Lecture 3: Kernelization

Making linear models non-linear

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Feature Maps

- Linear models: $\hat{y} = \mathbf{wx} + w_0 = \sum_{i=1}^{p} w_i x_i + w_0 = w_0 + w_1 x_1 + \ldots + w_p x_p$
- When we cannot fit the data well, we can add non-linear transformations of the features
- Feature map (or *basis expansion*) $\phi : X \to \mathbb{R}^d$

$$y = \mathbf{w}^T \mathbf{x} \to y = \mathbf{w}^T \phi(\mathbf{x})$$

- E.g. Polynomial feature map: all polynomials up to degree d and all products

$$[1, x_1, \ldots, x_p] \overset{\phi}{\to} [1, x_1, \ldots, x_p, x_1^2, \ldots, x_p^2, \ldots, x_p^d, x_1 x_2, \ldots, x_{p-1} x_p]$$

- Example with $p = 1, d = 3$:

$$y = w_0 + w_1 x_1 \overset{\phi}{\to} y = w_0 + w_1 x_1 + w_2 x_1^2 + w_3 x_1^3$$

Ridge regression example

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Weights: [0.418]
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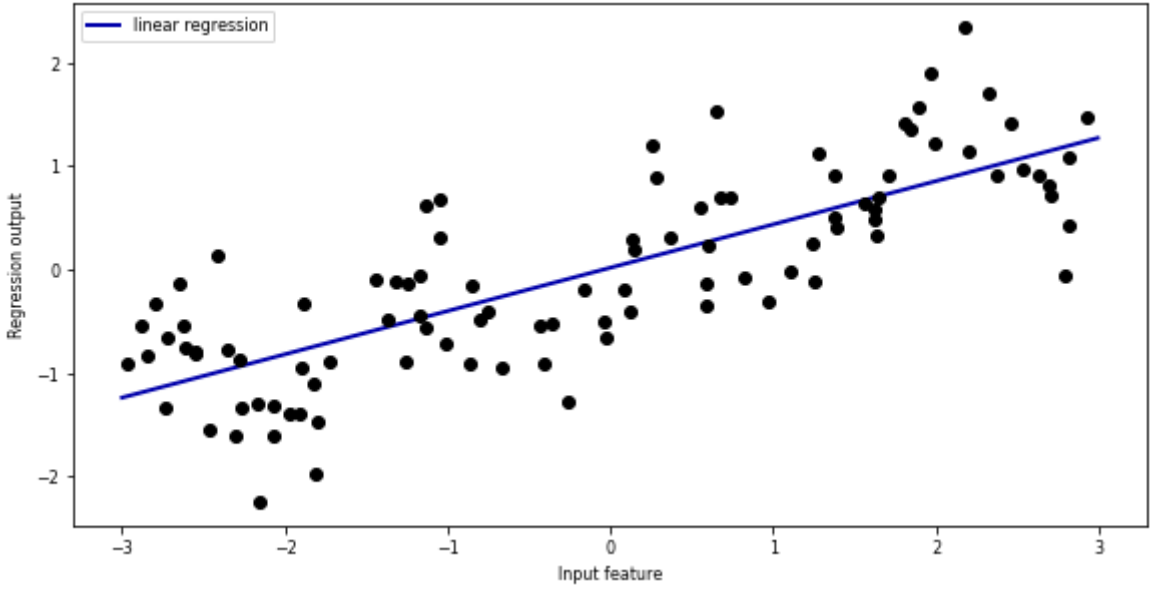

- Add all polynomials x^d up to degree 10 and fit again:
  - e.g. use sklearn `PolynomialFeatures`

	x0	x0^2	x0^3	x0^4	x0^5	x0^6	x0^7	x0^8
0	-0.752759	0.566647	-0.426548	0.321088	-0.241702	0.181944	-0.136960	0.103098
1	2.704286	7.313162	19.776880	53.482337	144.631526	391.124988	1057.713767	2860.360362
2	1.391964	1.937563	2.697017	3.754150	5.225640	7.273901	10.125005	14.093639
3	0.591951	0.350406	0.207423	0.122784	0.072682	0.043024	0.025468	0.015076
4	-2.063888	4.259634	-8.791409	18.144485	-37.448187	77.288869	-159.515582	329.222321

```
Weights: [ 0.643  0.297 -0.69  -0.264  0.41   0.096 -0.076 -0.014  0.004  0.001]
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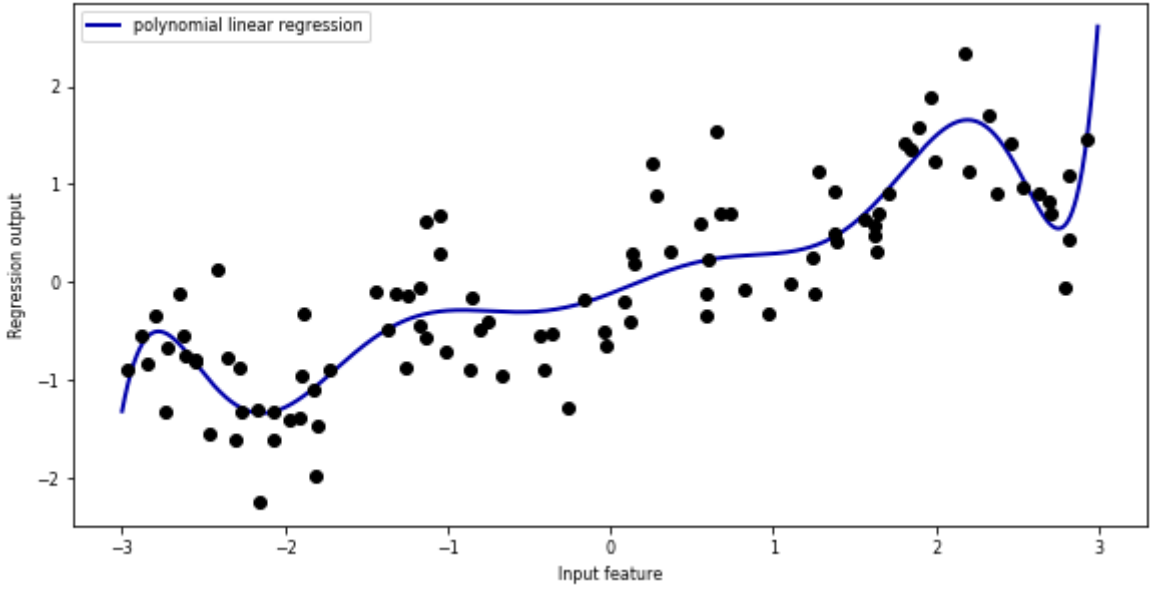


How expensive is this?

