Kernelization

Feature Maps

- Remember linear models?

$$\hat{y} = \mathbf{w}\mathbf{x} = \sum_{i=0}^{p} w_i \cdot x_i = w_0 \cdot x_0 + w_1 \cdot x_1 + \ldots + w_p \cdot x_p$$

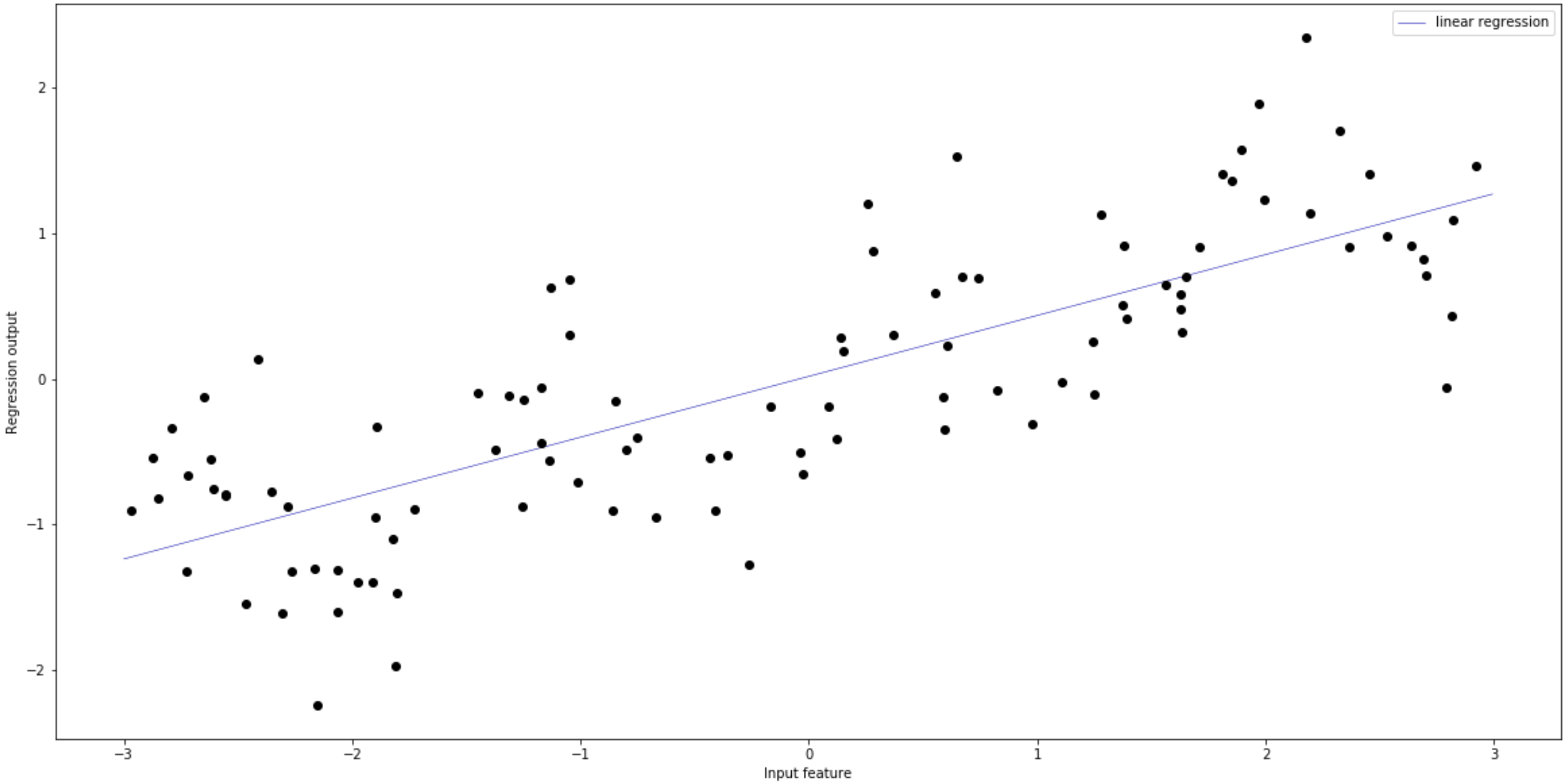
- When we cannot fit the data well with linear models, we can learn more complex models by simply adding more dimensions
- Feature map (or *basis expansion*) ϕ: $X \rightarrow \mathbb{R}^d$

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

- You still may need MANY dimensions to fit the data
  - Memory and computational cost
  - More likely overfitting

Example: Ridge regression

`Coefficients: [0.418]`



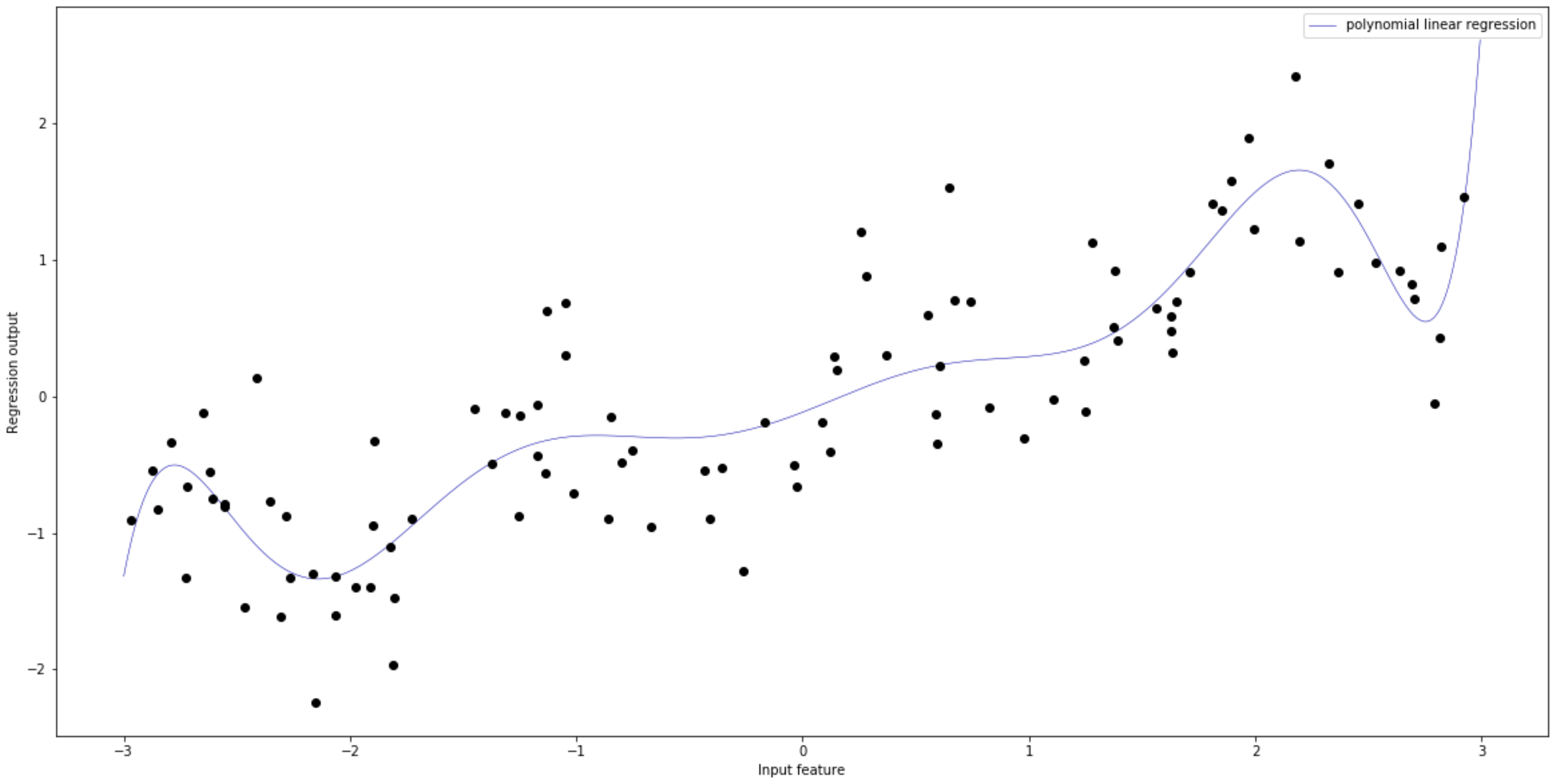
- Add all polynomials x^d up to degree D. How large should D be?
- We can also compute all polynomials and all interactions between features (e.g. $x \cdot x^2$). This leads to D^2 features.

