Support Vector Machines I

Dr. Chelsea Parlett-Pelleriti

Outline

- Maximal Margin Classifiers
- Support Vector Classifiers
- Support Vector Machines: Kernels and The Kernel Trick
- Common Kernels
  - Polynomial
  - Radial Basis Function

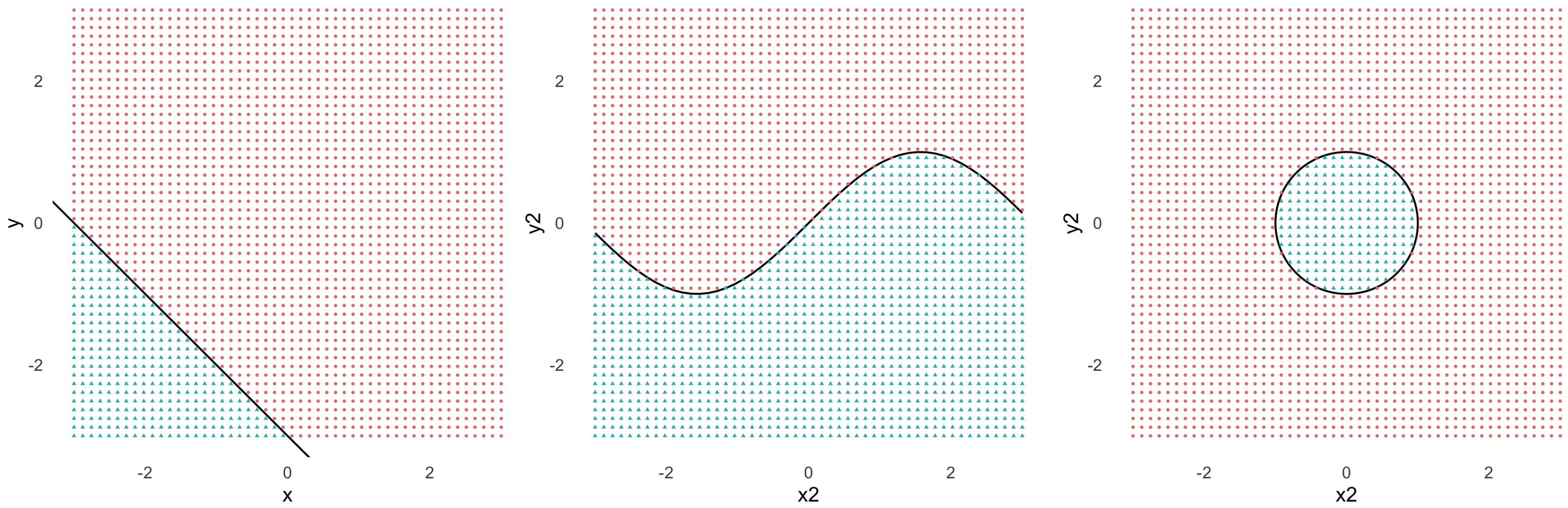
Hyperplanes

Flat: the hyperplane is not curved, it increases/decreases constantly in each direction

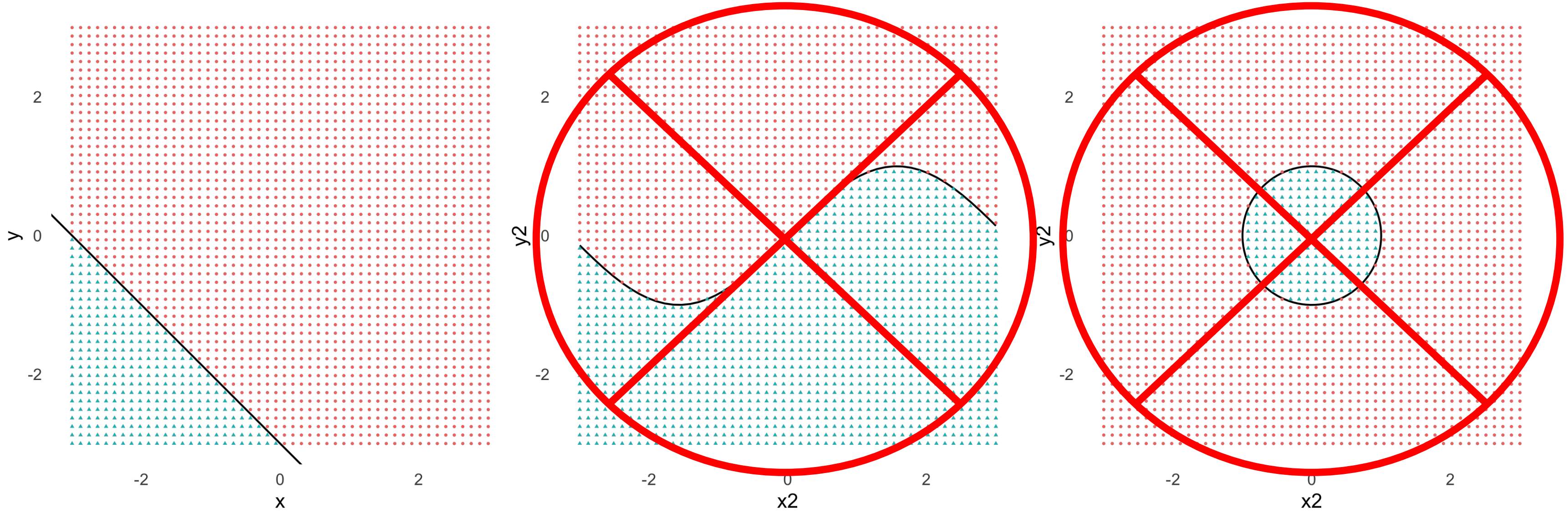
Affine: the hyperplane doesn't need to pass through the origin

Subspace: a subset of vectors in a larger vector space (closure under addition and scalar multiplication; here, a hyperplane with n-1 dimensions)