- You may need MANY dimensions to fit the data
    - Memory and computational cost
    - More weights to learn, more likely overfitting
- Ridge has a closed-form solution which we can compute with linear algebra:

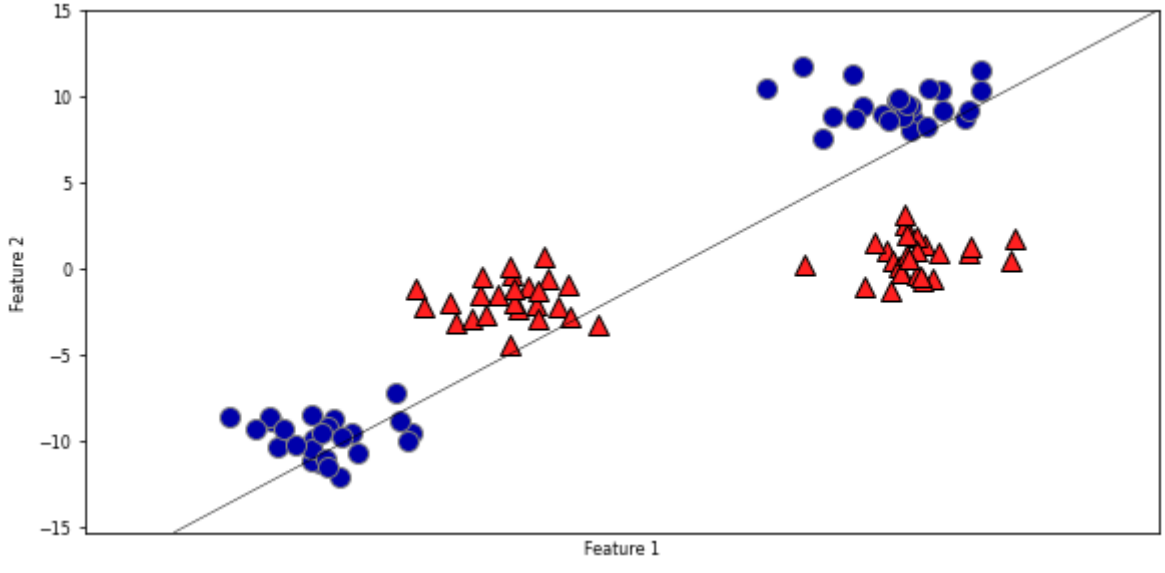
$$w^* = (X^T X + \alpha I)^{-1} X^T Y$$

- Since X has n rows (examples), and d columns (features), $X^T X$ has dimensionality dxd
- Hence Ridge is quadratic in the number of features, $\mathcal{O}(d^2 n)$
- After the feature map Φ, we get

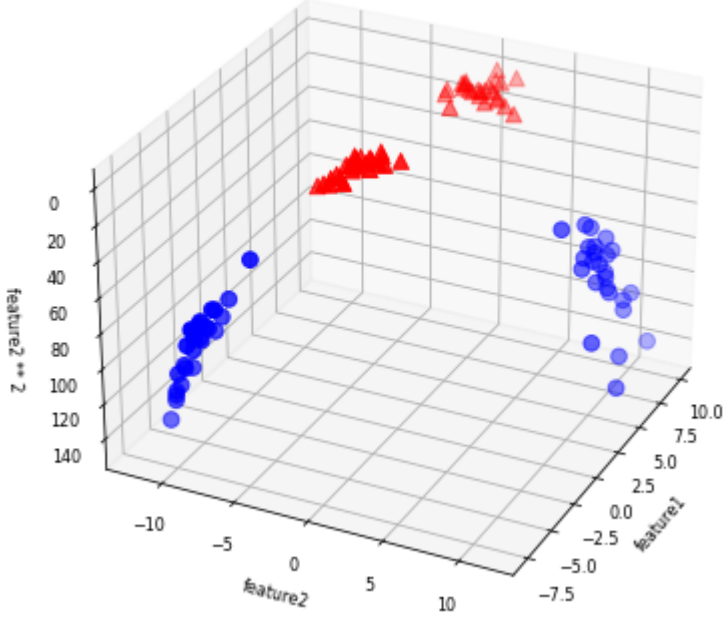
$$w^* = (\Phi(X)^T \Phi(X) + \alpha I)^{-1} \Phi(X)^T Y$$

- Since Φ increases d a lot, $\Phi(X)^T \Phi(X)$ becomes *huge*

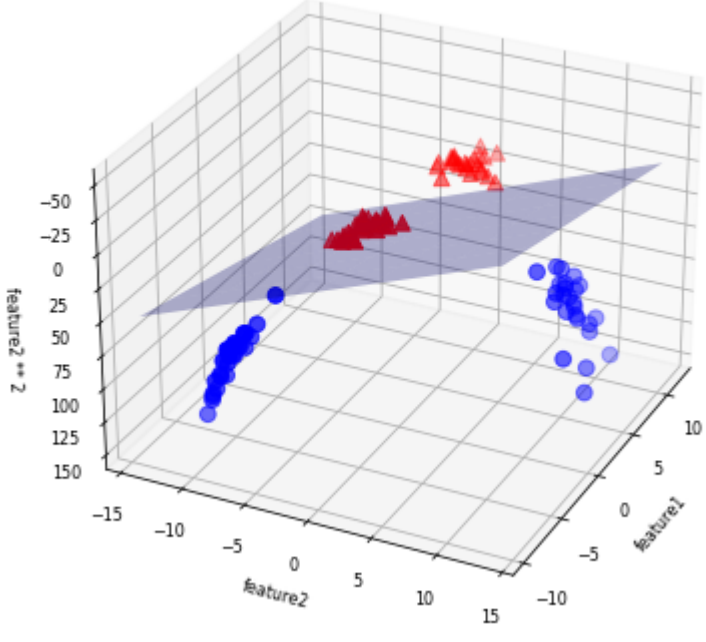
Linear SVM example (classification)



We can add a new feature by taking the squares of feature1 values

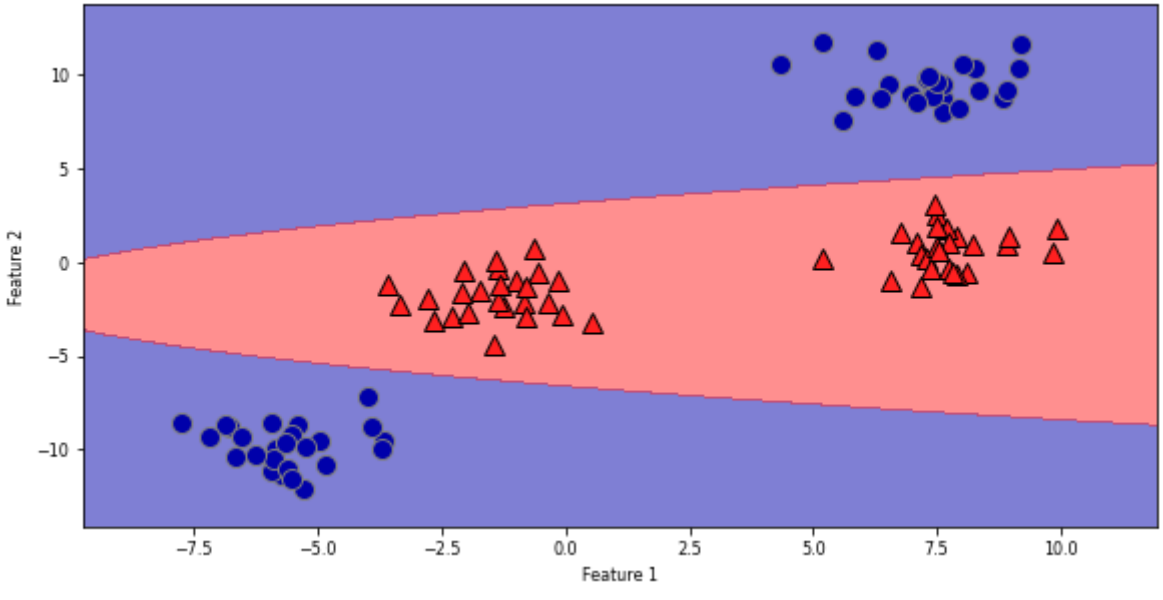


Now we can fit a linear model



As a function of the original features, the decision boundary is now a polynomial as well

$$y = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_2^2 > 0$$



The kernel trick

- Computations in explicit, high-dimensional feature maps are *expensive*
- For *some* feature maps, we can, however, compute *distances* between *points* cheaply
    - Without explicitly constructing the high-dimensional space at all
- Example: *quadratic* feature map for $\mathbf{x} = (x_1, \ldots, x_p)$:

$$\Phi(\mathbf{x}) = (x_1, \ldots, x_p, x_1^2, \ldots, x_p^2, \sqrt{2}x_1x_2, \ldots, \sqrt{2}x_{p-1}x_p)$$

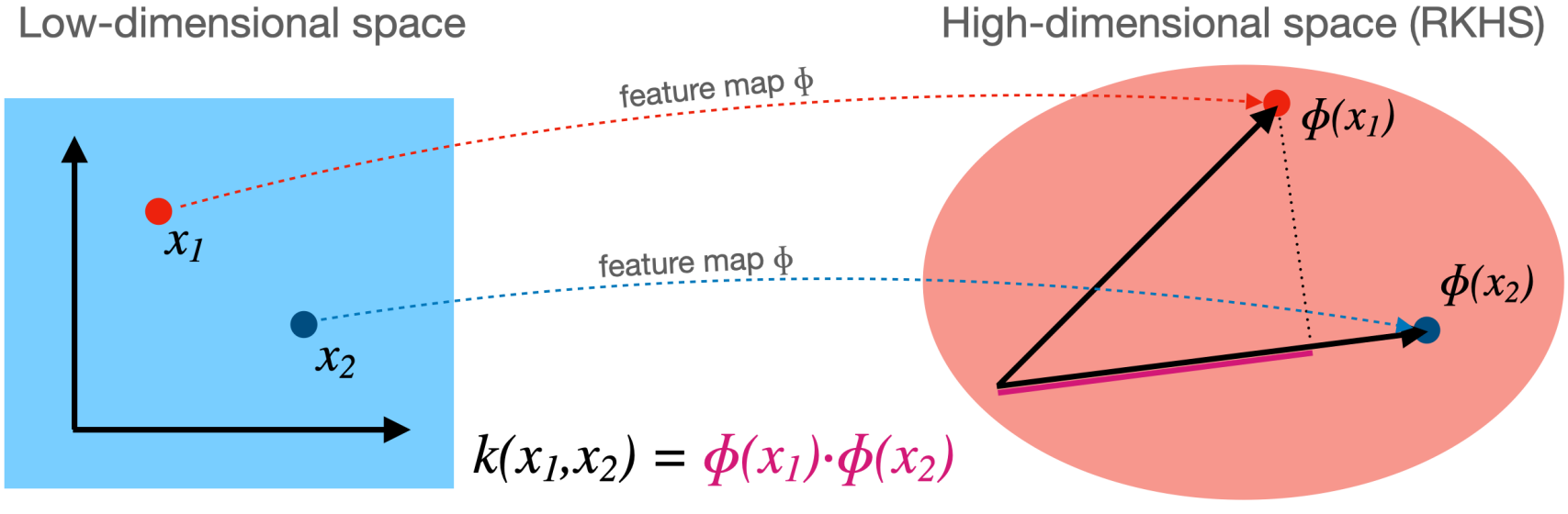
