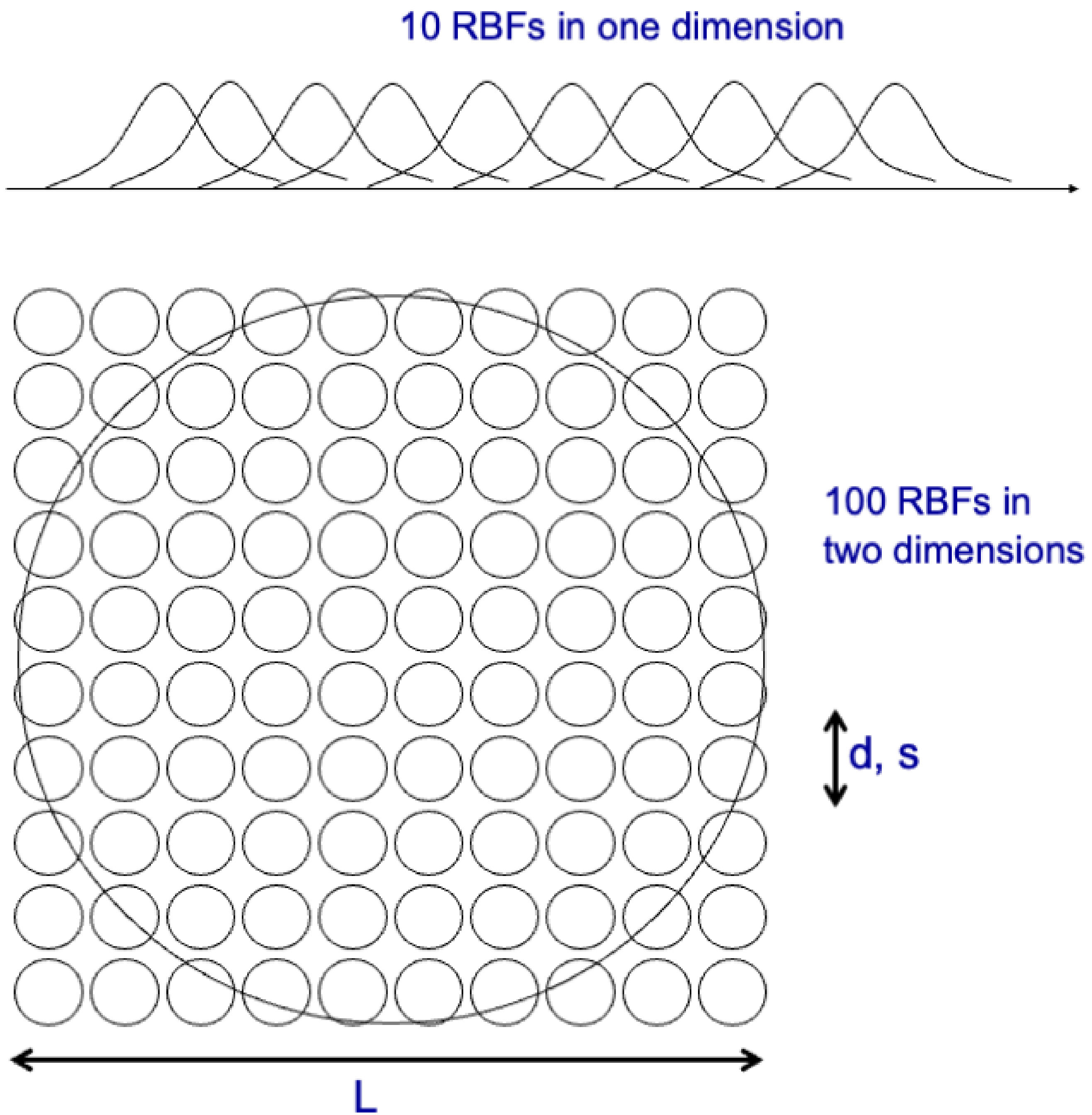
- Statistical machine learning analyses the distance between the expected distance between a model function, where the parameters were estimated based on some training data, and a given $\mathbf{f}$
- This is not the issue in approximation theory, and will be discussed in a later lecture

Analysis of Dimensionality

- Consider input space dimension M
- If in one dimensions, we need $M_\phi^{(\textit{one-dim})}$ RBFs (e.g., $M_\phi^{(\textit{one-dim})} = 10$), and we want to maintain the same complexity in higher dimensions, then we need

$$M_\phi = \left(M_\phi^{(\textit{one-dim})}\right)^M$$

RBFs in M dimensions


10 RBFs in one dimension
100 RBFs in two dimensions
d, s
L

Analysis of Dimensionality (cont'd)

- We get

$$M_\phi^{(\textit{one-dim})} = \mathcal{O}\left(\frac{1}{\epsilon_B^{1/m}}\right)$$

- Here, m is a characterization of the smoothness of the target class: m can be the set of all functions with continuous partial derivatives of orders up to m (derivatives of higher order can be discontinuous)

- This result can, e.g., be found in: "Why and When Can Deep-but Not Shallow-networks Avoid the Curse of Dimensionality: A Review" Tomaso Poggio et al., International Journal of Automation and Computing, 2017, Equation 5.