Out[7]:

	x0	x0^2	x0^3	x0^4	x0^5	x0^6	x0^7	x0^8	x0^9	x0^10
0	-0.75	0.57	-0.43	0.32	-0.24	0.18	-0.14	0.1	-0.078	0.058
1	2.7	7.3	20	53	1.4e+02	3.9e+02	1.1e+03	2.9e+03	7.7e+03	2.1e+04
2	1.4	1.9	2.7	3.8	5.2	7.3	10	14	20	27
3	0.59	0.35	0.21	0.12	0.073	0.043	0.025	0.015	0.0089	0.0053
4	-2.1	4.3	-8.8	18	-37	77	-1.6e+02	3.3e+02	-6.8e+02	1.4e+03

Fit Ridge again:

```
Coefficients: [ 0.643  0.297 -0.69  -0.264  0.41   0.096 -0.076 -0.014  0.
004  0.001]
```



How expensive is this?

- Ridge has a closed-form solution which we can compute with linear algebra:
$$w^* = (X^T X + \lambda I)^{-1} X^T Y$$
- 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
$$w^* = (\Phi(X)^T \Phi(X) + \lambda I)^{-1} \Phi(X)^T Y$$
- Since Φ increases d a *lot*, $\Phi(X)^T \Phi(X)$ becomes *huge*
- To be continued...

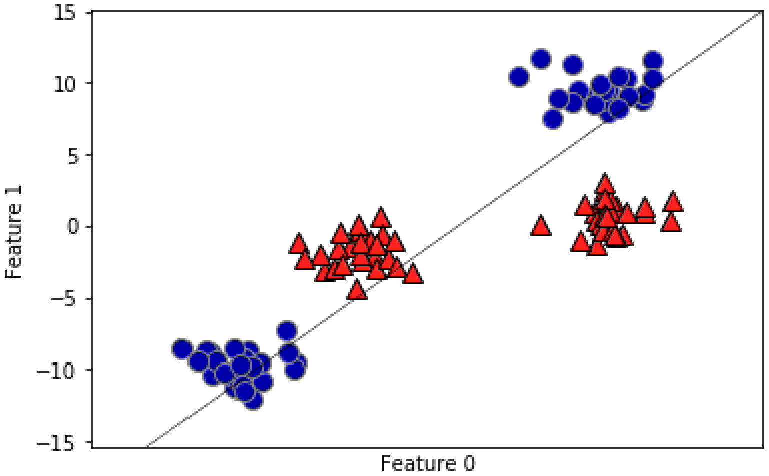
Linear models for Classification (recap)

Aims to find a (hyper)plane that separates the examples of each class.
For binary classification (2 classes), we aim to fit the following function:

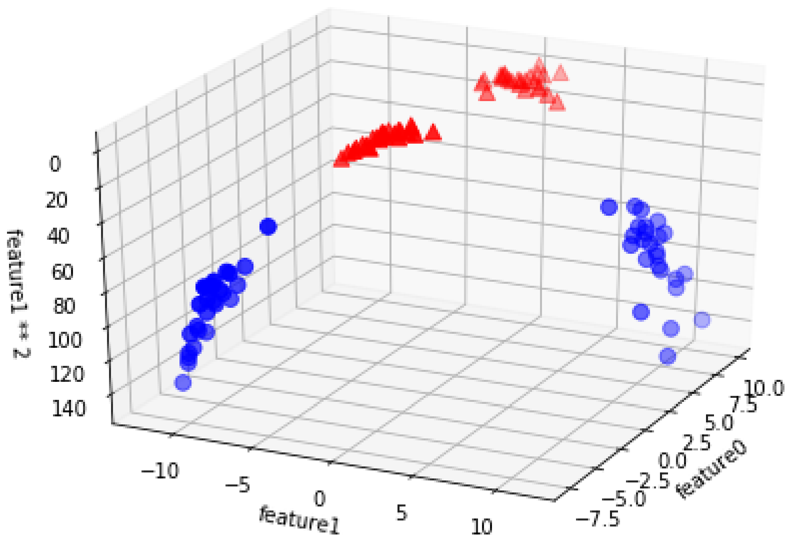
$$\hat{y} = w_0 * x_0 + w_1 * x_1 + ... + w_p * x_p + b > 0$$