- A *kernel function* exists for this feature map to compute dot products

$$k_{quad}(\mathbf{x_i}, \mathbf{x_j}) = \Phi(\mathbf{x_i}) \cdot \Phi(\mathbf{x_j}) = \mathbf{x_i} \cdot \mathbf{x_j} + (\mathbf{x_i} \cdot \mathbf{x_j})^2$$

- Skip computation of $\Phi(x_i)$ and $\Phi(x_j)$ and compute $k(x_i, x_j)$ directly

Kernelization

- Kernel k corresponding to a feature map Φ: $k(\mathbf{x_i}, \mathbf{x_j}) = \Phi(\mathbf{x_i}) \cdot \Phi(\mathbf{x_j})$
- Computes dot product between x_i, x_j in a high-dimensional space $\mathcal{H}$
    - Kernels are sometimes called *generalized dot products*
    - $\mathcal{H}$ is called the *reproducing kernel Hilbert space* (RKHS)
- The dot product is a measure of the *similarity* between x_i, x_j
    - Hence, a kernel can be seen as a similarity measure for high-dimensional spaces
- If we have a loss function based on dot products $\mathbf{x_i} \cdot \mathbf{x_j}$ it can be *kernelized*
    - Simply replace the dot products with $k(\mathbf{x_i}, \mathbf{x_j})$



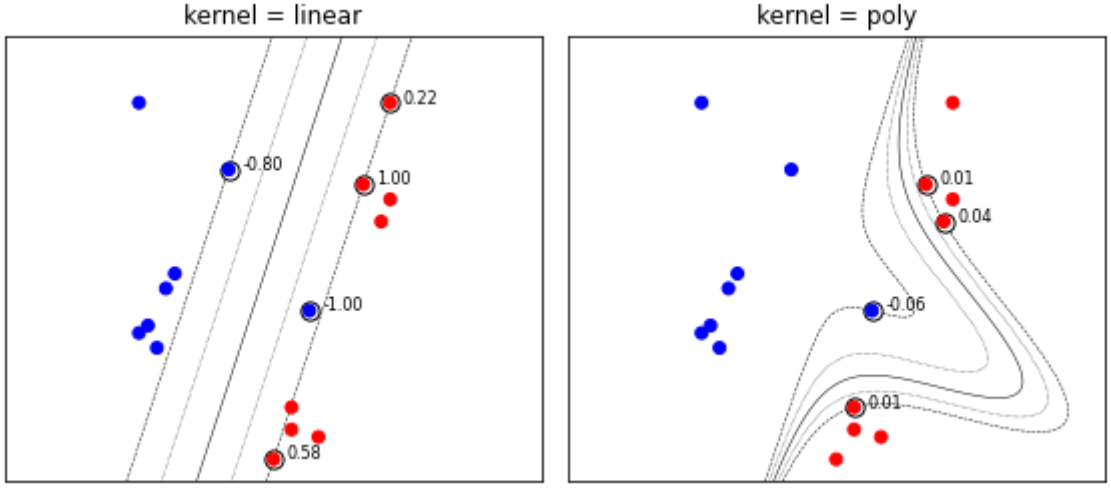
Example: SVMs

- Linear SVMs (dual form, for l support vectors with dual coefficients a_i and classes y_i):

$$\mathcal{L}_{Dual}(a_i) = \sum_{i=1}^{l} a_i - \frac{1}{2} \sum_{i,j=1}^{l} a_i a_j y_i y_j (\mathbf{x_i} . \mathbf{x_j})$$

- Kernelized SVM, using any existing kernel k we want:

$$\mathcal{L}_{Dual}(a_i, k) = \sum_{i=1}^{l} a_i - \frac{1}{2} \sum_{i,j=1}^{l} a_i a_j y_i y_j k(\mathbf{x_i}, \mathbf{x_j})$$



Which kernels exist?

