RBF with K centers

N parameters $w_1, \cdots, w_N$ based on N data points

Use $K \ll N$ centers: $\boldsymbol{\mu}_1, \cdots, \boldsymbol{\mu}_K$ instead of $\mathbf{x}_1, \cdots, \mathbf{x}_N$

$$h(\mathbf{x}) = \sum_{k=1}^{K} w_k \exp\left(-\gamma \left\|\mathbf{x} - \boldsymbol{\mu}_k\right\|^2\right)$$

1. How to choose the centers $\boldsymbol{\mu}_k$

2. How to choose the weights w_k

Choosing the centers

Minimize the distance between $\mathbf{x}_n$ and the **closest** center $\boldsymbol{\mu}_k$: | K-means clustering |

Split $\mathbf{x}_1, \cdots, \mathbf{x}_N$ into clusters $S_1, \cdots, S_K$

Minimize $\displaystyle\sum_{k=1}^{K} \sum_{\mathbf{x}_n \in S_k} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$

Unsupervised learning ☺

NP-hard ☹

An iterative algorithm

Lloyd's algorithm: Iteratively minimize $\sum_{k=1}^{K} \sum_{\mathbf{x}_n \in S_k} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$ w.r.t. $\boldsymbol{\mu}_k, S_k$

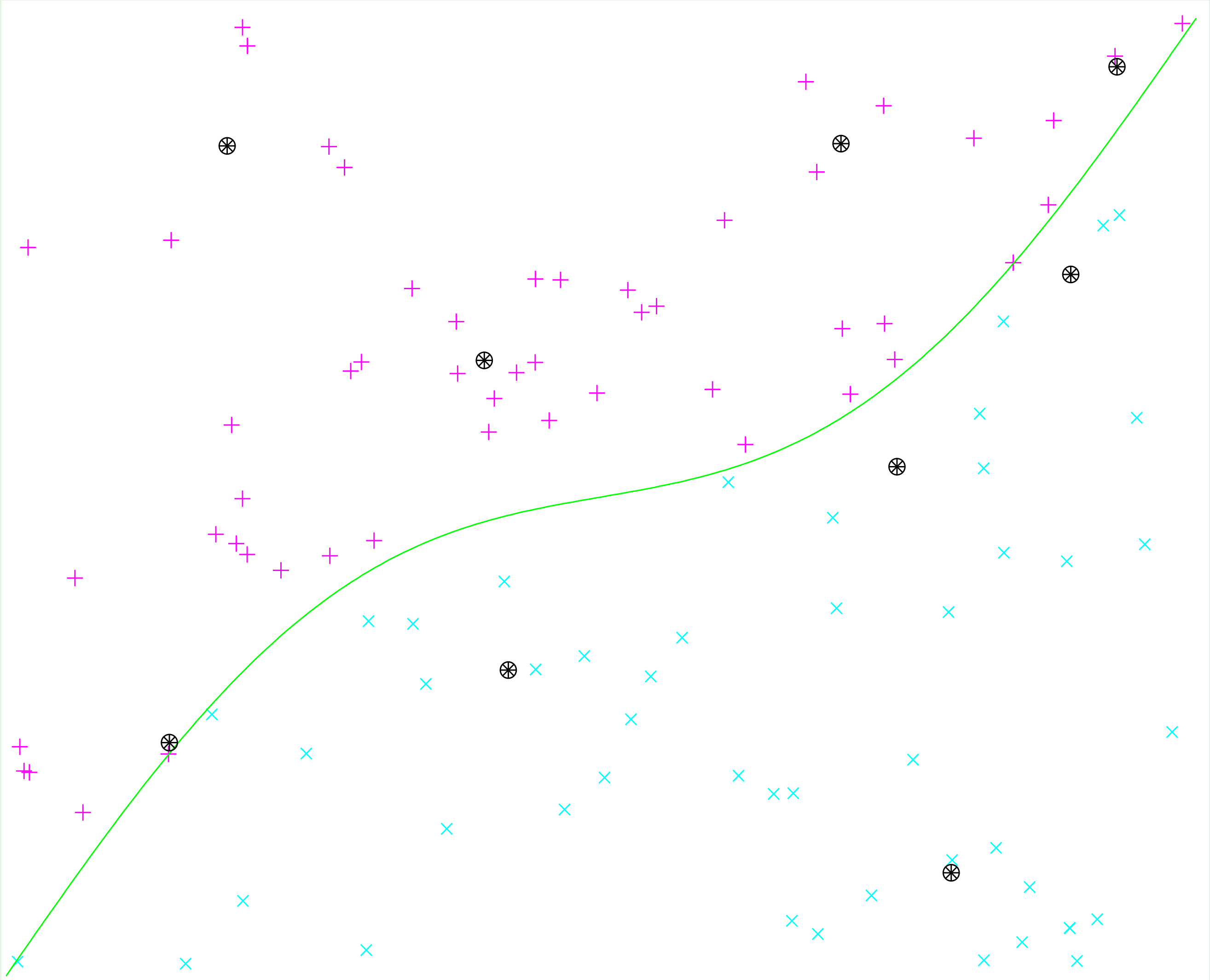
$$\boldsymbol{\mu}_k \leftarrow \frac{1}{|S_k|} \sum_{\mathbf{x}_n \in S_k} \mathbf{x}_n$$