When $\hat{y} < 0$, predict class -1, otherwise predict class +1

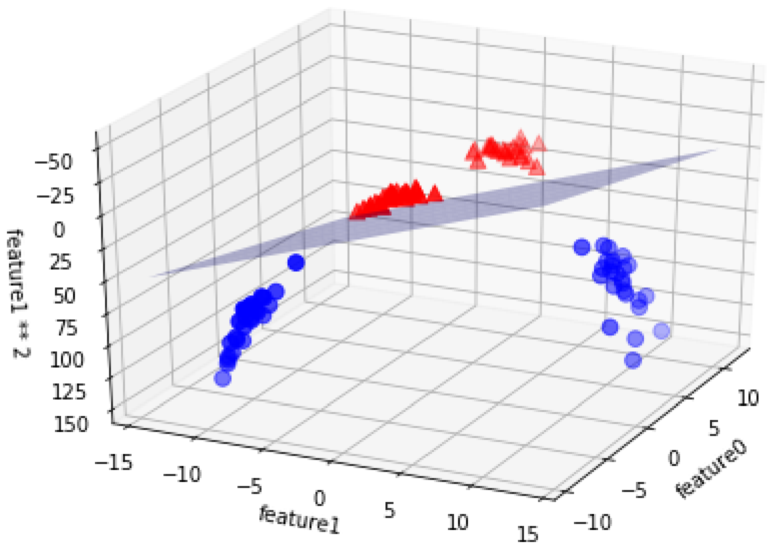
Again, we can add dimensions when our linear model doesn't fit the data well



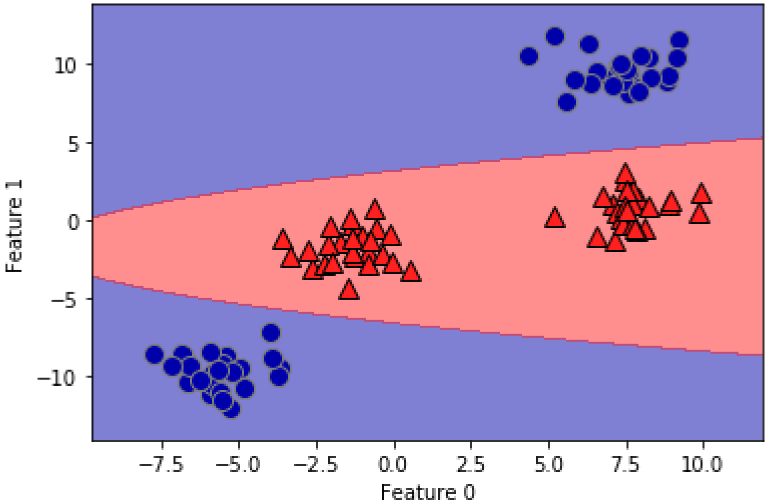
We can add a new feature by taking the squares of feature1 values



Now we can fit a linear model

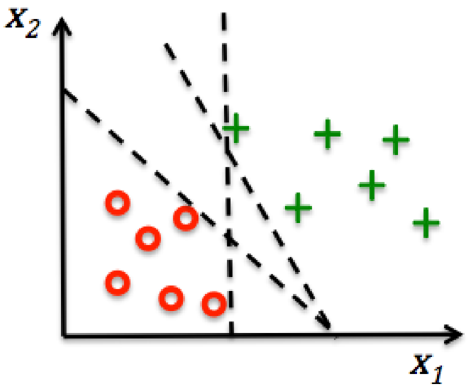


As a function of the original features, the linear SVM model is not actually linear anymore, but more of an ellipse

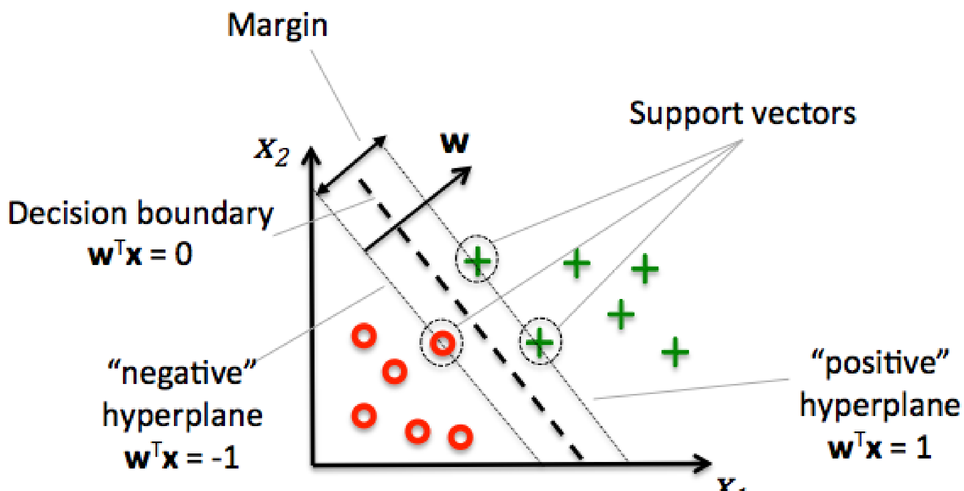


Support vector machines (recap)

- In several other linear models, we minimized (misclassification) error
- In SVMs, the optimization objective is to maximize the *margin*
- The **margin** is the distance between the separating hyperplane and the *support vectors*
- The **support vectors** are the training samples closest to the hyperplane
- Intuition: large margins generalize better, small margins may be prone to overfitting



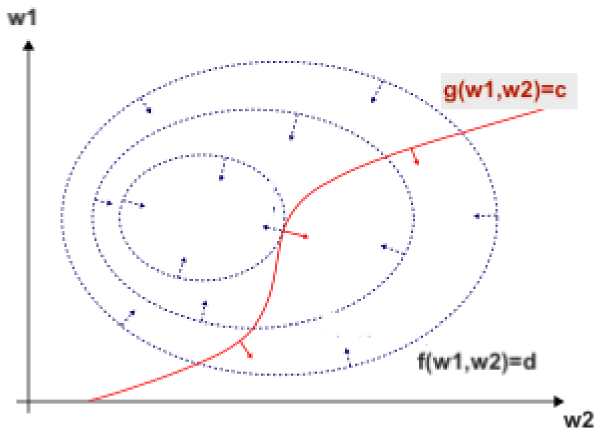
Which hyperplane?