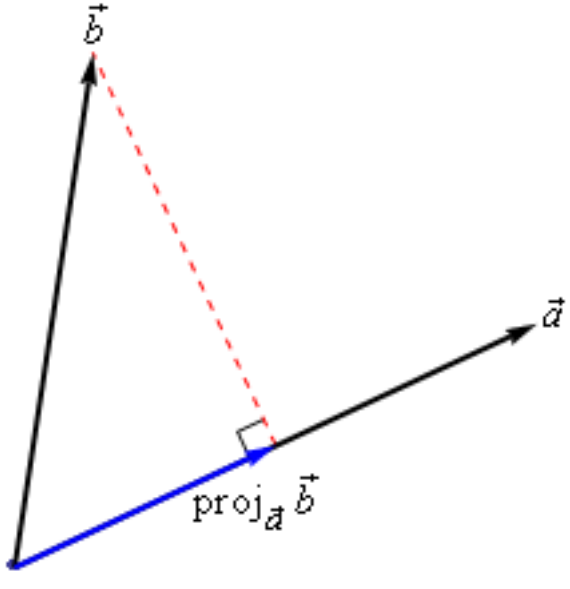
- A (Mercer) kernel is any function $k : X \times X \to \mathbb{R}$ with these properties:
    - Symmetry: $k(\mathbf{x_1}, \mathbf{x_2}) = k(\mathbf{x_2}, \mathbf{x_1}) \ \ \forall \mathbf{x_1}, \mathbf{x_2} \in X$
    - Positive definite: the kernel matrix K is positive semi-definite
        - Intuitively, $k(\mathbf{x_1}, \mathbf{x_2}) \geq 0$
- The kernel matrix (or Gram matrix) for n points of $x_1, \ldots, x_n \in X$ is defined as:

$$K = XX^T = \begin{bmatrix} k(\mathbf{x_1}, \mathbf{x_1}) & \ldots & k(\mathbf{x_1}, \mathbf{x_n}) \\ \vdots & \ddots & \vdots \\ k(\mathbf{x_n}, \mathbf{x_1}) & \ldots & k(\mathbf{x_n}, \mathbf{x_n}) \end{bmatrix}$$

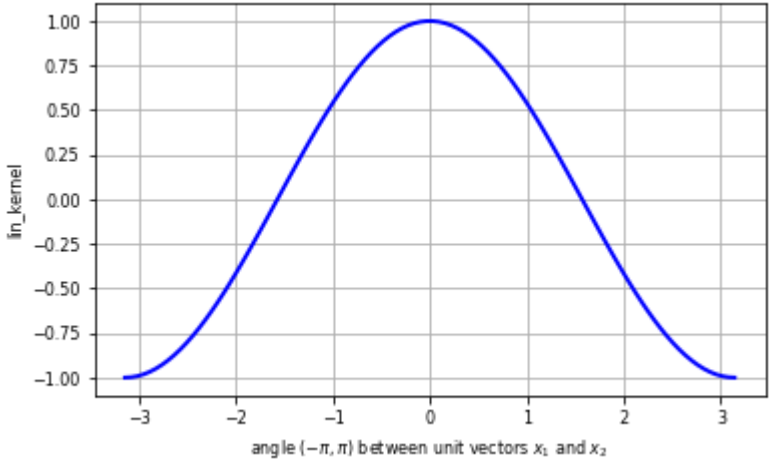
- Once computed ($\mathcal{O}(n^2)$), simply lookup $k(\mathbf{x_1}, \mathbf{x_2})$ for any two points
- In practice, you can either supply a kernel function or precompute the kernel matrix

Linear kernel

- Input space is same as output space: $X = \mathcal{H} = \mathbb{R}^d$
- Feature map $\Phi(\mathbf{x}) = \mathbf{x}$
- Kernel: $k_{linear}(\mathbf{x_i}, \mathbf{x_j}) = \mathbf{x_i} \cdot \mathbf{x_j}$
- Geometrically, the dot product is the *projection* of $\mathbf{x_j}$ on hyperplane defined by $\mathbf{x_i}$
    - Becomes larger if $\mathbf{x_i}$ and $\mathbf{x_j}$ are in the same 'direction'



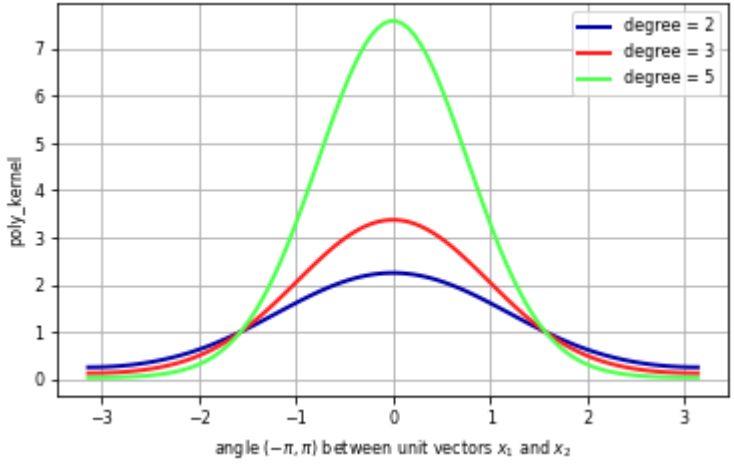
- Linear kernel between point (0,1) and another unit vector an angle a (in radians)
    - Points with similar angles are deemed similar



Polynomial kernel

- If k_1, k_2 are kernels, then $\lambda . k_1$ ($\lambda \geq 0$), $k_1 + k_2$, and $k_1 . k_2$ are also kernels
- The **polynomial kernel** (for degree $d \in \mathbb{N}$) reproduces the polynomial feature map