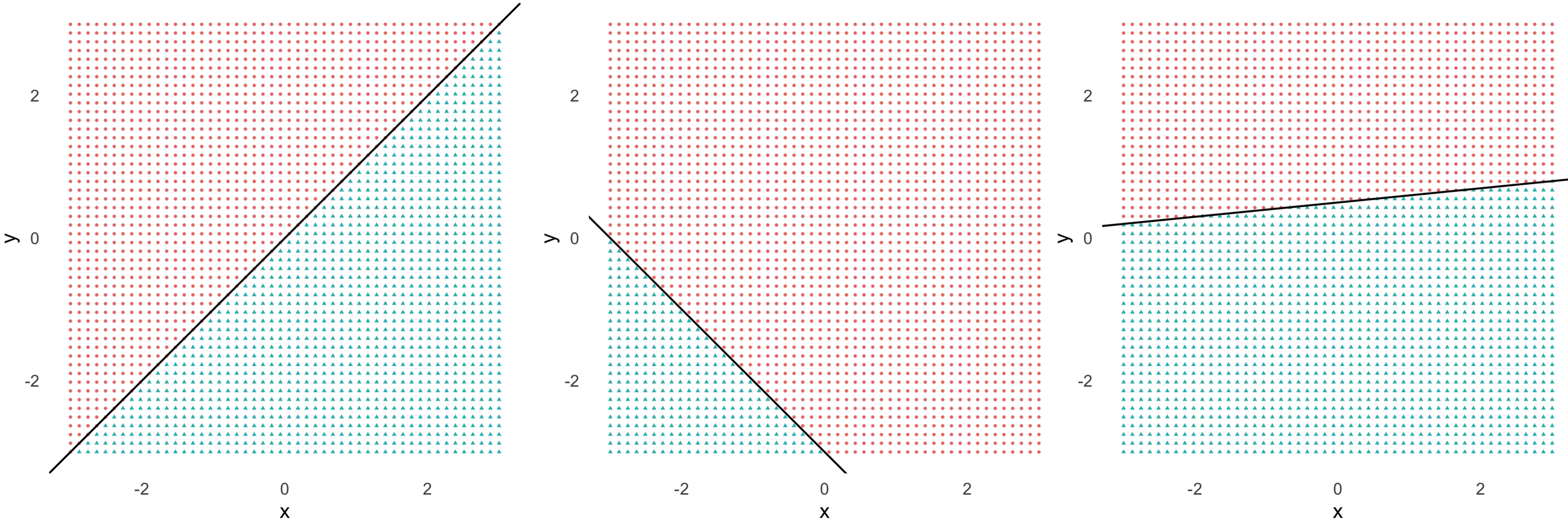
Quick Check: Which of these are flat affine subspaces?



Quick Check: Which of these are flat affine subspaces?