Analysis of Dimensionality (cont'd)

- We can write this as

$$M_\phi^{(\textit{one-dim})} = \mathcal{O}\left(\textit{accuracy}^{\textit{roughness}}\right)$$

where we have defined *accuracy* $= 1/\epsilon_B$ and *roughness* $= 1/m$

Analysis of Dimensionality: Main Result

- Overall, the total number of basis function is then

$$M_\phi = \mathcal{O}\left(\mathit{accuracy}^{M \times \mathit{roughness}}\right)$$

- Note, that, for a fixed desired accuracy (e.g., $\mathit{accuracy} = 10$), the number of basis functions increases exponentially with $M \times \mathit{roughness}$

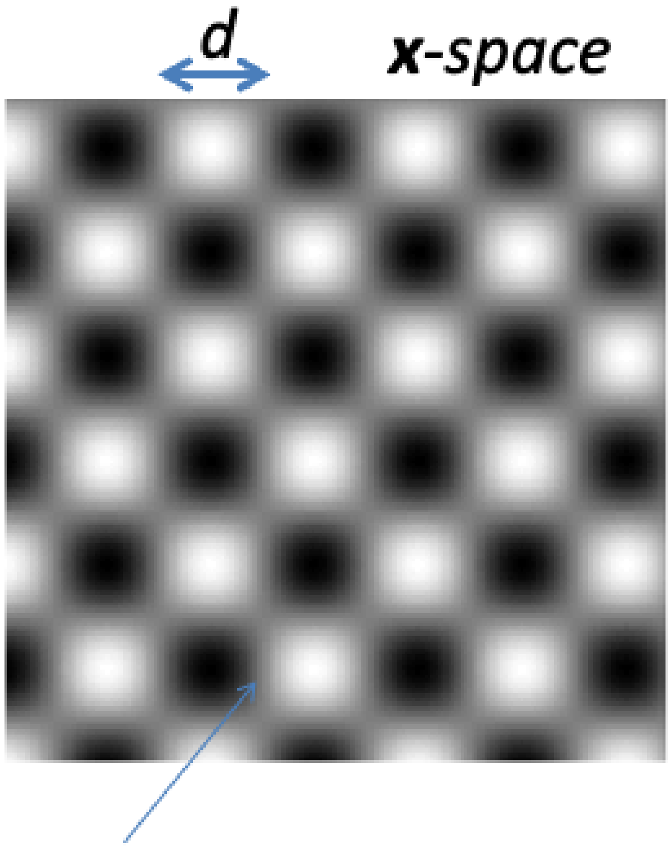
- Sometimes it is more instructive to look at the logarithm

$$\log M_\phi = \mathcal{O}\left(M \times \mathit{roughness} \times \log(\mathit{accuracy})\right)$$

Case I: Curse of Dimensionality

- $\mathcal{F}$: dimensionality M is large, and *roughness* is large
- $\mathcal{M}$: Considering that ($M \times$ *roughness*) is in the exponent, M_ϕ is unrealistically large
- This is the famous Bellman's "Curse of Dimensionality"

20-Dimensional Checker Board Function:
"Curse of Dimensionality"



2-D slice through a 20-Dimensional input space

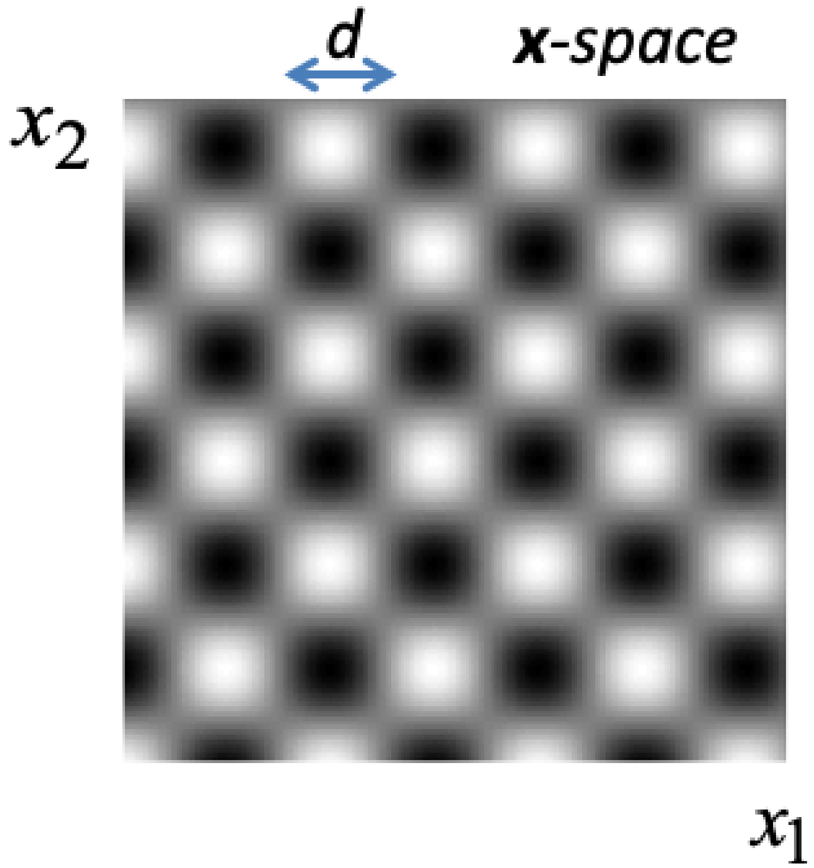
M is high (M=20), roughness is large

The required number of basis function is huge

Case II: Blessing of Dimensionality

- $\mathcal{F}$: dimensionality M is small but *roughness* is large
- In this case ($M \times$ *roughness*) might be acceptable
- $\mathcal{M}$: This is what I would call the "Blessing of Dimensionality": a complex nonlinear classification problem (large *roughness*) can be solved by a transformation of the low-dimensional input space (M) into a high-dimensional space (M_ϕ) where the problem might even become linearly separable