$$S_k \leftarrow \{\mathbf{x}_n : \|\mathbf{x}_n - \boldsymbol{\mu}_k\| \leq \text{all } \|\mathbf{x}_n - \boldsymbol{\mu}_\ell\|\}$$

Convergence $\longrightarrow$ **local minimum**

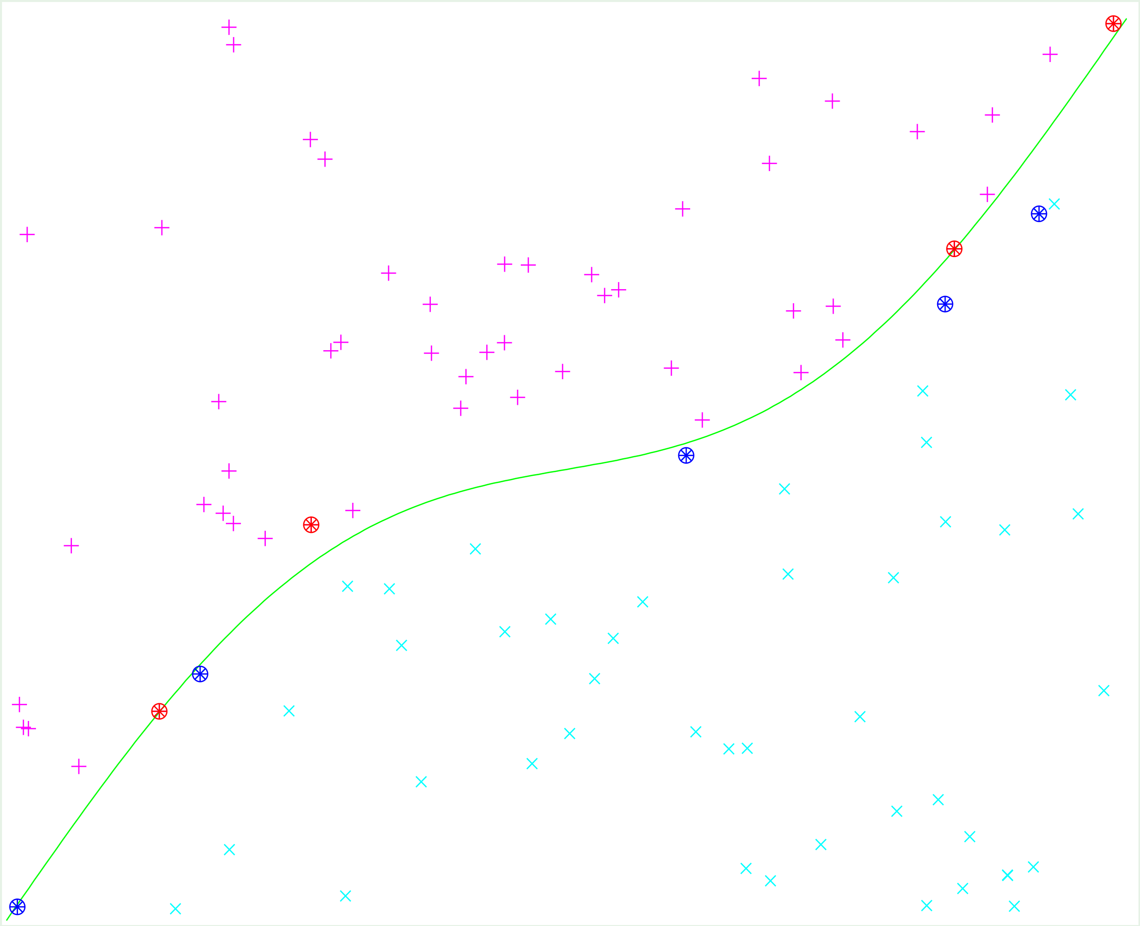
Lloyd's algorithm in action

1. Get the data points
2. Only the inputs!
3. Initialize the centers
4. Iterate
5. These are your $\boldsymbol{\mu}_k$'s

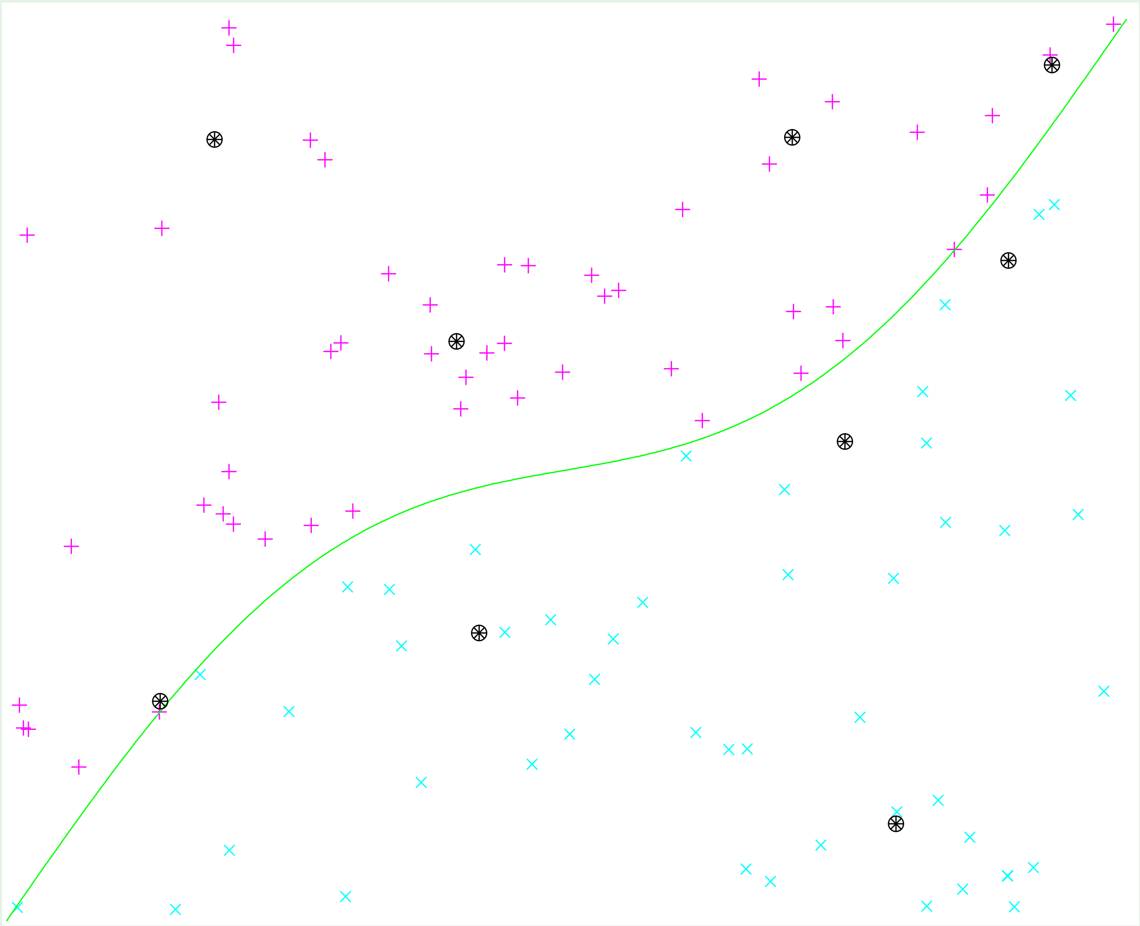


Centers versus support vectors

support vectors



RBF centers



Choosing the weights

$$\sum_{k=1}^{K} w_k \ \exp\left(-\gamma \ \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2\right) \approx \ y_n$$

N equations in $K < N$ unknowns

$$\underbrace{\begin{bmatrix} \exp(-\gamma \ \|\mathbf{x}_1 - \boldsymbol{\mu}_1\|^2) & \dots & \exp(-\gamma \ \|\mathbf{x}_1 - \boldsymbol{\mu}_K\|^2) \\ \exp(-\gamma \ \|\mathbf{x}_2 - \boldsymbol{\mu}_1\|^2) & \dots & \exp(-\gamma \ \|\mathbf{x}_2 - \boldsymbol{\mu}_K\|^2) \\ \vdots & \vdots & \vdots \\ \exp(-\gamma \ \|\mathbf{x}_N - \boldsymbol{\mu}_1\|^2) & \dots & \exp(-\gamma \ \|\mathbf{x}_N - \boldsymbol{\mu}_K\|^2) \end{bmatrix}}_{\Phi} \underbrace{\begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_K \end{bmatrix}}_{\mathbf{w}} \approx \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}}_{\mathbf{y}}$$

If $\Phi^{\top}\Phi$ is invertible, $\boxed{\mathbf{w} = (\Phi^{\top}\Phi)^{-1}\Phi^{\top}\mathbf{y}}$ **pseudo-inverse**