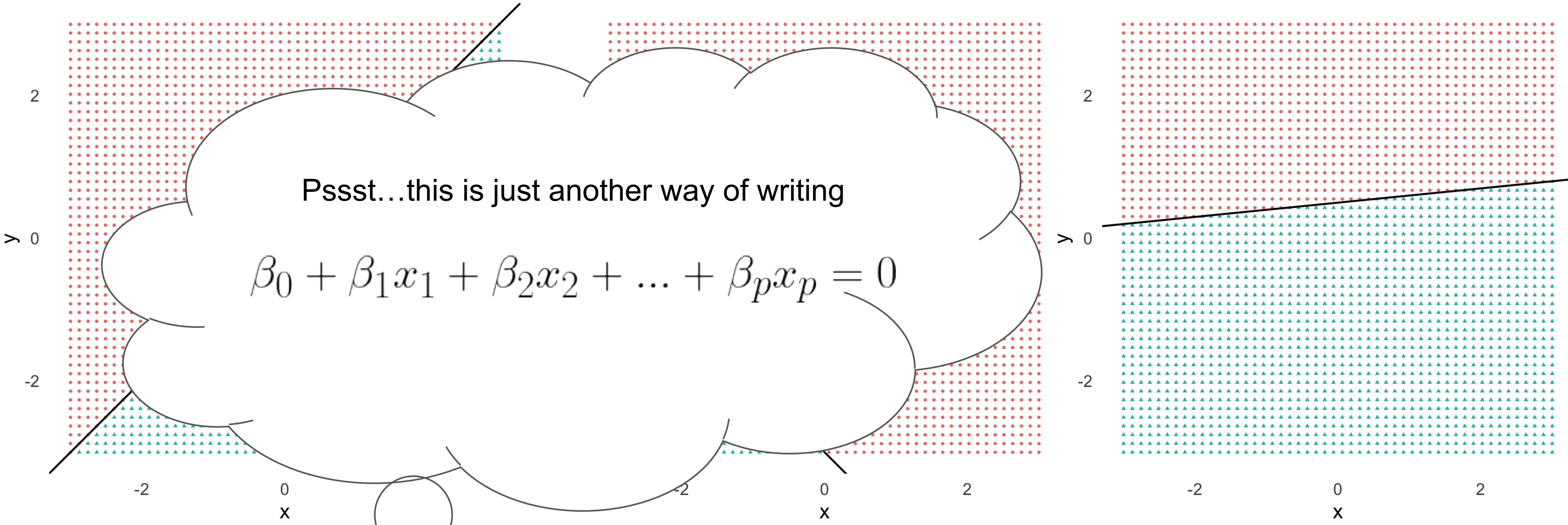


Hyperplanes Divide Spaces in Half



$$\mathbf{w}^T x + b = 0$$

Hyperplanes Divide Spaces in Half

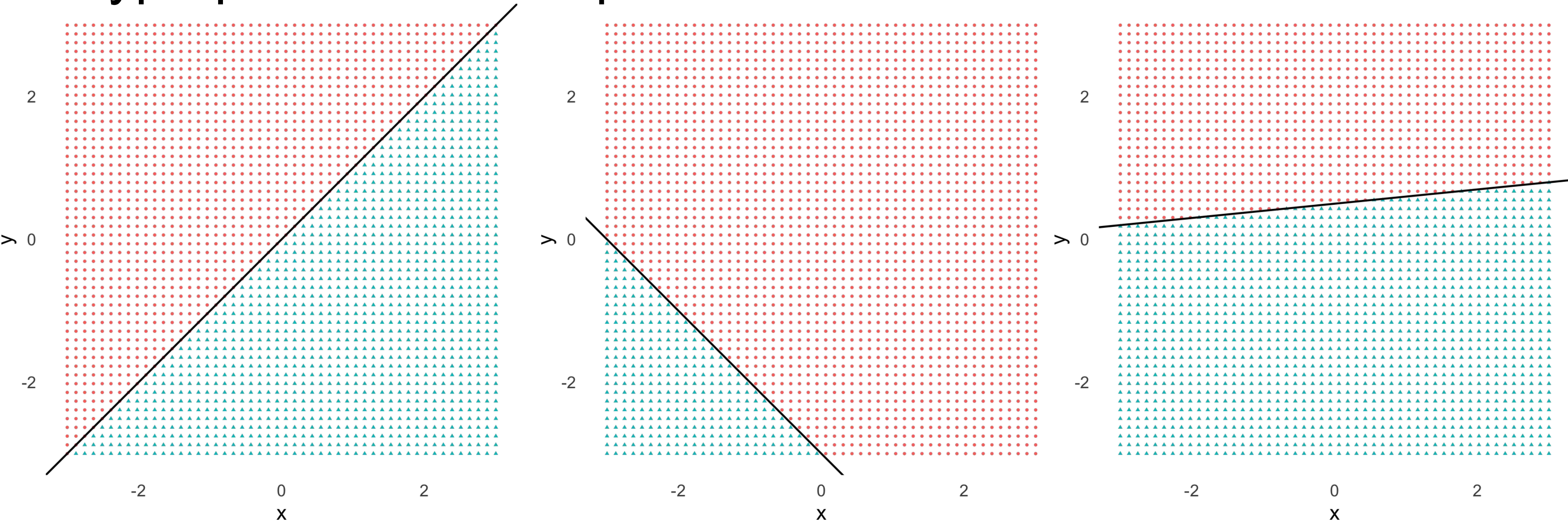


Pssst…this is just another way of writing

$$\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_p x_p = 0$$

$$\mathbf{w}^T x + b = 0$$

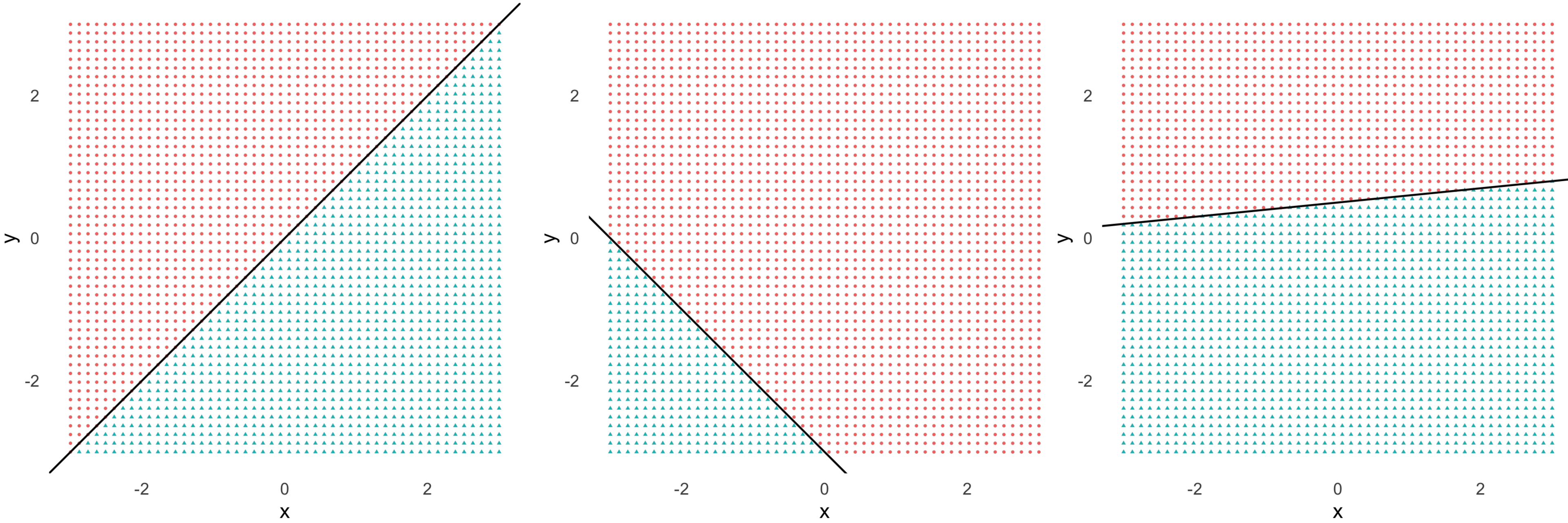
Hyperplanes Divide Spaces in Half



$$\mathbf{w}^T x_n + b > 0 \text{ if } t_n = 1$$

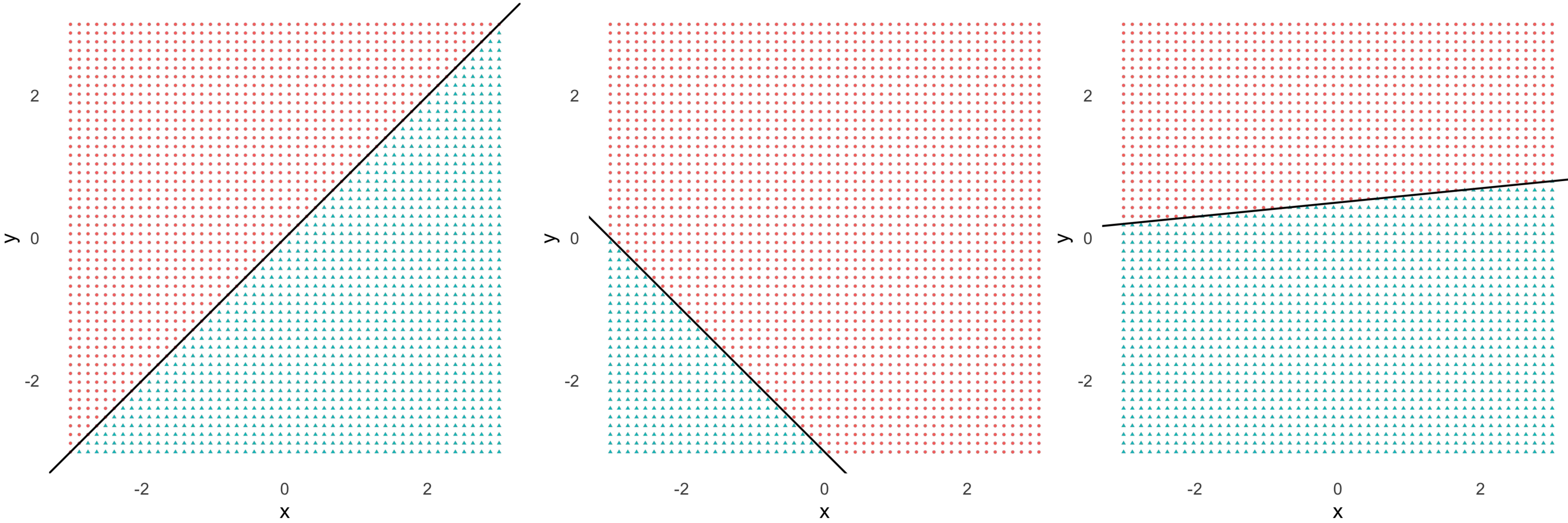
$$\mathbf{w}^T x_n + b < 0 \text{ if } t_n = -1$$