2-D Checker Board Function



Here *M=2 (roughness is large)* and with less than 100 RBF basis functions we might get a good fit

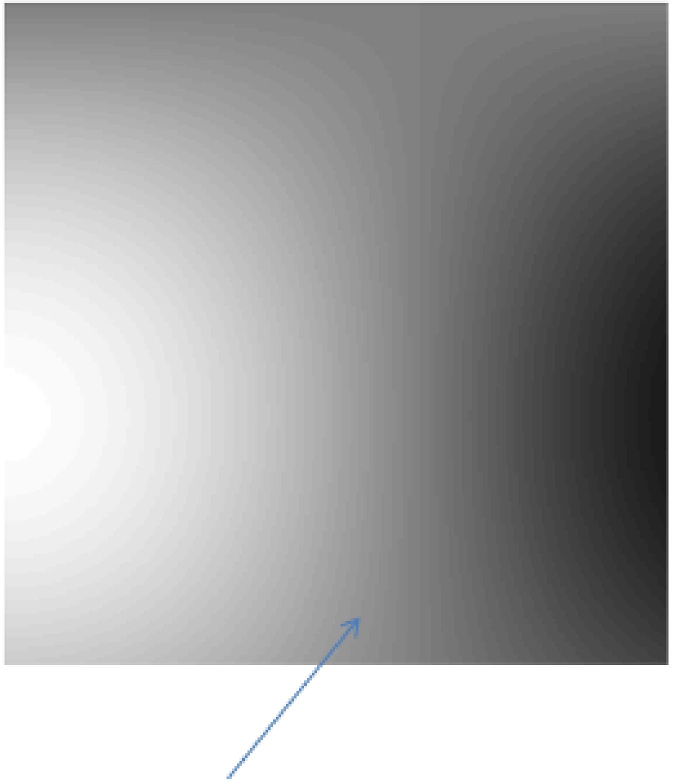
Case III: Smooth Target Function in High Dimensions

- $\mathcal{F}$: dimensionality M is large and *roughness* is small (the target function is smooth)
- A special case would be when the target functions are linear functions; then where $M_\phi = M + 1$; The target function exhibits a voting behavior: each input itself has a (small) contribution to the output
- $\mathcal{F}$: if the target functions can well be approximated by linear functions, the input dimension can be quite high ($M > 10000$)

Case IV (Simple): Smooth Target Function in Low Dimensions

- $\mathcal{F}$: dimensionality M is small and *roughness* is small (the target function is smooth)
- $\mathcal{M}$: Only a small number M_ϕ of smooth basis functions are required

x-space



2-D slice through a 20-D input space

M is large (M=20) and roughness is small

Here *M=20* is medium size and with less than 100 RBF basis functions we might get a good fit

Revisiting Case I

- Fortunately, even Case I is not as hopeless as it first appears, since, in reality, classes are more restricted
- Ia: $\mathcal{F}$: The target functions have high-frequency components, but only locally, and a sparse solution is feasible
- Ib: The input data points are restricted to a low-dimensional manifold (reflected in $P(\mathbf{x})$)
- Ic: $\mathcal{F}$: The target functions are composable (discussed in the lecture on deep learning)

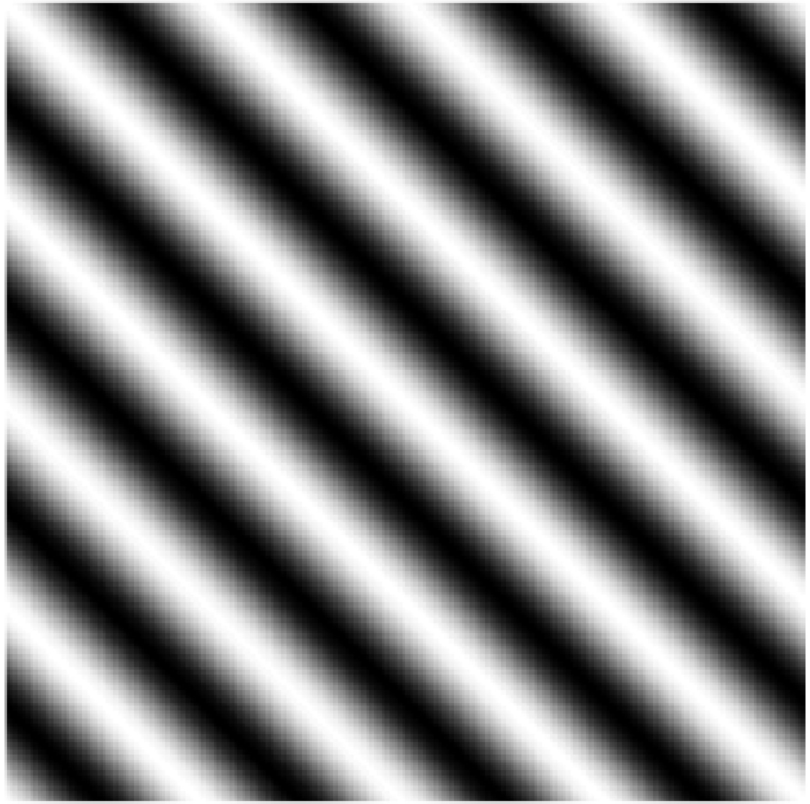
Case Ia: Sparse Basis: No Curse of Dimensionality with a Neural Network

- $\mathcal{F}$: both M and *roughness* are large, so the required M_ϕ is large, **but only** $H << M_\phi$ **basis functions have nonzero weights**; e.g., high complexity might only be present in a restricted region in input space

- $\mathcal{M}$: With a neural network model, the number of hidden units with nonzero weights (i.e., H) might even be independent of M!