SVM:
Maximize the margin

Geometric interpretation (for linearly separable data)

- Imagine a hyperplane defined by coefficients w (and bias b)
- We want it to have value 1 in the nearest positive example and value -1 in the nearest negative example
- The hyperplane with the largest margin maximizes $f = \frac{2}{||w||^2}$
  - The factor 2 is for scaling
- And we want that the hyperplane is >1 for all positive examples: $g(\mathbf{w}) = y^{(i)}(b + \mathbf{w}^{\mathbf{T}}\mathbf{x}^{\mathbf{(i)}}) > 1 \quad \forall i$
- Find the point (w_1, w_2) that satifies g but maximizes f



Loss function

A quadratic loss function with linear constraints can be solved using the *Lagrangian multipliers* methods, which has two solutions. The **Primal** objective is:

$$\mathcal{L}_{Primal} = \frac{1}{2}||\mathbf{w}||^2 - \sum_{i=1}^{n} a_i y_i (\mathbf{x_i} * \mathbf{w} + b) + \sum_{i=1}^{n} a_i$$

so that

$$a_i \geq 0$$

$$\mathbf{w} = \sum_{i=1}^{n} a_i y_i \mathbf{x_i}$$
$$\sum_{i=1}^{n} a_i y_i = 0$$

with n the number of training examples and a the *dual variables*, which act like weights for each training example. We find the optimal set of a's first, then the w's can be easily computed.

It has a Dual formulation as well (See 'Elements of Statistical Learning'):

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

so that

$$a_i \geq 0$$

$$\sum_{i=1}^{l} a_i y_i = 0$$

- Observe the term $\mathbf{x_i} . \mathbf{x_j}$. When the inputs only appear in inner products, we call the method *kernelized*

Making predictions

- a_i will be *0* if the point lies outside the margin, on the right side of the decision boundary
- The training samples for which a_i is not 0 are the *support vectors*

- Hence, the SVM model is completely defined by the support vectors and their coefficients

- Knowing the dual coefficients a_i (of which l are non-zero) we can find the weights w for the maximal margin separating hyperplane:

$$\mathbf{w} = \sum_{i=1}^{l} a_i y_i \mathbf{x_i}$$

- Hence, we can classify a new sample $\mathbf{u}$ by looking at the sign of $\mathbf{w} * \mathbf{u} + b$

SVMs and kNN

Remember, we will classify a new sample u by looking at the sign of:
$f(x) = \mathbf{w} * \mathbf{u} + b = \sum_{i=1}^{l} a_i y_i \mathbf{x_i} * \mathbf{u} + b$

Weighted k-nearest neighbor is a generalization of the k-nearest neighbor classifier. It classifies points by looking at the sign of:
$f(x) = \sum_{i=1}^{k} a_i y_i dist(x_i, u)$

Hence: SVM's predict exactly the same way as k-NN, only:

- They only consider the truly important points (the support vectors)
    - Thus *much* faster
- The number of neighbors is the number of support vectors
- The distance function is an *inner product of the inputs*

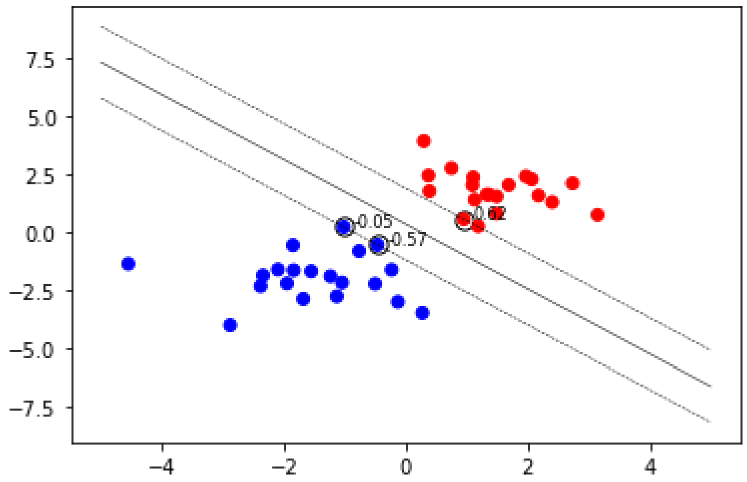
SVMs in scikit-learn

- We can use the `svm.SVC` classifier
    - or `svm.SVR` for regression
    - it only support the dual loss function
- To build a linear SVM use `kernel=linear`
- It returns the following:
    - `support_vectors_`: the support vectors
    - `dual_coef_`: the dual coefficients *a*, i.e. the `weigths` of the support vectors
    - `coef_`: only for linear SVMs, the feature weights w

```python
clf = svm.SVC(kernel='linear')
clf.fit(X, Y)
print("Support vectors:", clf.support_vectors_[:])
print("Coefficients:", clf.dual_coef_[:])
```

```
Support vectors:
[[-1.021  0.241]
 [-0.467 -0.531]
 [ 0.951  0.58 ]]
Coefficients:
[[-0.048 -0.569  0.617]]
```

SVM result. The circled samples are support vectors, together with their coefficients.



Dealing with nonlinearly separable data

- If the data is not linearly separable, (hard) margin maximization becomes meaningless
  - The constraints would contradict
- We can allow for violatings of the margin constraint by introducing a *slack variable* $\xi^{(i)}$ for every data point

$$b + \mathbf{w^T x^{(i)}} \geq 1 - \xi^{(i)} \quad if \quad y^{(i)} = 1$$
$$b + \mathbf{w^T x^{(i)}} \leq -1 + \xi^{(i)} \quad if \quad y^{(i)} = -1$$

The new objective (to be minimized) becomes:

$$\frac{||w||^2}{2} + C(\sum_i \xi^{(i)})$$

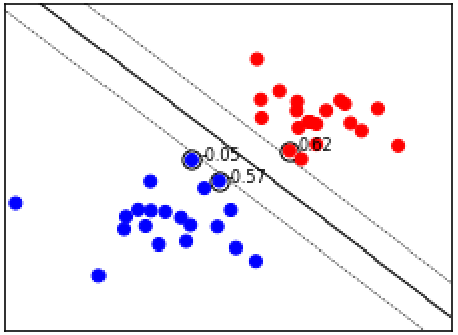
- C is a penalty for misclassification
  - Large C: large error penalties
  - Small C: less strict about violations (more regularization)
- This is known as the *soft margin* SVM (or *large margin* SVM)
  - Some support vectors are exactly on the margin hyperplane, with margin = 1
  - Others are margin violators, with margin < 1 and a positive slack variable: $\xi^{(i)} > 0$
    - If $\xi^{(i)} \geq 1$, they are misclassified