Hyperplanes Divide Spaces in Half



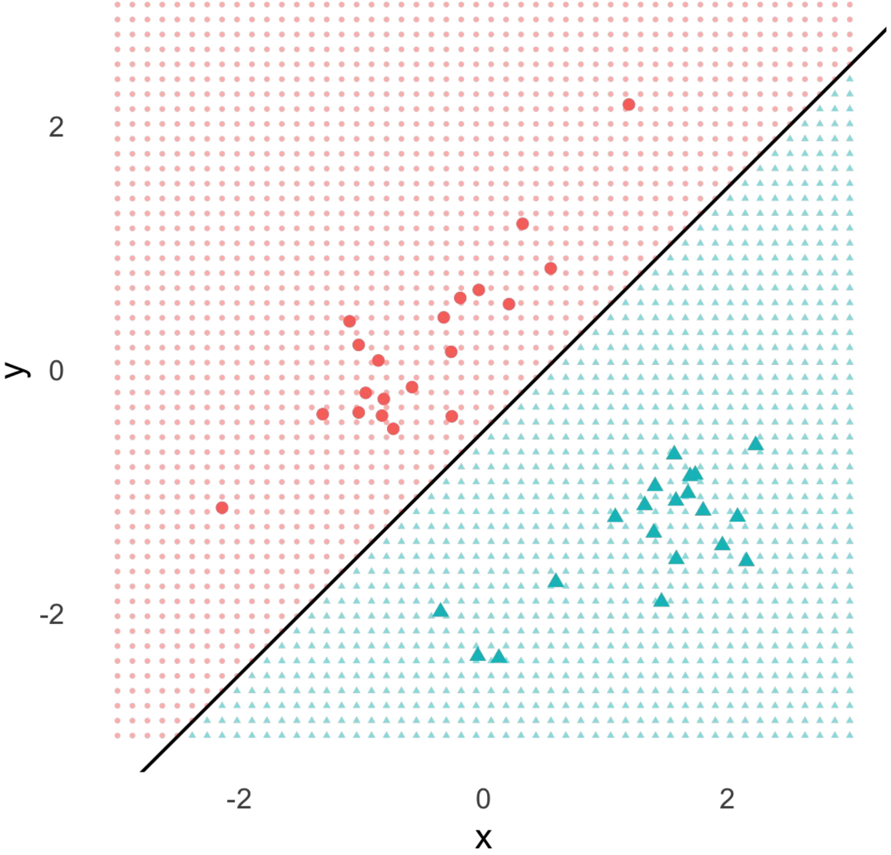
$$t_n(\mathbf{w}^T x_n + b) > 0$$

Hyperplanes Divide Spaces in Half

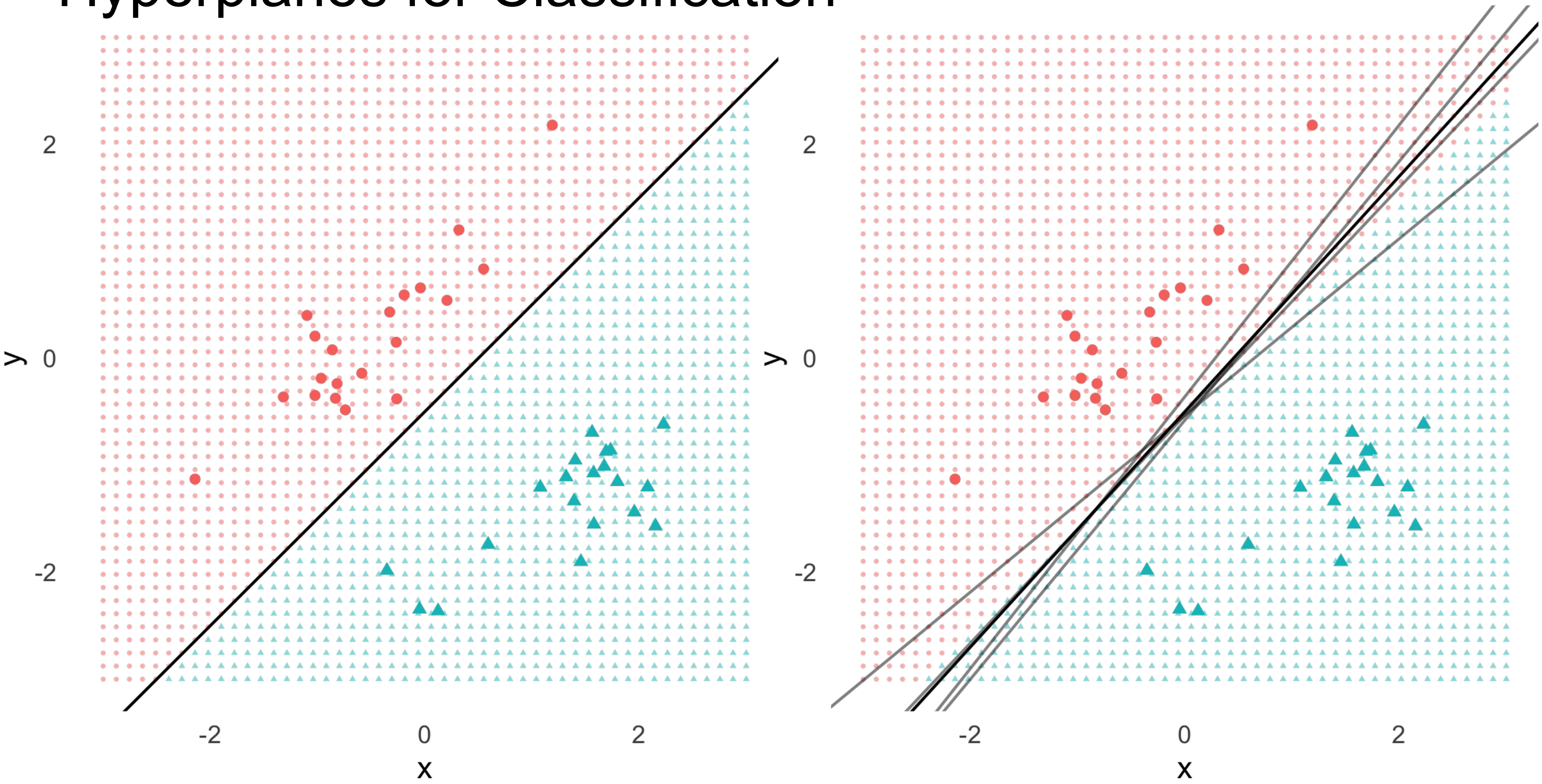


We can use these hyperplanes to classify data!