- As a model class, classical neural networks with H hidden units can adaptively find the "perfect" sparse basis during training (with backpropagation)

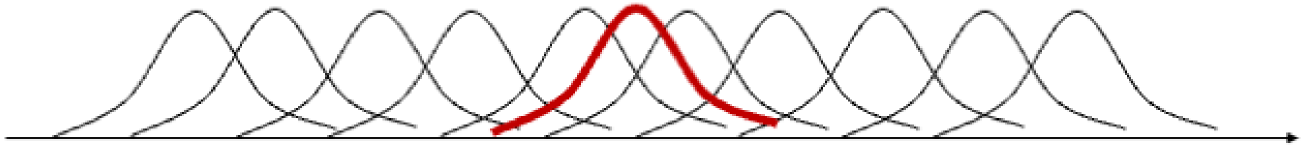
***x**-space*



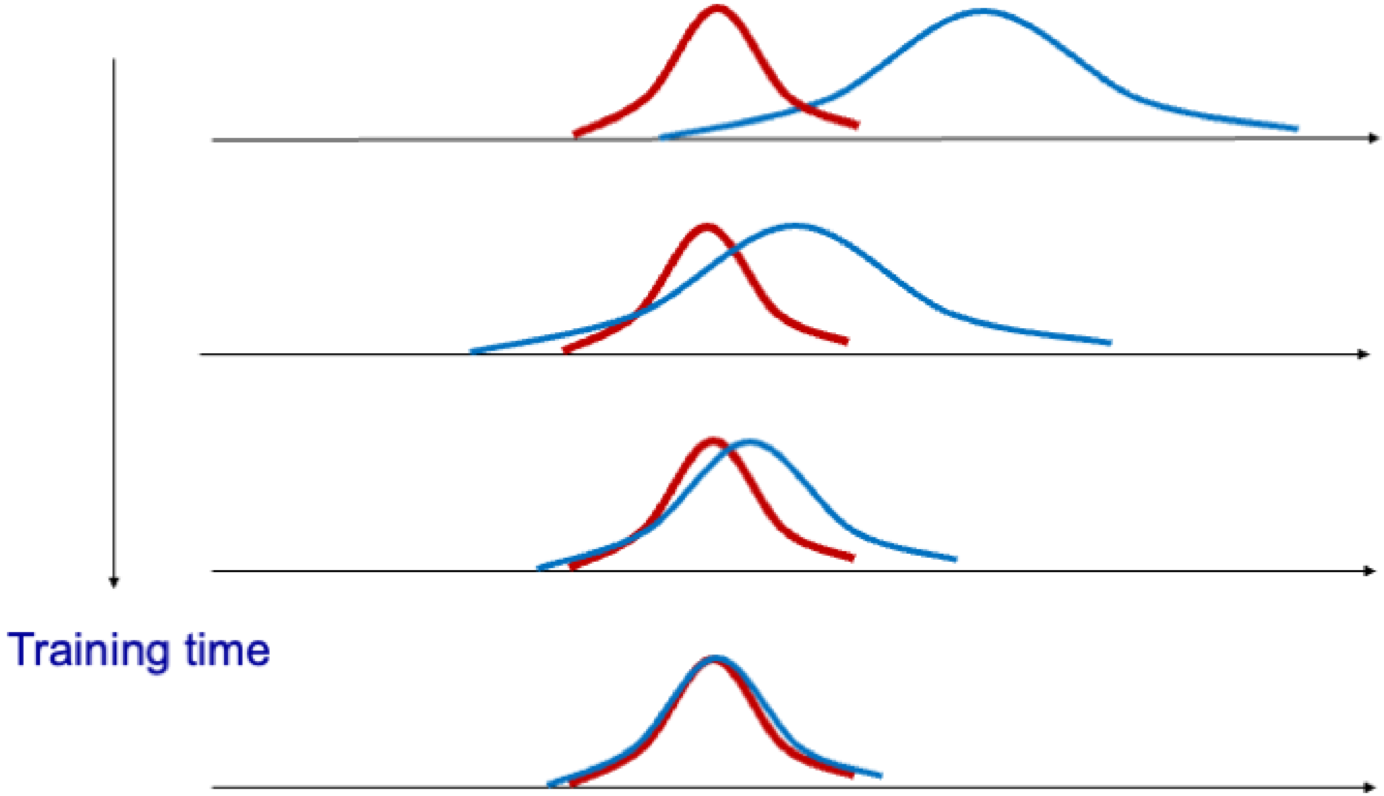
H=16 hidden units in a neural network might be sufficient