  - γ is a scaling hyperparameter (default $\frac{1}{p}$)
  - c_0 is a hyperparameter (default 1) to trade off influence of higher-order terms

$$k_{poly}(\mathbf{x_1}, \mathbf{x_2}) = (\gamma(\mathbf{x_1} \cdot \mathbf{x_2}) + c_0)^d$$



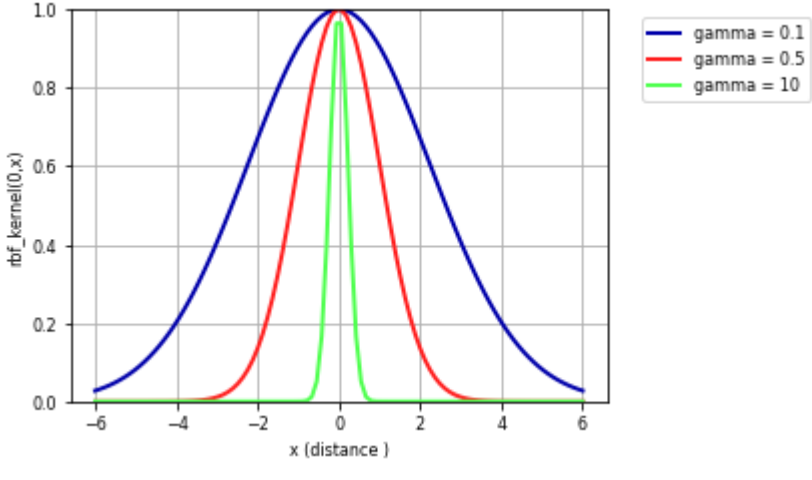
RBF (Gaussian) kernel

- The *Radial Basis Function* (RBF) feature map builds the Taylor series expansion of e^x

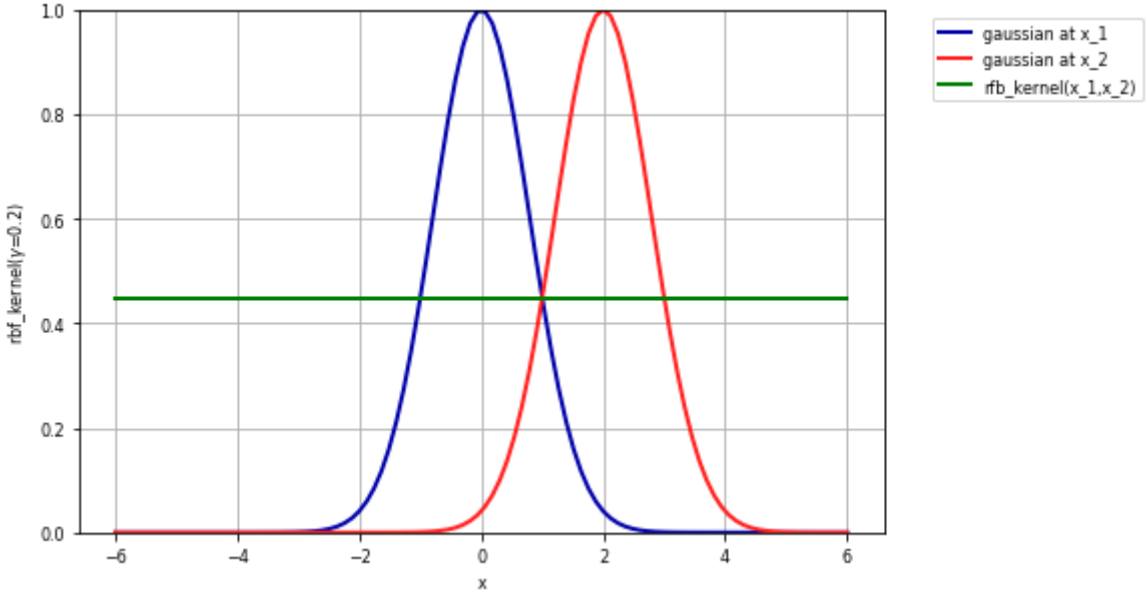
$$\Phi(x) = e^{-x^2/2\gamma^2}\left[1, \sqrt{\frac{1}{1!\gamma^2}}x, \sqrt{\frac{1}{2!\gamma^4}}x^2, \sqrt{\frac{1}{3!\gamma^6}}x^3, \dots\right]^T$$

- RBF (or *Gaussian*) kernel with *kernel width* $\gamma \geq 0$:

$$k_{RBF}(\mathbf{x_1}, \mathbf{x_2}) = exp(-\gamma||\mathbf{x_1} - \mathbf{x_2}||^2)$$

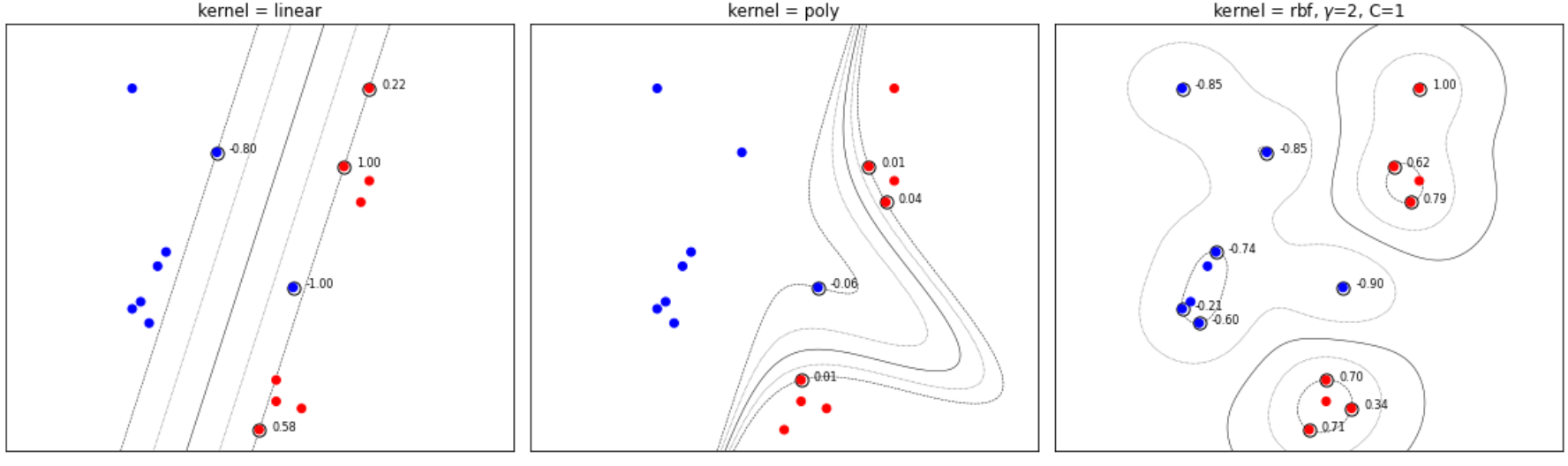


- The RBF kernel $k_{RBF}(\mathbf{x_1}, \mathbf{x_2}) = exp(-\gamma||\mathbf{x_1} - \mathbf{x_2}||^2)$ does not use a dot product
    - It only considers the distance between $\mathbf{x_1}$ and $\mathbf{x_2}$
    - It's a *local kernel* : every data point only influences data points nearby
        - linear and polynomial kernels are *global* : every point affects the whole space
    - Similarity depends on closeness of points and kernel width
        - value goes up for closer points and wider kernels (larger overlap)



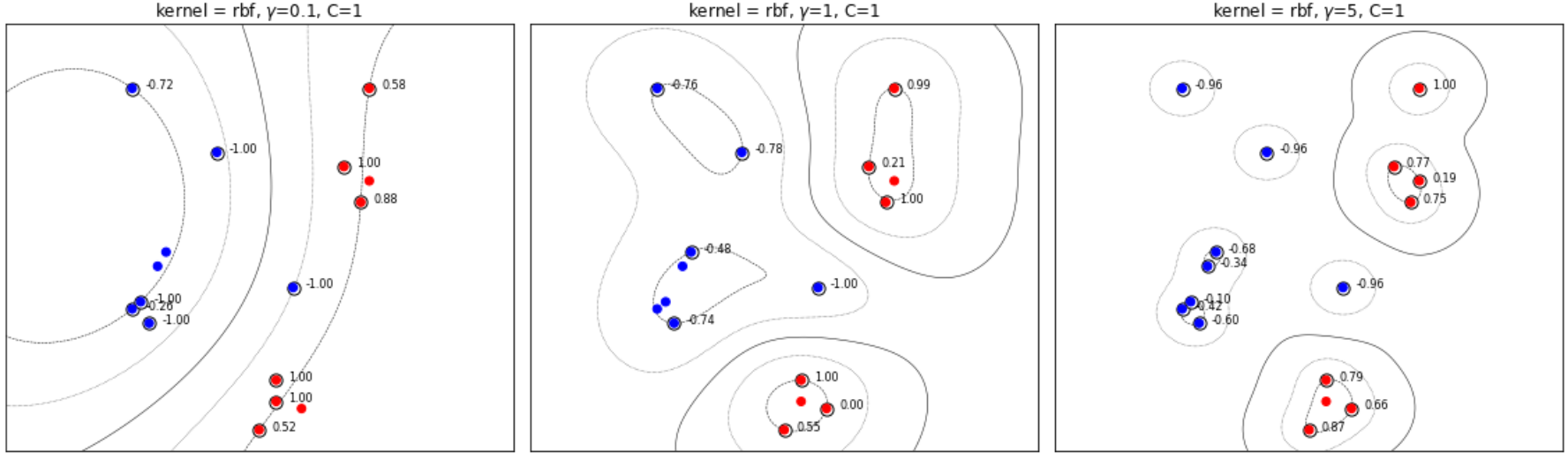
Kernelized SVMs in practice

- You can use SVMs with any kernel to learn non-linear decision boundaries



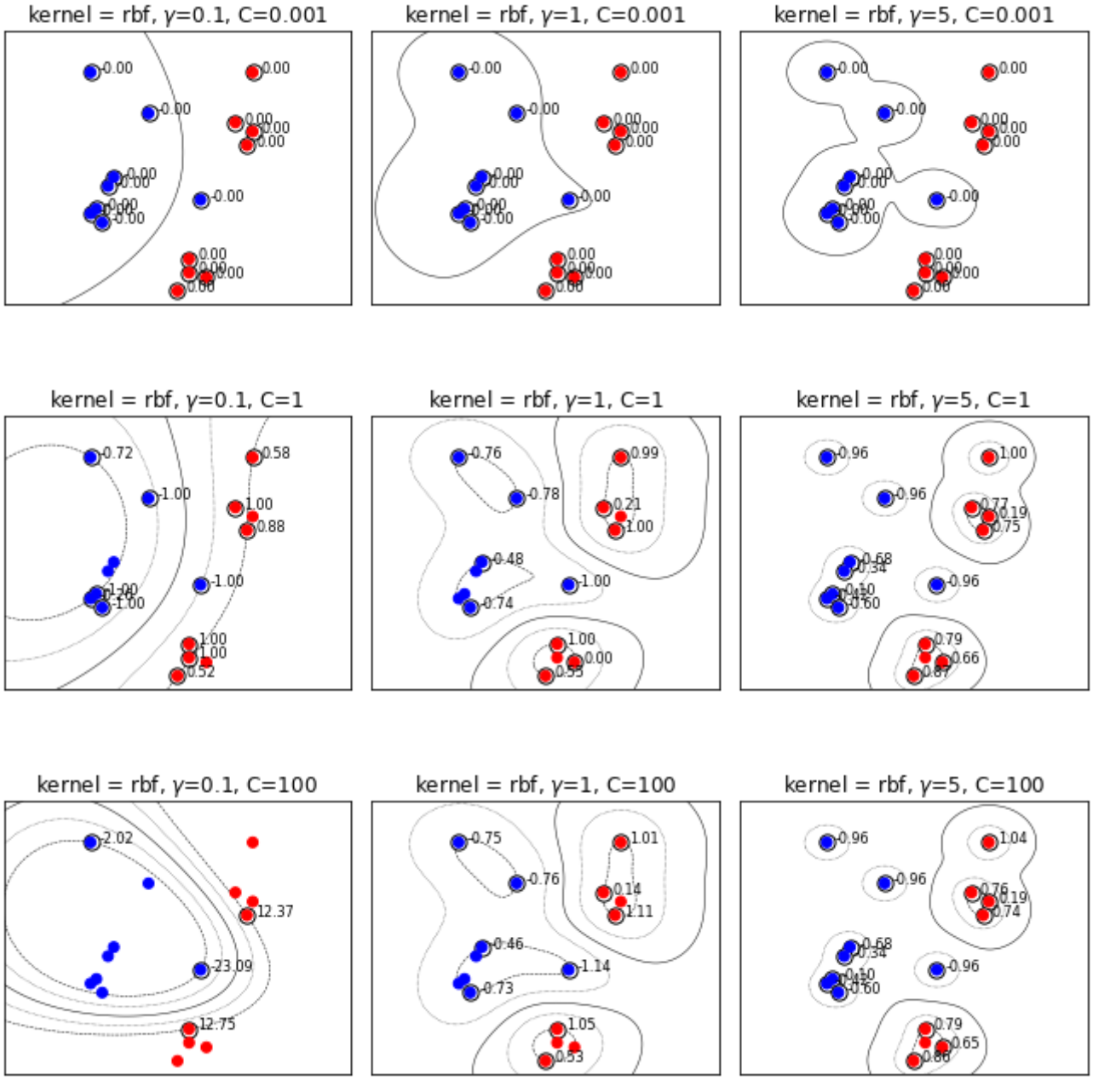
SVM with RBF kernel

- Every support vector *locally* influences predictions, according to kernel width (γ)
- The prediction for test point $\mathbf{u}$: sum of the remaining influence of each support vector
  - $f(x) = \sum_{i=1}^{l} a_i y_i k(\mathbf{x_i}, \mathbf{u})$