Hyperplanes for Classification



Hyperplanes for Classification



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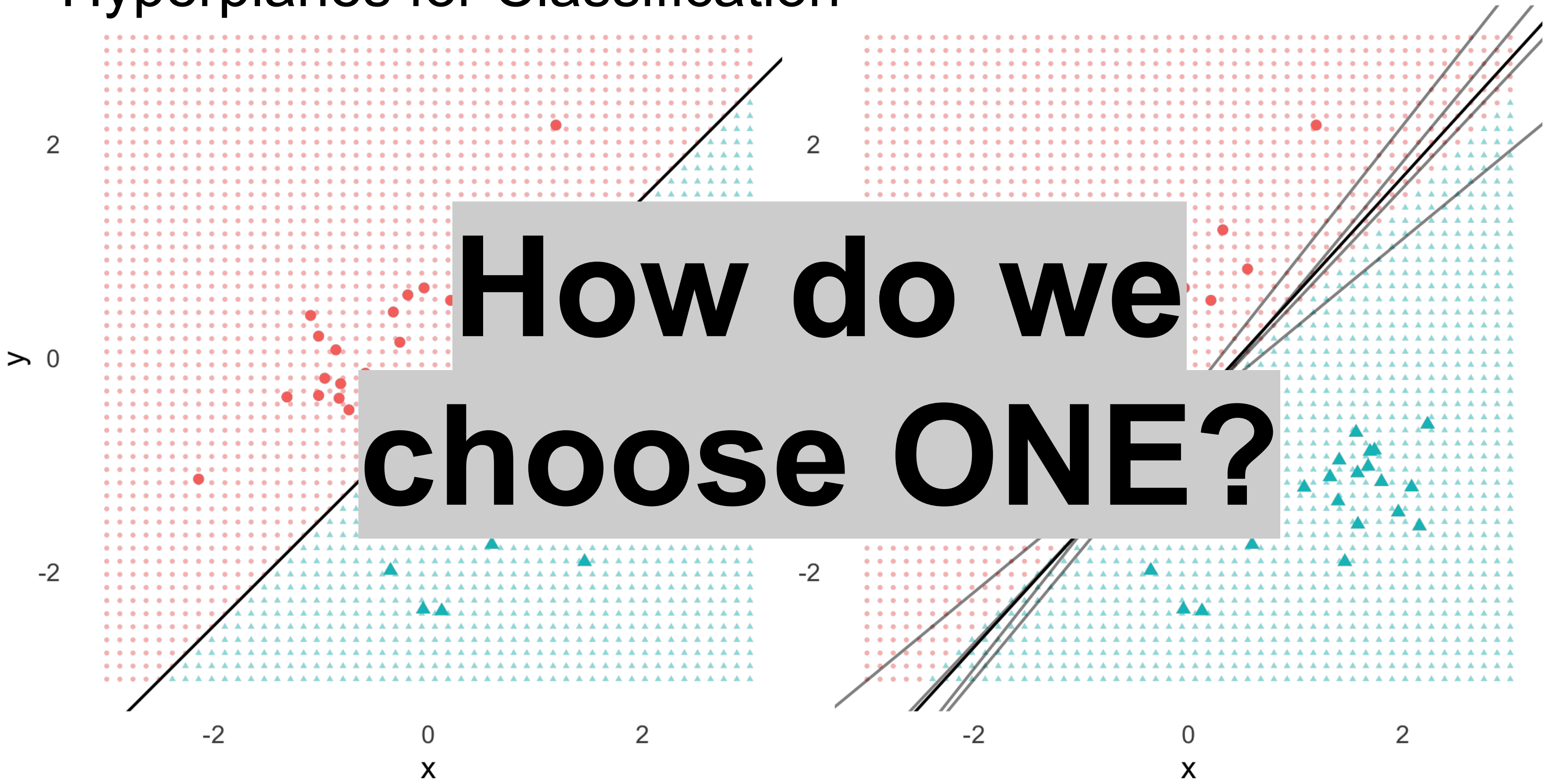


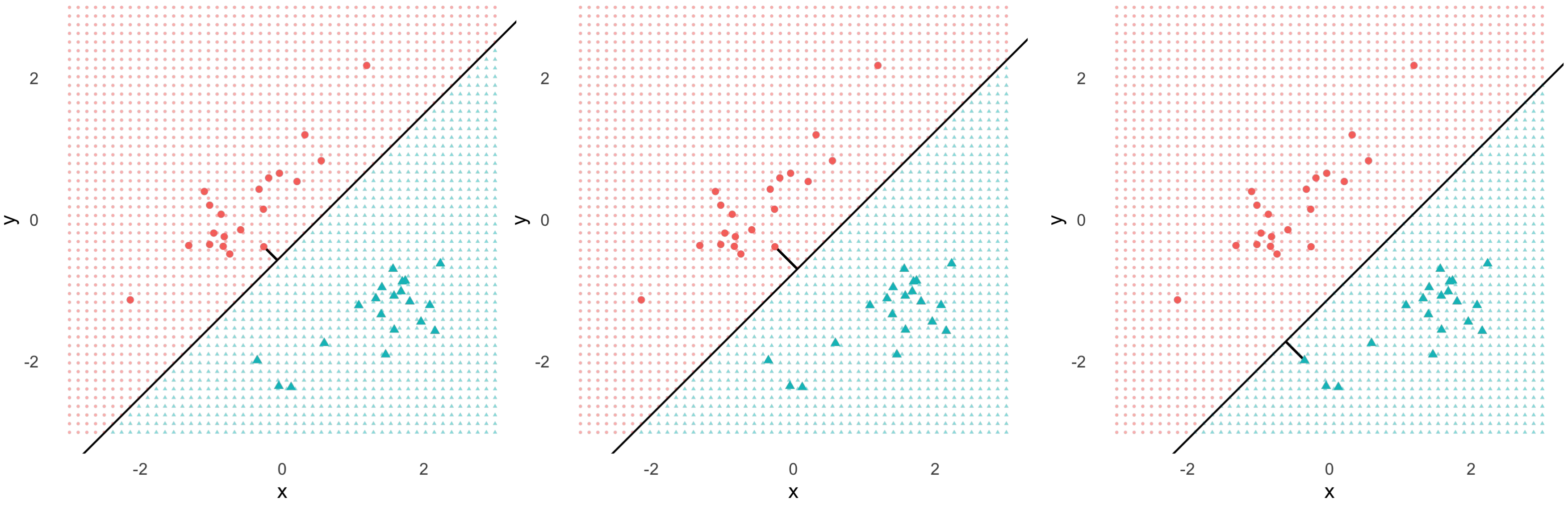
How do we choose ONE?