Although the input space might be high dimensional, complexity is limited

I need to allocate *10^M* fixed basis functions

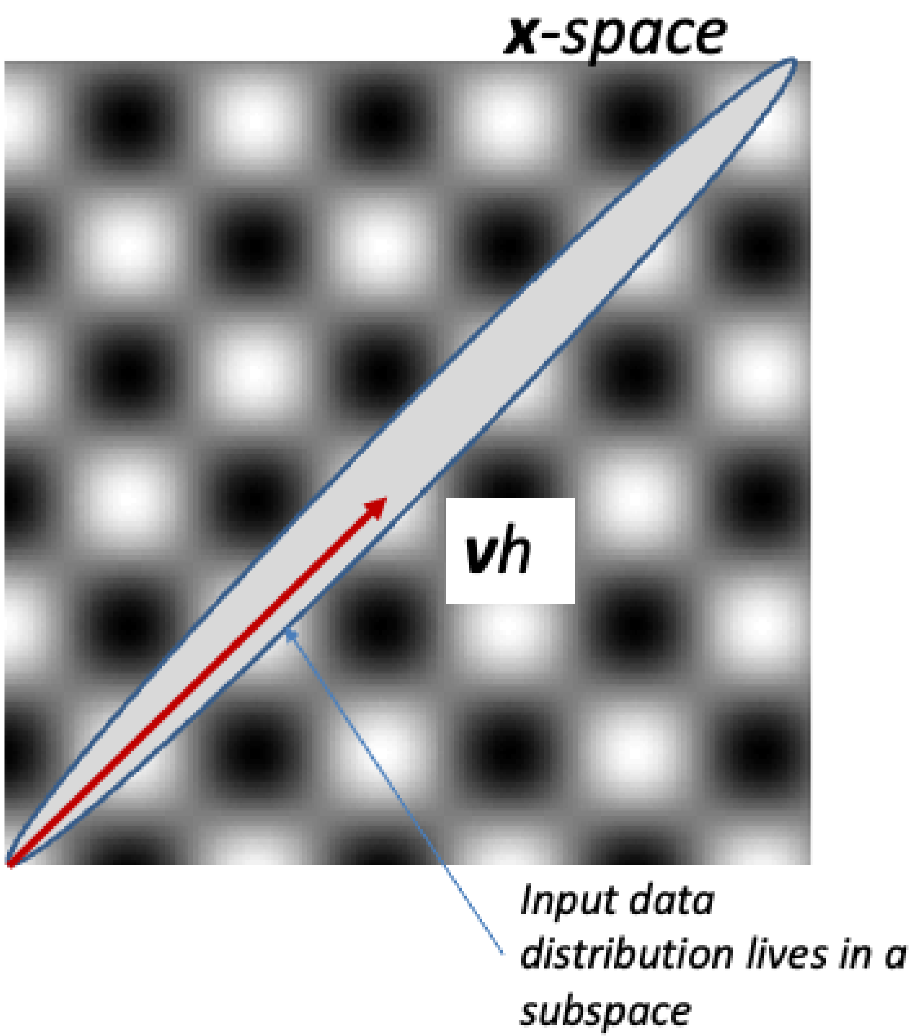


If I adapt center and width of *one* basis function, I can get a perfect fit



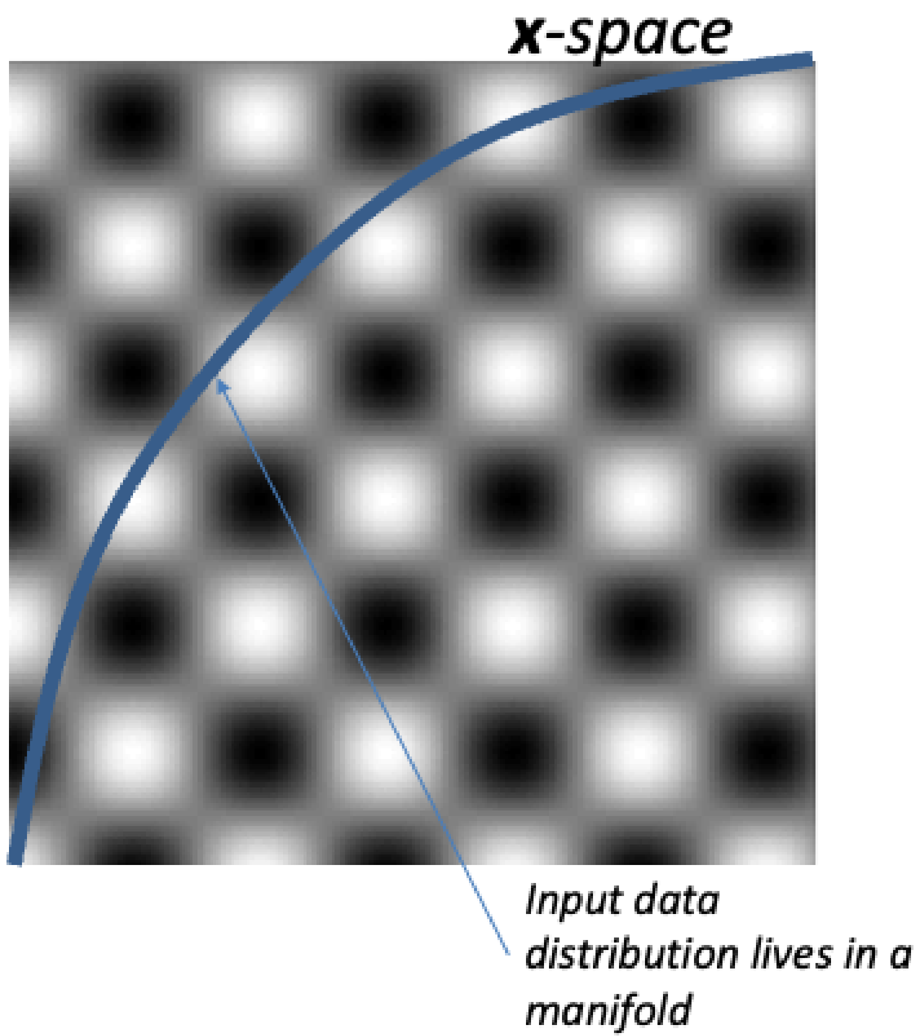
Case Ib: Manifold

- So far we did not assume any particular input data distribution: $P(\mathbf{x})$ might be a uniform distribution within the unit ball
- But sometimes $P(\mathbf{x})$ is restricted to a subspace of small dimension $M_h << M$; in the nonlinear case, the subspace is called a manifold (data is often on a manifold, when model accuracy is very high (like in OCR)
- $\mathcal{M}$: we might only need on the order of $\textit{accuracy}^{M_h \times \textit{roughness}}$ (instead of $\textit{accuracy}^{M \times \textit{roughness}}$) basis functions to cover the relevant region in input space
- Some model classes, like neural networks / deep neural networks, model data on a low-dimensional manifold quite effectively