C and regularization

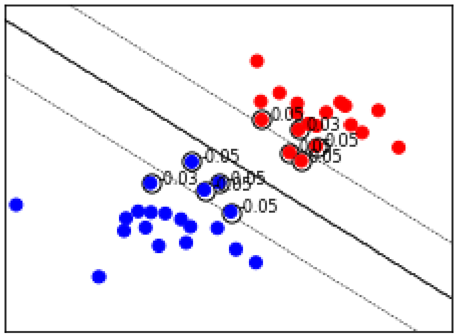
- Hence, we can use C to control the size of the margin and overfitting:
    - Small C: Increases bias, reduces variance, more underfitting
    - Large C: Reduces bias, increases variance, more overfitting
- The penalty term $C(\sum_i \xi^{(i)})$ acts as an L1 regularizer on the dual coefficients
    - Also known as hinge loss
    - This induces sparsity: large C values will set many dual coefficients to 0, hence fewer support vectors
    - Small C values will typically lead to more support vectors (more points fall within the margin)
    - Again, it depends on the data how flexible or strict you need to be
- The *least squares SVM* is a variant that does L2 regularization
    - Will have many more support vectors (with low weights)
    - In scikit-learn, this is only available for the `LinearSVC` classifier (`loss='squared_hinge'`)

Effect on linearly separable data

C = 1

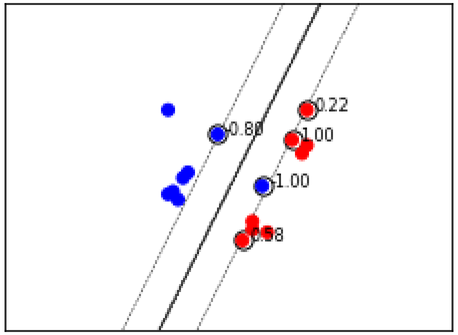


C = 0.05

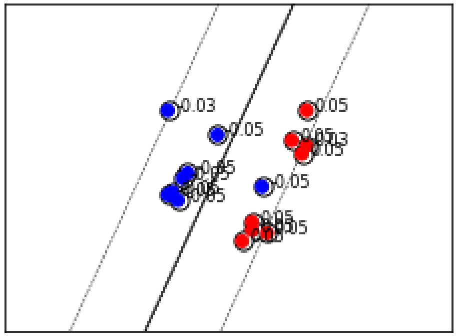


Effect on non-linearly separable data

C = 1



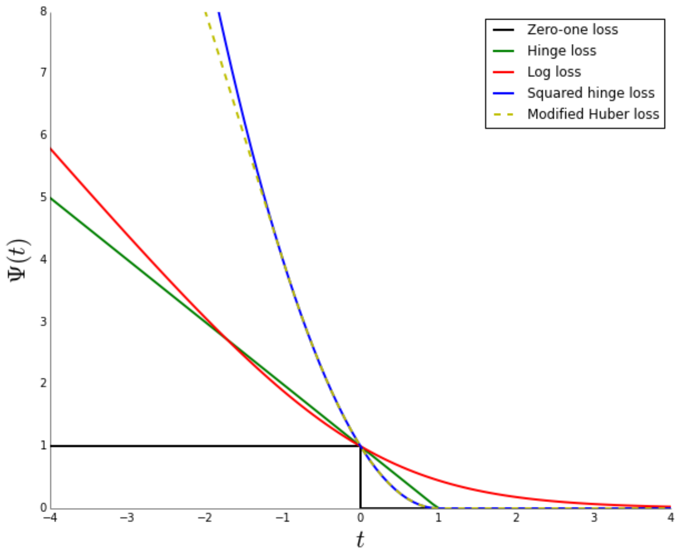
C = 0.05



Other loss functions

It is possible to *generalize* SVMs by training them with other loss functions and gradient descent as the optimizer

See the `SGDClassifier` (`SGDClassifier(loss='hinge')` will act like an SVM)



Kernelization

- A method is *kernelized* if inputs only appear inside inner products $x_i \cdot x_j$ $= \langle x_i, x_j \rangle$
- We said that SVMs can be *kernelized* through it's dual formulation:

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

- A *kernel function* corresponding to a transformation Φ is

$$k(x_i, x_j) = \langle \Phi(x_i), \Phi(x_j) \rangle$$

- $\Phi(x)$ can be used to generate many more features based on the original feature x
- Turns out, we can often evaluate $k(x_i, x_j)$ directly, *without* evaluating $\Phi(x_i), \Phi(x_j)$

Kernel trick

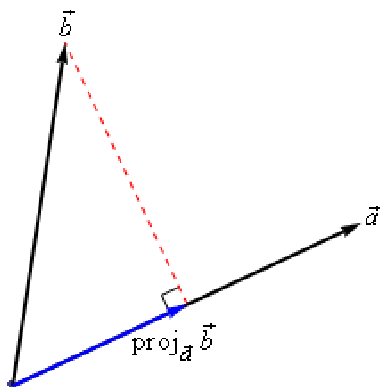
- Evaluating the kernel directly can be *much* cheaper.
- Example: a simple *quadratic* feature map for $x = (x1, \dots, xd)$ has dimension $\mathcal{O}(d^2)$:
$$\Phi(x) = (x_1, \dots, x_d, x_1^2, \dots, x_d^2, \sqrt{2}x_1x_2, \dots, \sqrt{2}x_{d-1}x_d)$$
- The corresponding quadratic kernel is:
$$k(x_i, x_j) = \langle \Phi(x_i), \Phi(x_j) \rangle = \langle x_i, x_j \rangle + \langle x_i, x_j \rangle^2$$
- We can skip the computation of $\Phi(x_i)$ and $\Phi(x_j)$ and compute $k(x_i, x_j)$ in $\mathcal{O}(d)$ instead of $\mathcal{O}(d^2)$!

Kernel functions

- It is useful to think of a kernel as a similarity score between 2 vectors (points)
    - Not mathematically equivalent
- There are many ways to design such a similarity score (also for text, graphs,...)
- Computationally *much* cheaper
- We can access very large (even infinite) feature spaces $\mathcal{H}$
- Thinking in terms of similarity is much more intuitive than thinking in high-dimensional feature spaces

Linear kernel

- Input space is same as output space: $X = \mathcal{H} = \mathbb{R}^d$
- Feature map $\Phi(x) = x$
- Kernel: $k(x_i, x_j) = x_i \cdot x_j = x_i^T x_j$
- Geometrically, we can view these as *projections* of x_j on a hyperplane defined by x_i
    - Nearby points will have nearby projections



Kernel matrix

For points of $x_1, \ldots, x_n \in X$ and an inner product $\langle \cdot, \cdot \rangle$, the kernel matrix (or Gram matrix) is defined as:

$$K = \begin{bmatrix} \langle x_1, x_1 \rangle & \ldots & \langle x_1, x_n \rangle \\ \vdots & \ddots & \vdots \\ \langle x_n, x_1 \rangle & \ldots & \langle x_n, x_n \rangle \end{bmatrix}$$