Maximal Margin Classifier

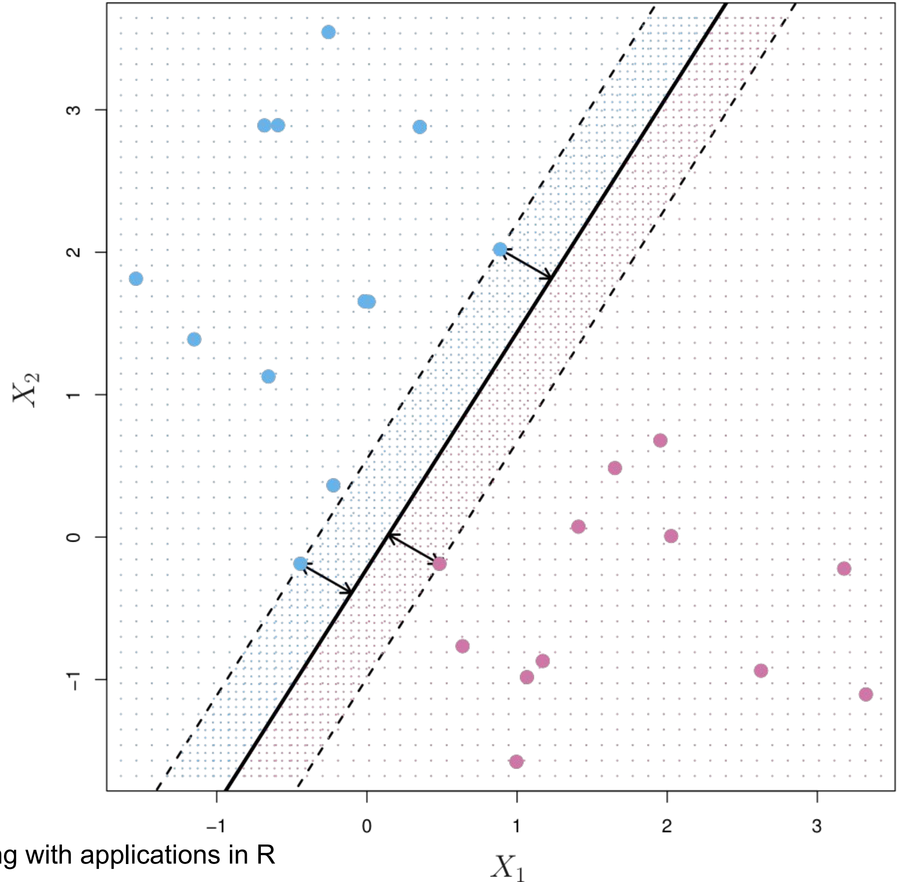
Maximal Margin Classifier

Problem: If a separating hyperplane exists, there will be ∞

Solution: Choose the one that's *furthest* from the training examples



Maximal Margin Classifier



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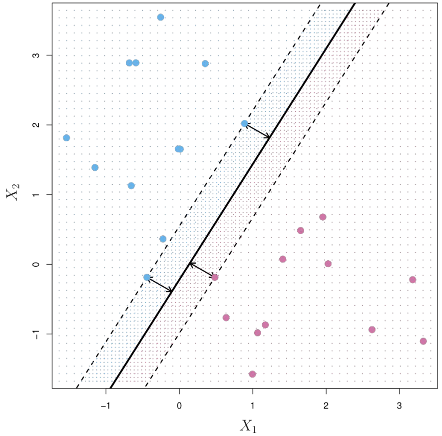
Maximal Margin Classifier Math

$$\underbrace{\frac{t_n\left(w^T x_n + b\right)}{\|w\|}}_{\substack{\text{distance btw} \\ x_n \text{ and line}}}$$



$$\underbrace{\underset{\mathbf{w},b}{\arg\max}\left\{\frac{1}{\|\mathbf{w}\|}\min_n\left[t_n\left(\mathbf{w}^T x_n + b\right)\right]\right\}}_{\text{maximize the minimum distance btw hyperplane and point}}$$

$$\text{subject to: } t_n\left(\mathbf{w}^T x_n + b\right) \geq 1$$

Easier to minimize

$$\underset{\mathbf{w},b}{\arg\min}\ \frac{1}{2}\|\mathbf{w}\|^2$$

Constrained Optimization

$$f(x, y) = 2x + y$$
$$g(x, y) = x^2 + y^2 = 1$$

Optimize $f(x, y, z)$ subject to $g(x, y, z) = k$

1

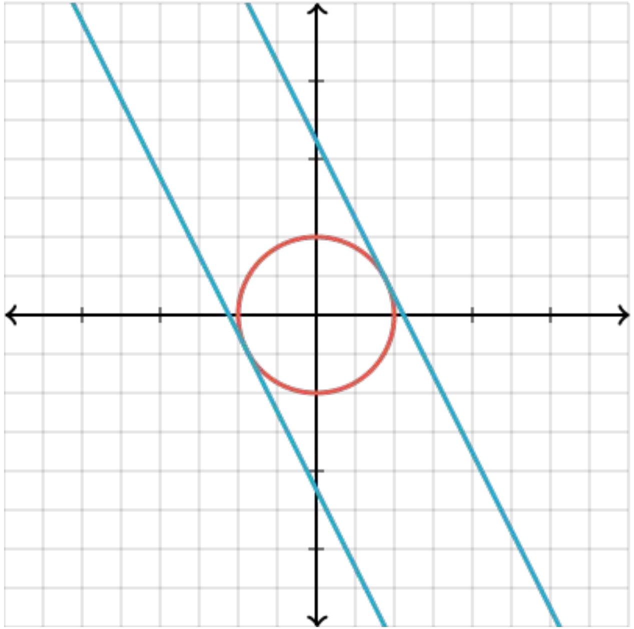


Image from Khan Academy's Lagrange Multiplier and Constrained Optimization Page: https://www.khanacademy.org/math/multivariable-calculus/applications-of-multivariable-derivatives/constrained-optimization/a/lagrange-multipliers-single-constraint

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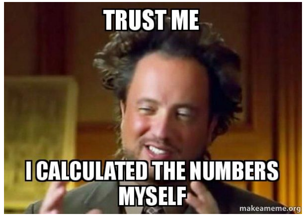
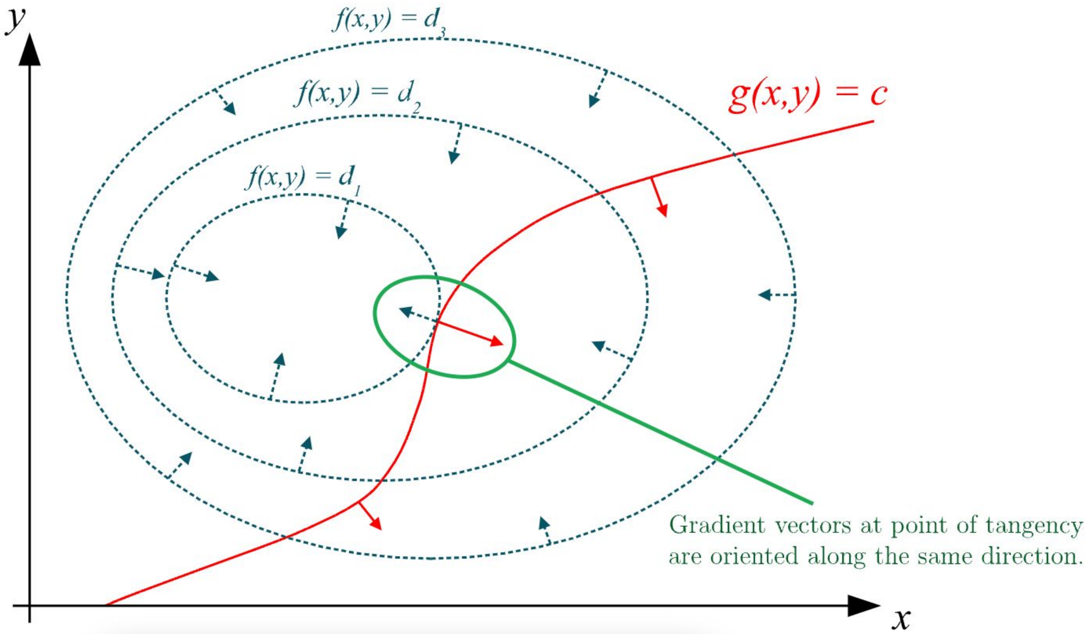