- Other approaches perform a preprocessing step (clustering, PCA, ICA, ...) to find the manifold (dimensionality reduction), and then apply any model class suitable for low-dimensional data



- Although the input space might be high dimensional, the data lives in a subspace
- The dimension of the subspace is M_h, here 1

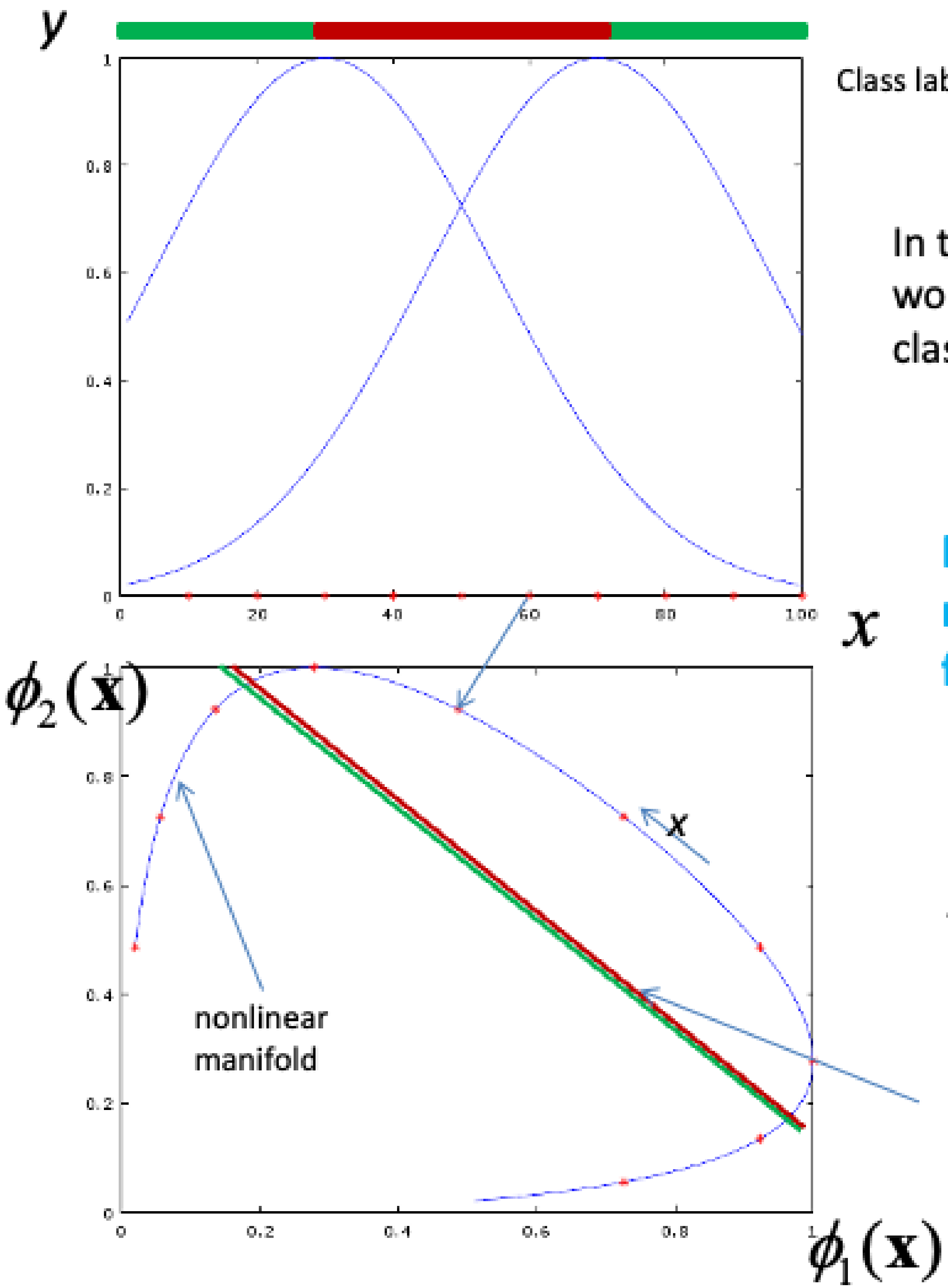
In case that the columns of V are orthonormal, there is a simple geometric interpretation



More general, the data lives in a manifold

Why Nature Generates Data on Manifolds

- We encountered this in the lecture on basis functions
- Assume that nature generates data in some low-dimensional space; nature then transforms this data to a high dimensional space by some nonlinear transformation
- This data then become the input data; then the input data might be on a manifold, as discussed in the lecture on basis functions!
- See lecture on manifold learning