- For the Euclidean inner product $k(x_i, x_j) = x_i^T x_j$, we have $K = XX^T$
- Size is nxn, irrespective of number of dimensions d
- Once kernel matrix is computed, cost depends on number of data points only

Kernels

More generally, a (Mercer) kernel on a space X is a function

$k : X \times X \to \mathbb{R}$

With the properties:

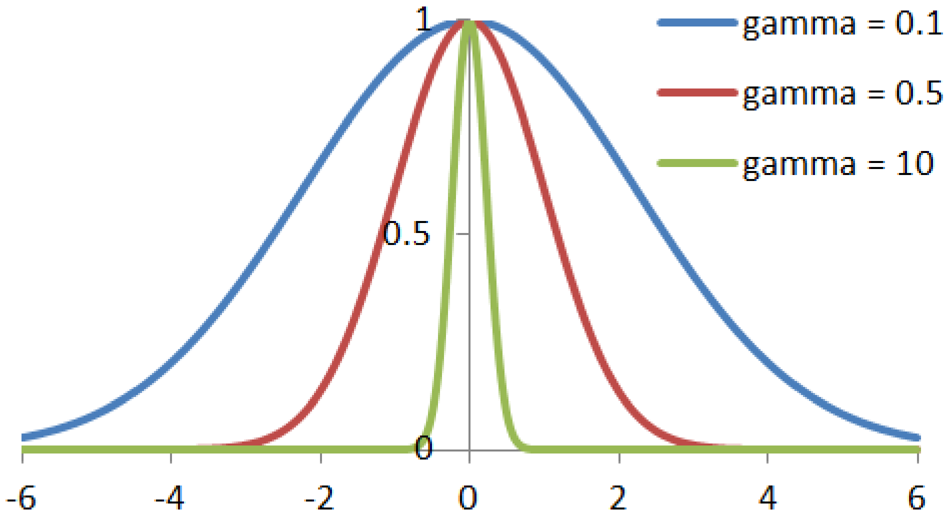
- Symmetry: $k(x_1, x_2) = k(x_2, x_1) \ \ \forall x_1, x_2 \in X$
- Positive definite: for each finite subset of data points $x_1, \ldots, x_n$, the kernel Gram matrix is positive semi-definite
    - Intuitively, $k(x_1, x_2) \geq 0$

This is also what we expect from similarity functions

Kernels: examples

- The inner product is a kernel. The standard inner product is the **linear kernel**:
  $k(x_1, x_2) = x_1^T x_2$
- Kernels can be constructed from other kernels k_1 and k_2:
  - For $\lambda \geq 0$, $\lambda . k_1$ is a kernel
  - $k_1 + k_2$ is a kernel
  - $k_1 . k_2$ is a kernel (thus also k_1^n)
- This allows to construct the **polynomial kernel**:
  $k(x_1, x_2) = (x_1^T x_2 + b)^d$, for $b \geq 0$ and $d \in \mathbb{N}$

- The 'radial base function' (or **Gaussian**) kernel is defined as: $k(x_1, x_2) = exp(-\gamma||x_1 - x_2||^2)$, for $\gamma \geq 0$

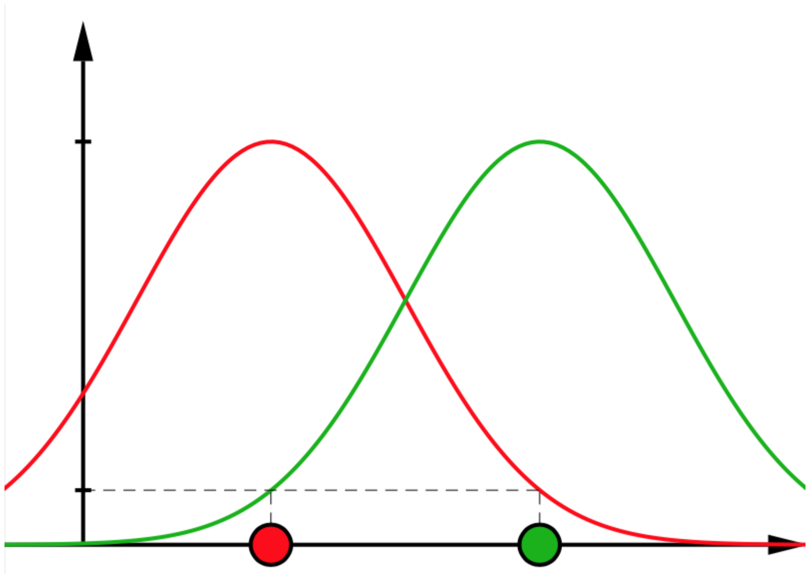


The Kernel Trick (summary)

- Explictly adding nonlinear features can make linear models much more powerful, but also much more expensive
- Given a kernelized ML algorithm, we can swap out the inner product for a new kernel function.
- Kernel functions allow us to directly compute distances (scalar products) in an implicit high dimensional space (you don't actually construct it)
- A *kernel function* is a distance (similarity) function with special properties for which this trick is possible
    - Polynomial kernel: computes all polynomials up to a certain degree of the original features
    - Gaussian kernel, or radial basis function (RBF): considers all possible polynomials of all degrees
        - Infinite high dimensional space (Hilbert space), where the importance of the features decreases for higher degrees

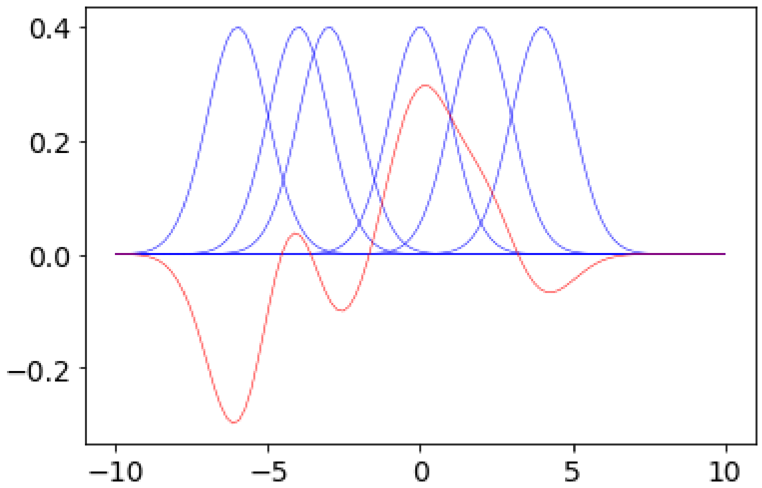
Gaussian kernel: intuition

- Each point generates a function, the inner product is where they intersect
- The closer the points are, the more similar they are