Optimize $f(x, y, z)$ subject to $g(x, y, z) = k$

2



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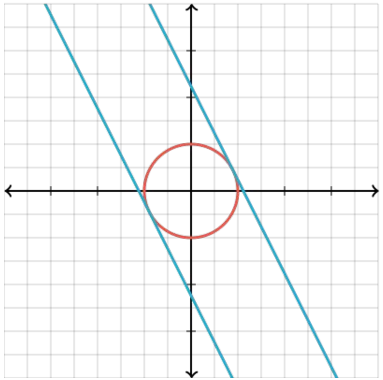
Optimize $f(x, y, z)$ subject to $g(x, y, z) = k$

3 $$\nabla f(x_0, y_0) = \lambda \nabla g(x_0, y_0)$$

Constrained Optimization

Optimize $f(x, y, z)$ subject to $g(x, y, z) = k$



$$f(x, y) = 2x + y$$

$$g(x, y) = x^2 + y^2 = 1$$

3

$$\nabla f(x_0, y_0) = \lambda \nabla g(x_0, y_0)$$

$$\nabla f(x, y) = \begin{bmatrix} \frac{\partial}{\partial x} 2x + y \\ \frac{\partial}{\partial y} 2x + y \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

$$\nabla g(x, y) = \begin{bmatrix} \frac{\partial}{\partial x} x^2 + y^2 \\ \frac{\partial}{\partial y} x^2 + y^2 \end{bmatrix} = \begin{bmatrix} 2x \\ 2y \end{bmatrix}$$

Constrained Optimization

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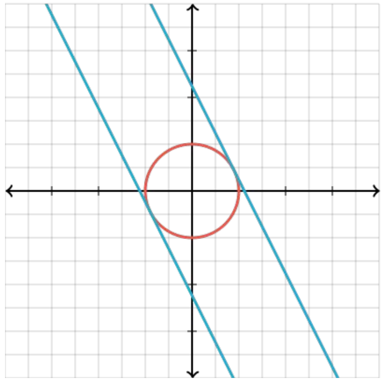

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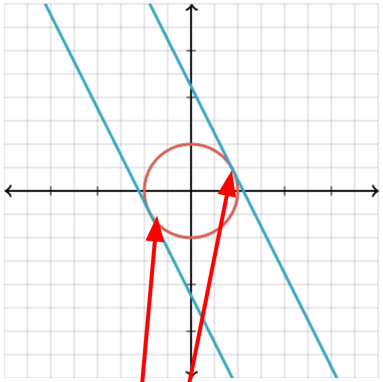

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$$f(x,y) = 2x + y$$
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Constrained Optimization

Optimize $f(x,y,z)$ subject to $g(x,y,z) = k$

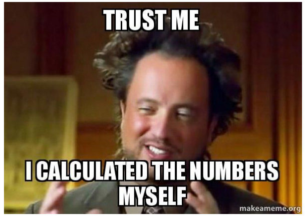
4

$$\mathcal{L}(x,y,\lambda) = f(x,y) - \lambda(g(x,y) - c)$$

$$\mathcal{L}(x,y,\lambda) = 2x + y - \lambda(x^2 + y^2 - 1)$$

For example

Constrained Optimization



Optimize $f(x, y, z)$ subject to $g(x, y, z) = k$

4

$$\mathcal{L}(x, y, \lambda) = f(x, y) - \lambda(g(x, y) - c)$$

$$\mathcal{L}_\lambda(x, y, \lambda) = \frac{\partial \mathcal{L}}{\partial \lambda} = 0 - (g(x, y) - c) = -g(x, y) + c$$

$$\mathcal{L}_\lambda(x, y, \lambda) = -g(x, y) + c = 0 \text{ when } \mathrm{g(x,y)} = \mathrm{c}$$

Constrained Optimization

Optimize $f(x, y, z)$ subject to $g(x, y, z) = k$

4

$$\mathcal{L}(x, y, \lambda) = f(x, y) - \lambda(g(x, y) - c)$$

$$\mathcal{L}_x(x, y, \lambda) = 0$$

$$\frac{\partial}{\partial x}(f(x, y) - \lambda(g(x, y) - c)) = 0$$

$$f_x(x, y) - \lambda g_x(x, y) = 0$$

$$f_x(x, y) = \lambda g_x(x, y)$$

Constrained Optimization

Optimize $f(x, y, z)$ subject to $g(x, y, z) = k$

4

$$\nabla \mathcal{L} = \begin{bmatrix} \dfrac{\partial}{\partial x}(2x + y - \lambda(x^2 + y^2 - 1)) \\ \\ \dfrac{\partial}{\partial y}(2x + y - \lambda(x^2 + y^2 - 1)) \\ \\ \dfrac{\partial}{\partial \lambda}(2x + y - \lambda(x^2 + y^2 - 1)) \end{bmatrix} = \begin{bmatrix} 2 - 2\lambda x \\ 1 - 2\lambda y \\ -x^2 - y^2 + 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

SVMs as Constrained Optimization

$$\arg\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

$$t_n(w^T x_n + b) \geq 1 \text{ for all n}$$

$$\mathcal{L}(\mathbf{w}, b, \mathbf{a}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N} a_n \left\{t_n(w^T x_n + b) - 1\right\}$$

SVMs as Constrained Optimization

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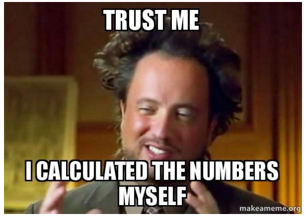
$$t_n(w^T x_n + b) \geq 1 \ \text{ for all n}$$



$$\mathcal{L}(\mathbf{w}, b, \alpha) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N} \alpha_n \left\{ t_n(w^T x_n + b) - 1 \right\}$$

$$\mathbf{w} = \sum_{n=1}^{N} a_n t_n x_n$$

$$0 = \sum_{n=1}^{N} a_n t_n$$

$$L(\tilde{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{M} \underbrace{a_n a_m}_{\text{lagrange multipliers}} \overbrace{t_n t_m}^{\text{targets}} \underbrace{x_n \cdot x_m}_{\text{dot product between two vectors}}$$