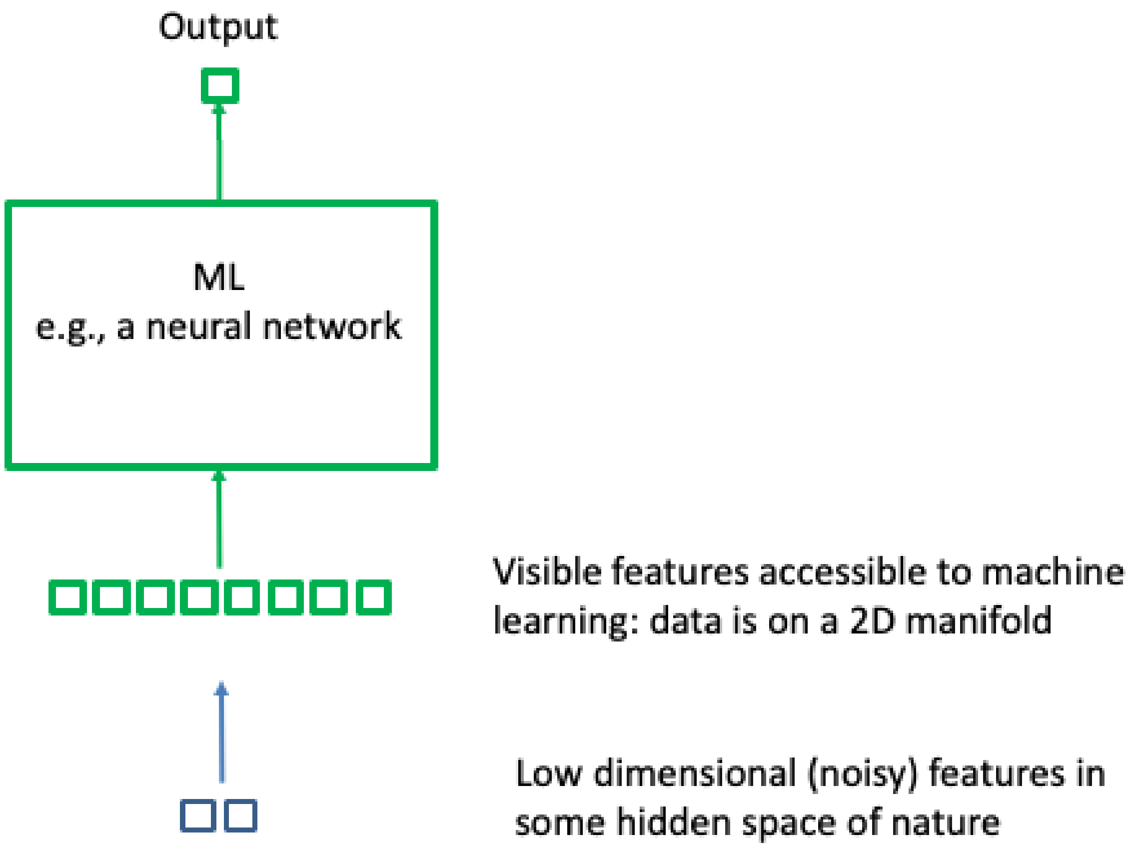
In the 1-D input space, a linear classifier would not be able to separate the two classes

From a linear 1-D input space (top) to a nonlinear 1-D manifold in 2-D basis function space (bottom)

In basis function space, classes can linearly be separated!

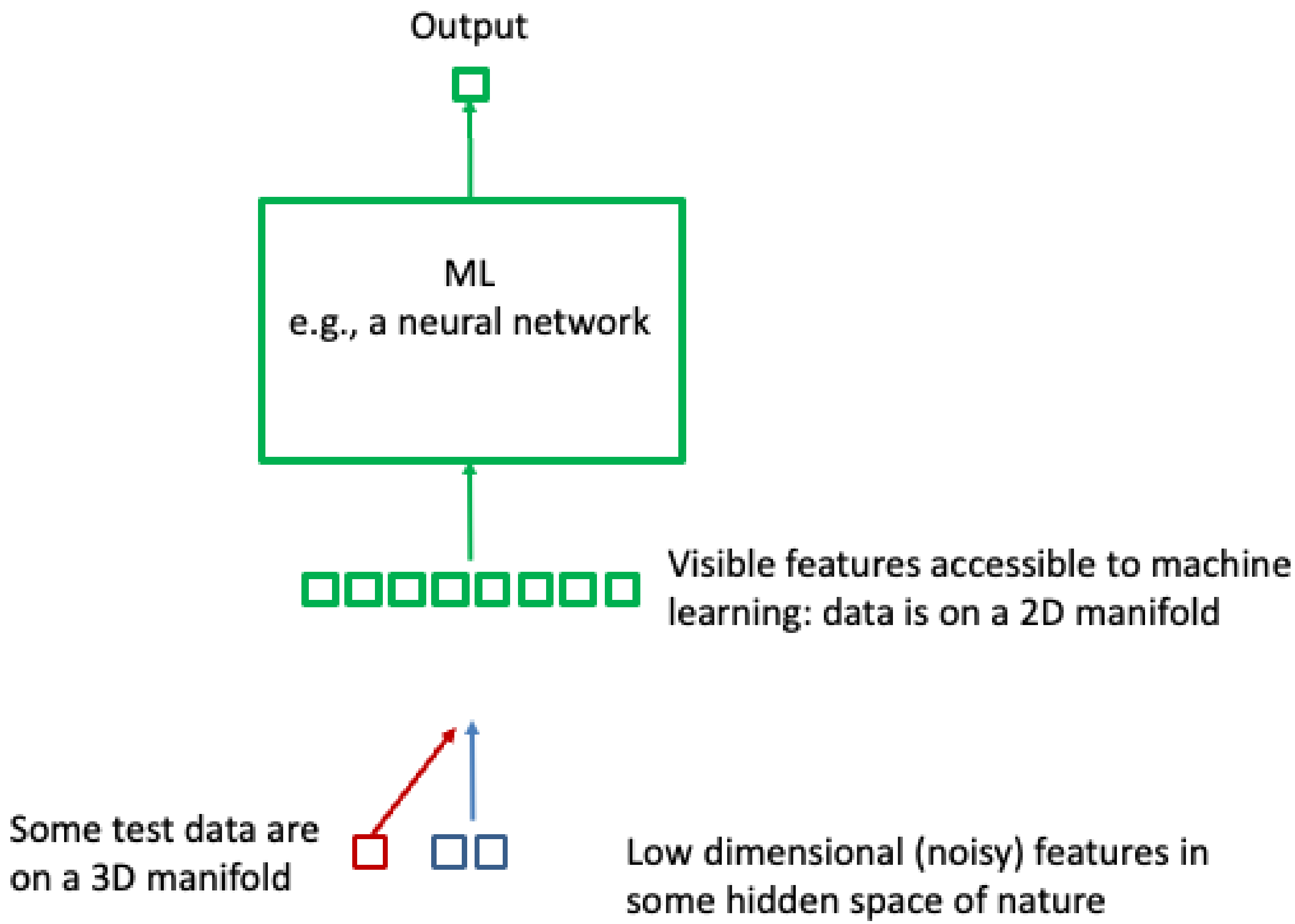
The image of the 1-D input data space is a 1-D **nonlinear manifold**