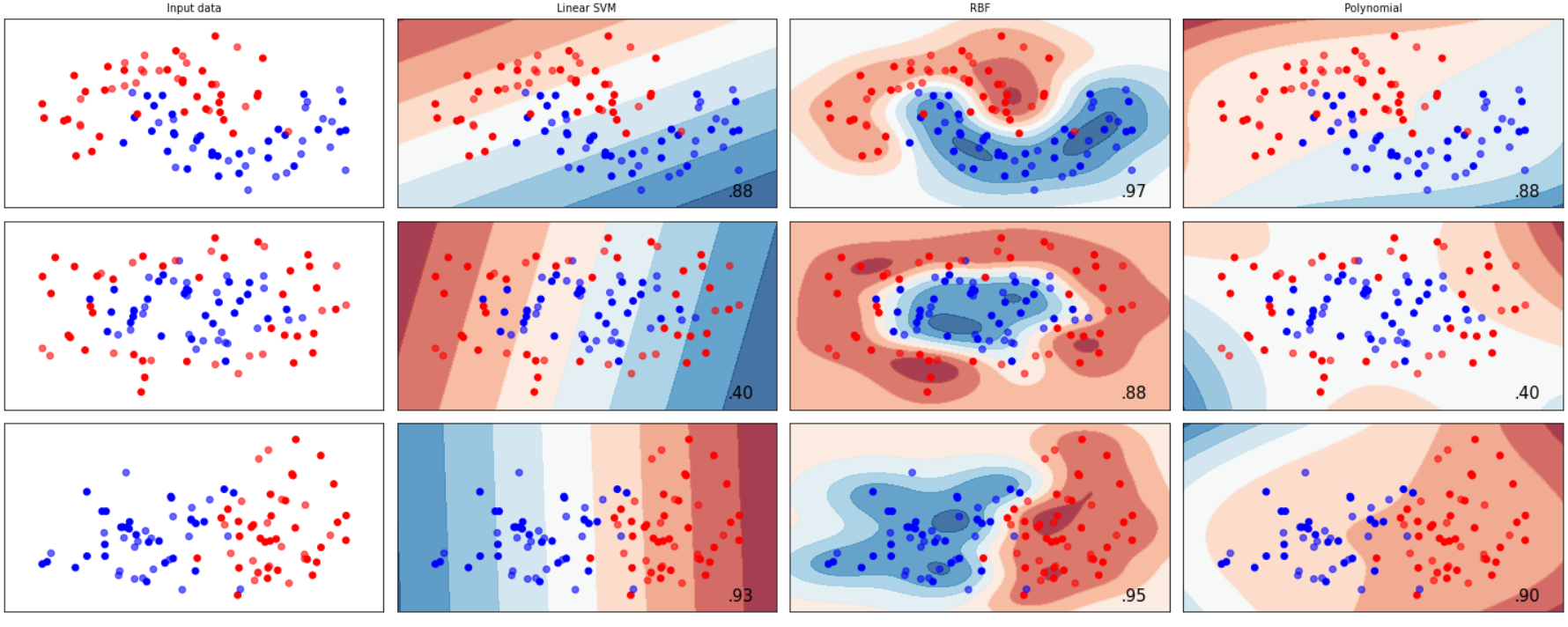


Tuning RBF SVMs

- gamma (kernel width)
    - high values cause narrow Gaussians, more support vectors, overfitting
    - low values cause wide Gaussians, underfitting
- C (cost of margin violations)
    - high values punish margin violations, cause narrow margins, overfitting
    - low values cause wider margins, more support vectors, underfitting


kernel = rbf, γ=0.1, C=0.001
kernel = rbf, γ=1, C=0.001
kernel = rbf, γ=5, C=0.001
kernel = rbf, γ=0.1, C=1
kernel = rbf, γ=1, C=1
kernel = rbf, γ=5, C=1
kernel = rbf, γ=0.1, C=100
kernel = rbf, γ=1, C=100
kernel = rbf, γ=5, C=100

Kernel overview



SVMs in practice

- C and gamma *always* need to be tuned
    - Interacting regularizers. Find a good C, then finetune gamma
- SVMs expect all features to be approximately on the same scale
    - Data needs to be scaled beforehand
- Allow to learn complex decision boundaries, even with few features
    - Work well on both low- and high dimensional data
    - Especially good at small, high-dimensional data
- Hard to inspect, although support vectors can be inspected
- In sklearn, you can use `SVC` for classification with a range of kernels
    - `SVR` for regression

Other kernels

- There are many more possible kernels
- If no kernel function exists, we can still *precompute* the kernel matrix
    - All you need is some similarity measure, and you can use SVMs
- Text kernels:
    - Word kernels: build a bag-of-words representation of the text (e.g. TFIDF)
        - Kernel is the inner product between these vectors
    - Subsequence kernels: sequences are similar if they share many sub-sequences
        - Build a kernel matrix based on pairwise similarities
- Graph kernels: Same idea (e.g. find common subgraphs to measure similarity)