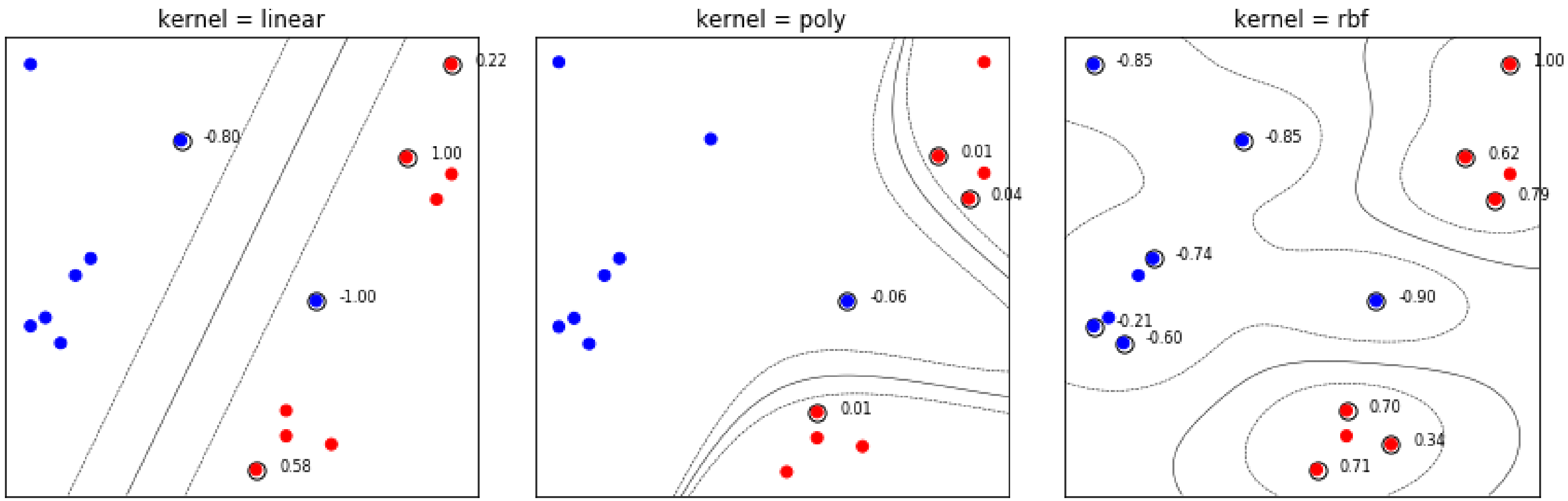
Example (for regression):

- We have 6 input points: [-6,-4,-3,0,2,4]
    - We fit a kernel over each (blue)
- We learn a coefficient for each: e.g. [-.8,.5,-0.5,.7,0.3,-0.2]
- Resulting preditions (red curve)
- Linear kernels will produce a linear function, Gaussian kernels can produce very complex functions.



Example (for classification):

- In the RBF SVM, every support vector generates a 2D Gaussian, the final prediction is the sum of those
- At prediction time, you evaluate each Gaussian (a kind of distance between the new point and the support vector) and sum up the values



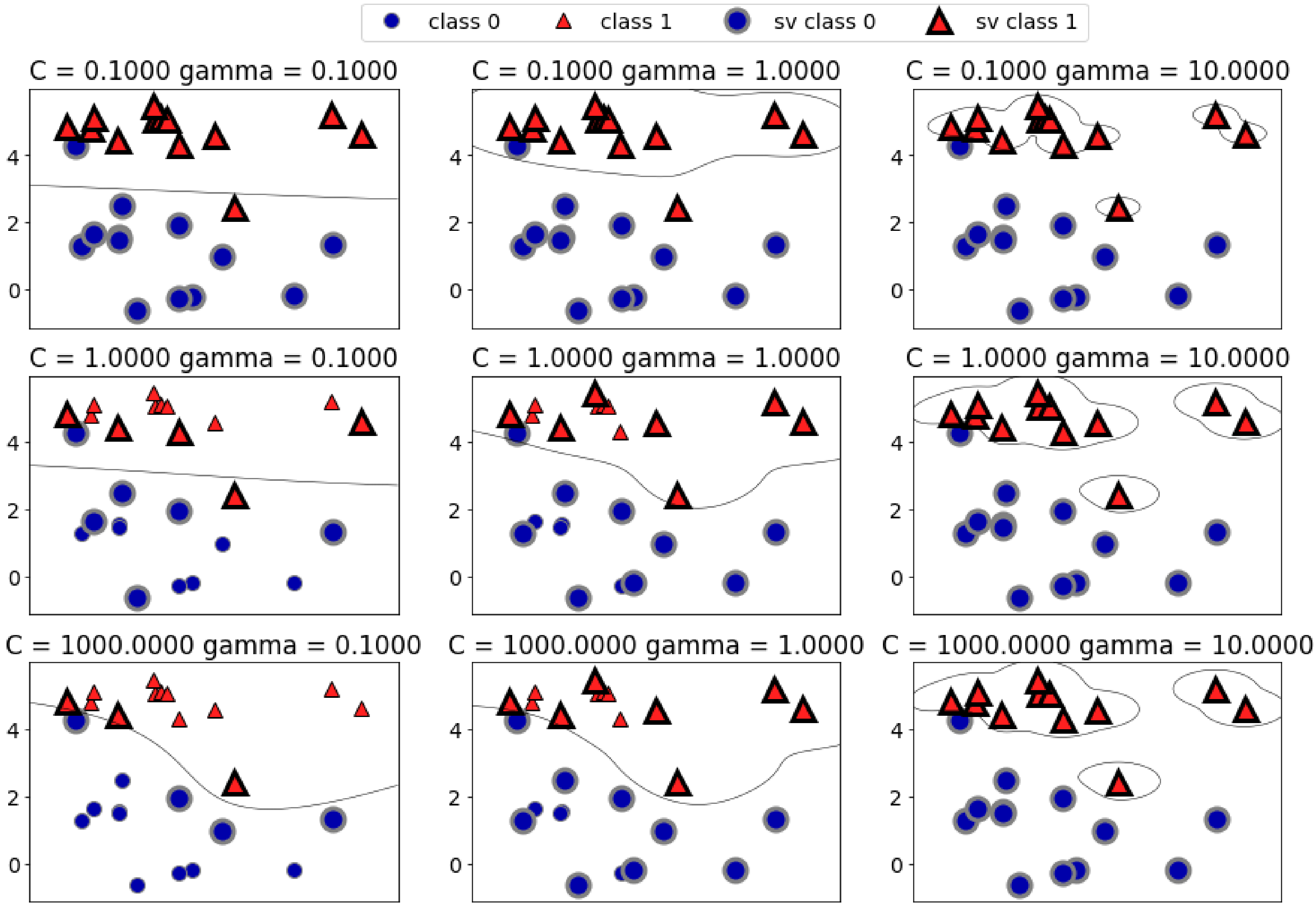
Local vs Global kernels

- With a linear or polynomial kernel, one support vector can affect the whole model space
  - These are called *global kernels*
- The RBF kernel only affects the region around the support vector (depending on how wide it is)
  - This a called a *local* kernel
  - Can capture local abnormalities that a global kernel can't
  - Also overfits easily if the kernels are very narrow