Data provided by nature is on a 2D manifold



Adversarial problem

- Training data provided by nature is on a 2D manifold
- Test data is on a 3D manifold



Manifold: Adversarial Examples

- But there is a danger: if we consider test data outside of the manifold, then performance might degrade quickly
- So although, $\epsilon_{P(\mathbf{x})}$ might be small, ϵ_B could be large!
- A common issue is: even on a test set (generated from the available data) the performance is excellent, but if I apply my model to new data collected independently, performance is much worse (even if $f(\mathbf{x})$ did not change)
- This might explain the bad performance of DNNs on adversarial examples
- Sometimes this problem is also called covariate shift (covariates are the inputs)

Conclusions

- Basis functions perform a nonlinear transformation from input space to basis function space
- To avoid the Curse of Dimensionality and if one uses fixed basis functions, ($M \times$ *roughness*) should not be very large
- Neural networks are effective when the basis is sparse (Ia (sparse basis)) or when data is on a manifold (Ib (data on a low-dimensional manifold))
- The next table evaluates linear models, distance-based methods (like nearest neighbor methods), models with fixed basis functions, neural networks, deep neural networks, and kernel approaches

Target \ Model	Lin	Neighb.	fixed BF	Neural Nets	Deep NNs	Kernels
I (curse)	-	-	-	-	-	-
II (blessing)	-	+	+	+	+	+
III (smooth)	+	-	+	+	+	+
IV (simple)	+	+	+	+	+	+
Ia (sparse basis)	-	-	-	+	+	-
Ib (manifold)	-	- (+dr)	- (+dr)	+	+	+
Ic (compos.)	-	-	-	-	+	-

- (+dr) stands for possibly good results with suitable dimensionality reduction by a preprocessing step;
- Case Ic are compositional functions, introduced in the lecture on deep neural networks
- Kernels are introduced in a later lecture

Appendix: Entropies

- Assume n discretization steps for each of the M input dimensions, e.g., $x_j \in 0, 1, 2, ..., n-1$
- With K discretization steps for the foutput , e.g., $f \in 0, 1, 2, ..., K-1$, we can realize $K^{(n^M)}$ functions, with entropy (number of required bits) (each function has the same probability for being generated)

$$\text{Entropy}_{\mathcal{F}} = \log_2 K^{(n^M)} = n^M \log_2 K$$

- For each possible input, we simply need $\log_2 K$ bits and there are n^M possible inputs
- Interesting: It is not the accuracy of the representation (i.e., K) that "kills" us, it is the dimensionality M reflected in the number of possible inputs (i.e., n^M)
- For a model class of fixed basis functions,

$$\text{Entropy}_{\mathcal{M}} = \log_2 K^{(M_\phi)} = M_\phi \log_2 K$$

if we represent each weight with $\log_2 K$ bits

Appendix: VC-dimension

- For systems with fixed basis functions and binary classification, $\mathit{dim}_{VC} = M_P = M_\phi$ is the VC-dimension (proportional to our entropy) of the model class
- Note that the VC-dimension is a property of the model class $\mathcal{M}$ and not of the function class $\mathcal{F}$
- If we have $N = M_\phi = \mathit{dim}_{VC}$ data points, the design matrix $\mathbf{\Phi}^T\mathbf{\Phi}$ is a square matrix and might be invertible; in that case, no matter what the assignment of training labels $\mathbf{y}$, we perfectly fit the classification labels (e.g., with regression)
- VC-theory states that one needs at least dim_{VC} data points for a valid generalization; this makes sense, since, without regularization, there are an infinite number of solutions when $M_\phi < N$
- Formally, dim_{VC} is defined as the cardinality of the largest set of points that the model class can shatter (i.e., perfectly model for any assignments of targets)