- These days, deep learning embeddings are more frequently used

The Representer Theorem

- We can kernelize many other loss functions as well
- The *Representer Theorem* states that if we have a loss function $\mathcal{L}'$ with
    - $\mathcal{L}$ an *arbitrary* loss function using some function f of the inputs $\mathbf{x}$
    - $\mathcal{R}$ a (non-decreasing) regularization score (e.g. L1 or L2) and constant λ

$$\mathcal{L}'(\mathbf{w}) = \mathcal{L}(y, f(\mathbf{x})) + \lambda \mathcal{R}(||\mathbf{w}||)$$

- Then the weights $\mathbf{w}$ can be described as a linear combination of the training samples:

$$\mathbf{w} = \sum_{i=1}^{n} a_i y_i f(\mathbf{x_i})$$

- Note that this is exactly what we found for SVMs: $\mathbf{w} = \sum_{i=1}^{l} a_i y_i \mathbf{x_i}$
- Hence, we can also kernelize Ridge regression, Logistic regression, Perceptrons, Support Vector Regression, ...

Kernelized Ridge regression

- The linear Ridge regression loss (with $\mathbf{x_0} = 1$):

$$\mathcal{L}_{Ridge}(\mathbf{w}) = \sum_{i=0}^{n}(y_i - \mathbf{w}\mathbf{x_i})^2 + \lambda\|w\|^2$$

- Filling in $\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x_i}$ yields the dual formulation:

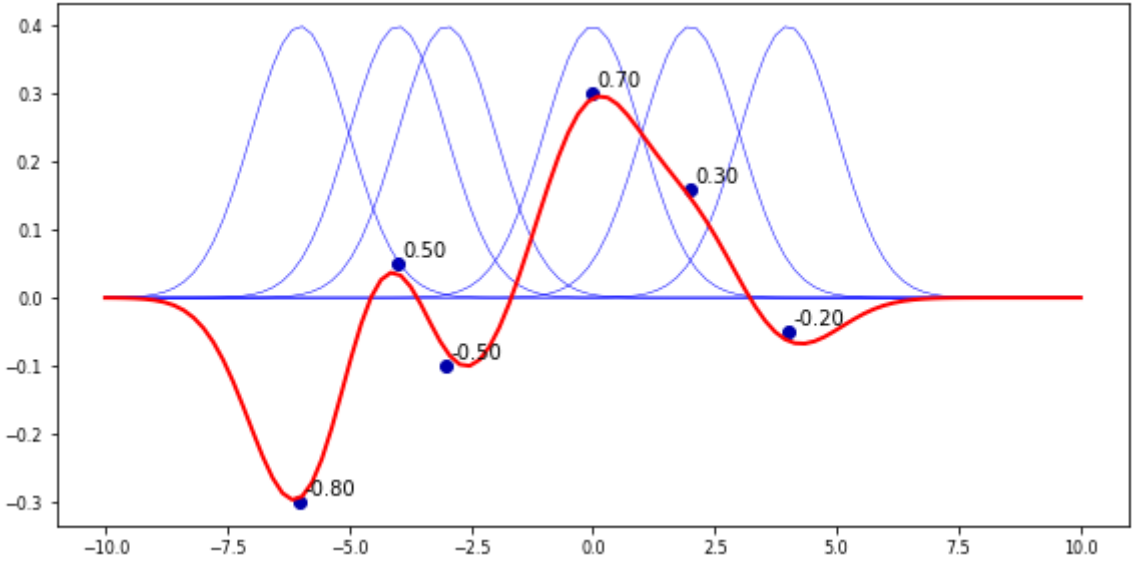
$$\mathcal{L}_{Ridge}(\mathbf{w}) = \sum_{i=1}^{n}(y_i - \sum_{j=1}^{n} \alpha_j y_j \mathbf{x_i}\mathbf{x_j})^2 + \lambda \sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x_i}\mathbf{x_j}$$

- Generalize $\mathbf{x_i} \cdot \mathbf{x_j}$ to $k(\mathbf{x_i}, \mathbf{x_j})$

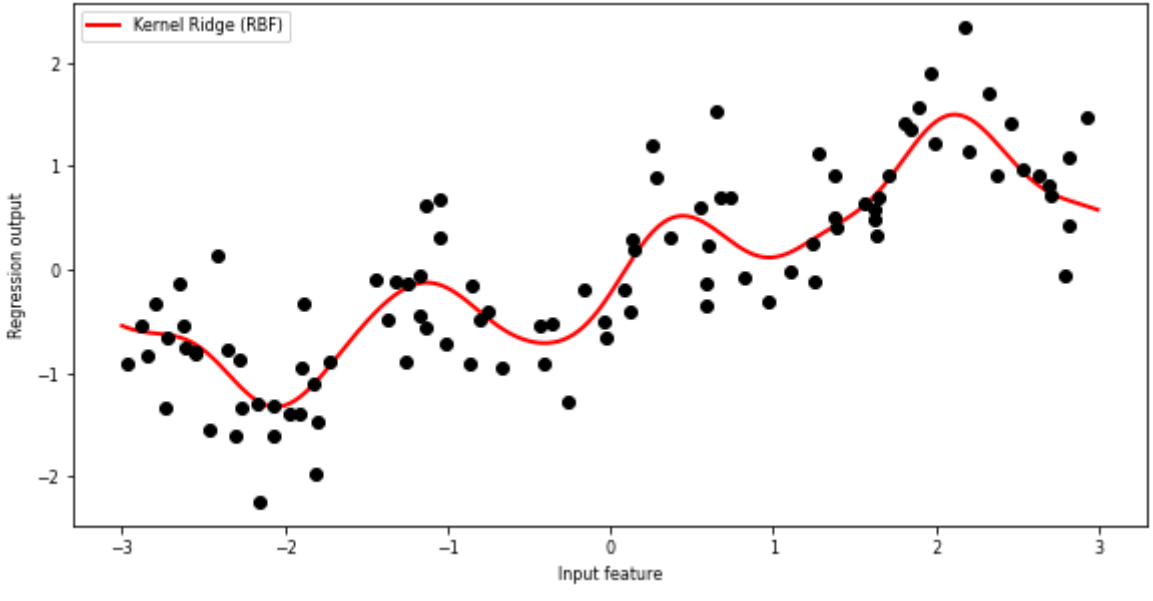
$$\mathcal{L}_{KernelRidge}(\alpha, k) = \sum_{i=1}^{n}(y_i - \sum_{j=1}^{n} \alpha_j y_j k(\mathbf{x_i}, \mathbf{x_n}))^2 + \lambda \sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j k(\mathbf{x_i}, \mathbf{x_j})$$