Tuning SVM parameters

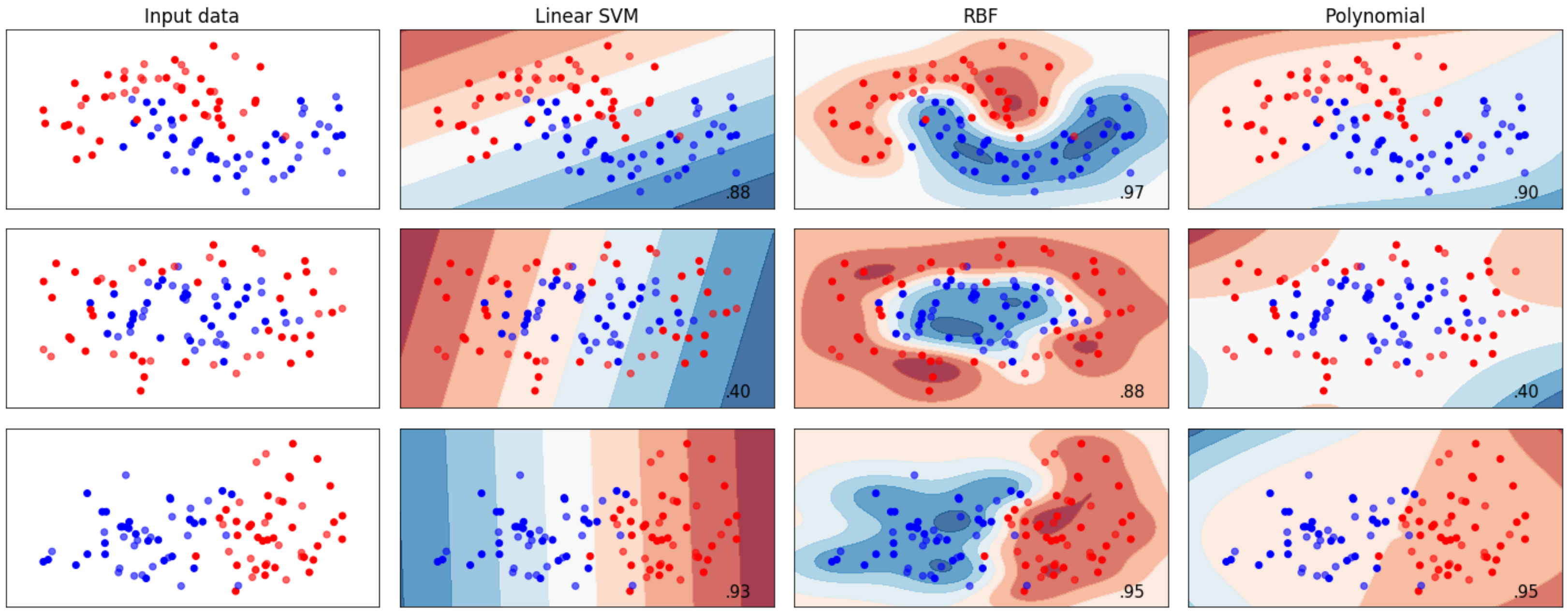
Several important parameters:

- gamma ((inverse) kernel width): high values means that points are further apart
    - High values mean narrow Gaussians, i.e. the influence of one point is very small
        - You need many support vectors
    - Leads to complex decision boundaries, overfitting
- C (our linear regularizer): 'cost' of misclassifying training examples
    - High C: force SVM to classify more examples correctly
        - Requires more support vectors, thus complex decision boundaries
- For polynomial kernels, the *degree* (exponent) defines the complexity of the models


class 0
class 1
sv class 0
sv class 1
C = 0.1000 gamma = 0.1000
C = 0.1000 gamma = 1.0000
C = 0.1000 gamma = 10.0000
C = 1.0000 gamma = 0.1000
C = 1.0000 gamma = 1.0000
C = 1.0000 gamma = 10.0000
C = 1000.0000 gamma = 0.1000
C = 1000.0000 gamma = 1.0000
C = 1000.0000 gamma = 10.0000
4
2
0

- Low gamma (left): wide Gaussians, very smooth decision boundaries
- High gamma (right): narrow Gaussians, boundaries focus on single points (high complexity)
- Low C (top): each support vector has very limited influence: many support vectores, almost linear decision boundary
- High C (bottom): Stronger influence, decision boundary bends to every support vector

Kernel overview



Preprocessing Data for SVMs

- SVMs are very sensitive to hyperparameter settings
- They expect all features to be approximately on the same scale
- Data point similarity (e.g. RBF kernel) is computed the same way in all dimensions
- If some dimension is scaled differently, it will have a much larger/smaller impact
- We'll get back to this in Lecture 4 (pipelines).

Strengths, weaknesses and parameters

- SVMs allow complex decision boundaries, even with few features.
- Work well on both low- and high-dimensional data
- Don't scale very well to large datasets (>100000)
- Require careful preprocessing of the data and tuning of the parameters.
- SVM models are hard to inspect

Important parameters:

- regularization parameter C
- choice of the kernel and kernel-specific parameters
  - Typically string correlation with C

Generalized linear models

We can generalize the SVM objective as follows:

$$\mathcal{J}(w) = \mathcal{R}(||w||) + \mathcal{L}(\langle w, \Phi(x_1)\rangle, \ldots, \langle w, \Phi(x_n)\rangle)$$

Where $\mathcal{R}$ is a (non-decreasing) regularization score and $\mathcal{L}$ is an *arbitrary* loss function

- The *Representer Theorem* says that if J(w) has a minimizer, it has a minimizer of the form
$$w^* = \sum_{i=1}^{n} \alpha_i \Phi(x_i)$$
- This is what we already discovered for SVMs (but with a lot more work)

Generalized linear models

- In the same way, we can define:
    - Kernelized SVMs
    - Kernelized Ridge regression
    - 1-layer neural networks
        - The 'kernel' here is the activation function
- We can also define kernels for text, graphs, and many other types of data