Example of kernelized Ridge

- Prediction (red) is now a linear combination of kernels (blue): $y = \sum_{j=1}^{n} \alpha_j y_j k(\mathbf{x}, \mathbf{x_j})$
- We learn a dual coefficient for each point



- Fitting our regression data with `KernelRidge`

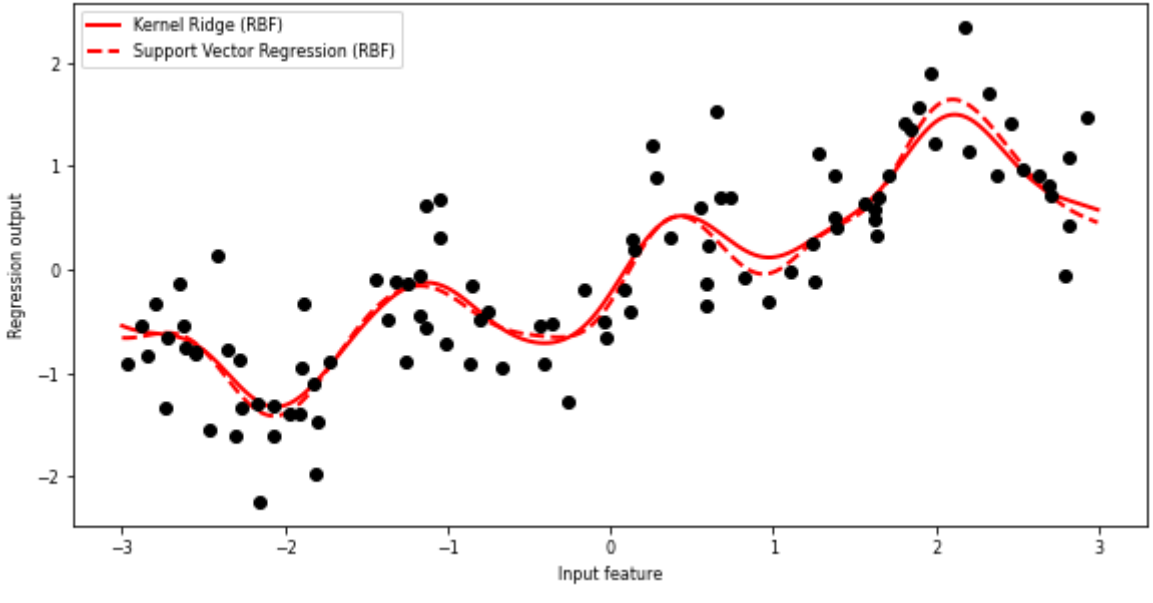


Other kernelized methods

- Same procedure can be done for logistic regression
- For perceptrons, $\alpha \rightarrow \alpha + 1$ after every misclassification

$$\mathcal{L}_{DualPerceptron}(x_i, k) = max(0, y_i \sum_{j=1}^{n} \alpha_j y_j k(\mathbf{x_j}, \mathbf{x_i}))$$

- Support Vector Regression behaves similarly to Kernel Ridge



Summary

- Feature maps $\Phi(x)$ transform features to create a higher-dimensional space
    - Allows learning non-linear functions or boundaries, but very expensive/slow
- For some $\Phi(x)$, we can compute dot products without constructing this space
    - Kernel trick: $k(\mathbf{x_i}, \mathbf{x_j}) = \Phi(\mathbf{x_i}) \cdot \Phi(\mathbf{x_j})$
    - Kernel k (generalized dot product) is a measure of similarity between $\mathbf{x_i}$ and $\mathbf{x_j}$
- There are many such kernels
    - Polynomial kernel: $k_{poly}(\mathbf{x_1}, \mathbf{x_2}) = (\gamma(\mathbf{x_1} \cdot \mathbf{x_2}) + c_0)^d$
    - RBF (Gaussian) kernel: $k_{RBF}(\mathbf{x_1}, \mathbf{x_2}) = exp(-\gamma||\mathbf{x_1} - \mathbf{x_2}||^2)$
    - A kernel matrix can be precomputed using any similarity measure (e.g. for text, graphs,...)
- Any loss function where inputs appear only as dot products can be kernelized
    - E.g. Linear SVMs: simply replace the dot product with a kernel of choice
- The Representer theorem states which *other* loss functions can also be kernelized and how
    - Ridge regression, Logistic regression, Perceptrons,...