$$a_n \geq 0, \ \text{ for } n = 1, \ldots, N$$

$$\sum_{n=1}^{N} a_n t_n = 0$$

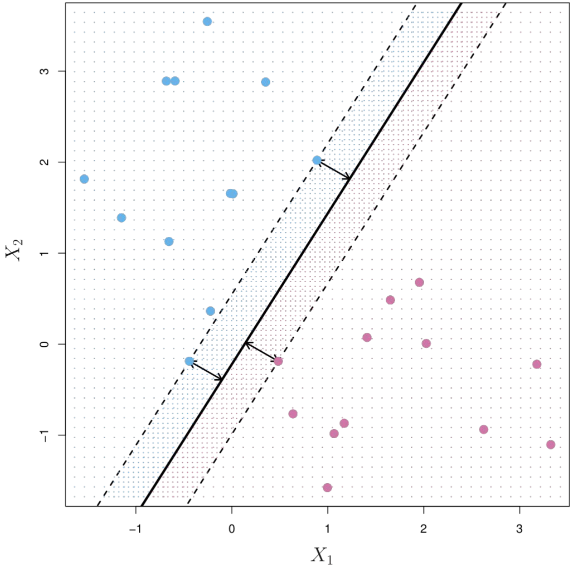
SVMs as Constrained Optimization

$$\underset{\mathbf{w},b}{\arg\min}\ \frac{1}{2}\|\mathbf{w}\|^2$$

$$t_n(w^T x_n + b) \geq 1 \quad \text{for all n}$$

$$\mathcal{L}(\mathbf{w}, b, \alpha) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N} \alpha_n \left\{ t_n(w^T x_n + b) - 1 \right\}$$

$$\overbrace{y(\mathbf{w}) = \sum_{n=1}^{N} a_n t_n \ \ x \cdot x_n \ \ + b}^{\text{formula to classify new data point } x}$$



$$a_n \geq 0$$

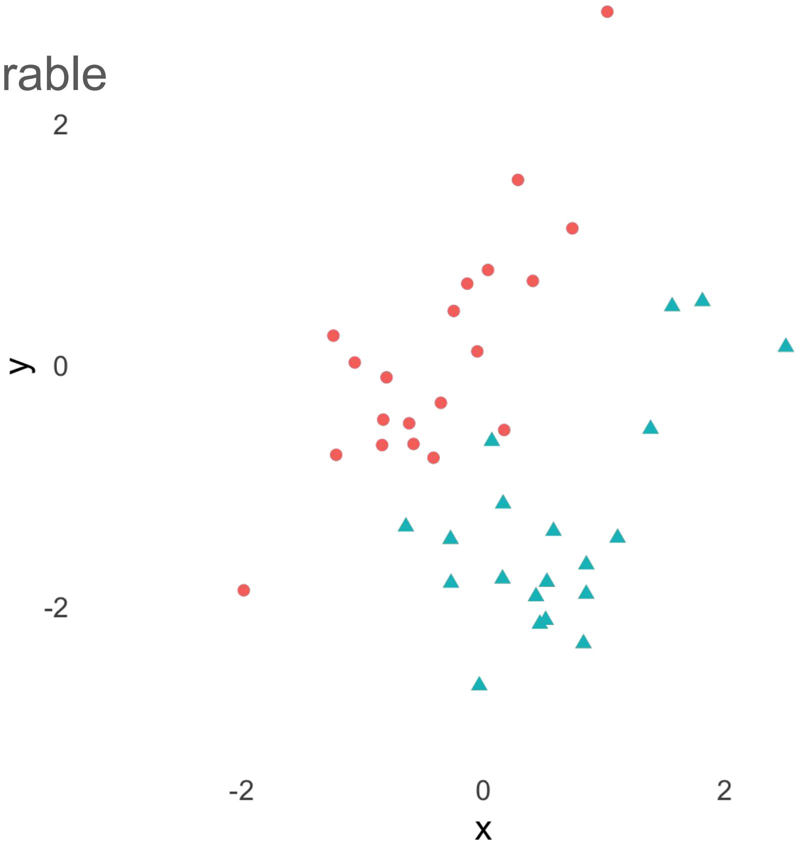
$$t_n y(x_n) - 1 \geq 0$$

2 $$a_n \left\{ t_n y(x_n) - 1 \right\} = 0$$

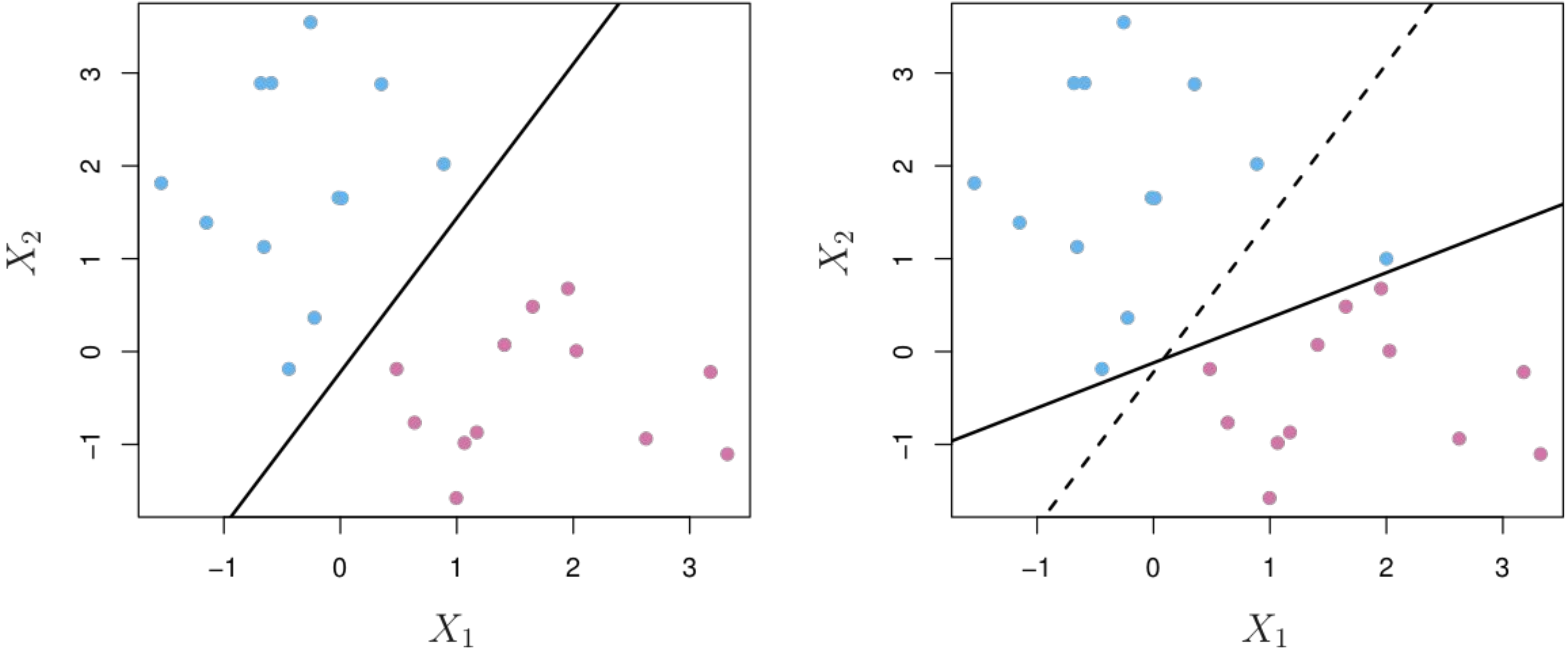
Support Vector Classifier

Support Vector Classifier

Problem: Non-Separable



Support Vector Classifier



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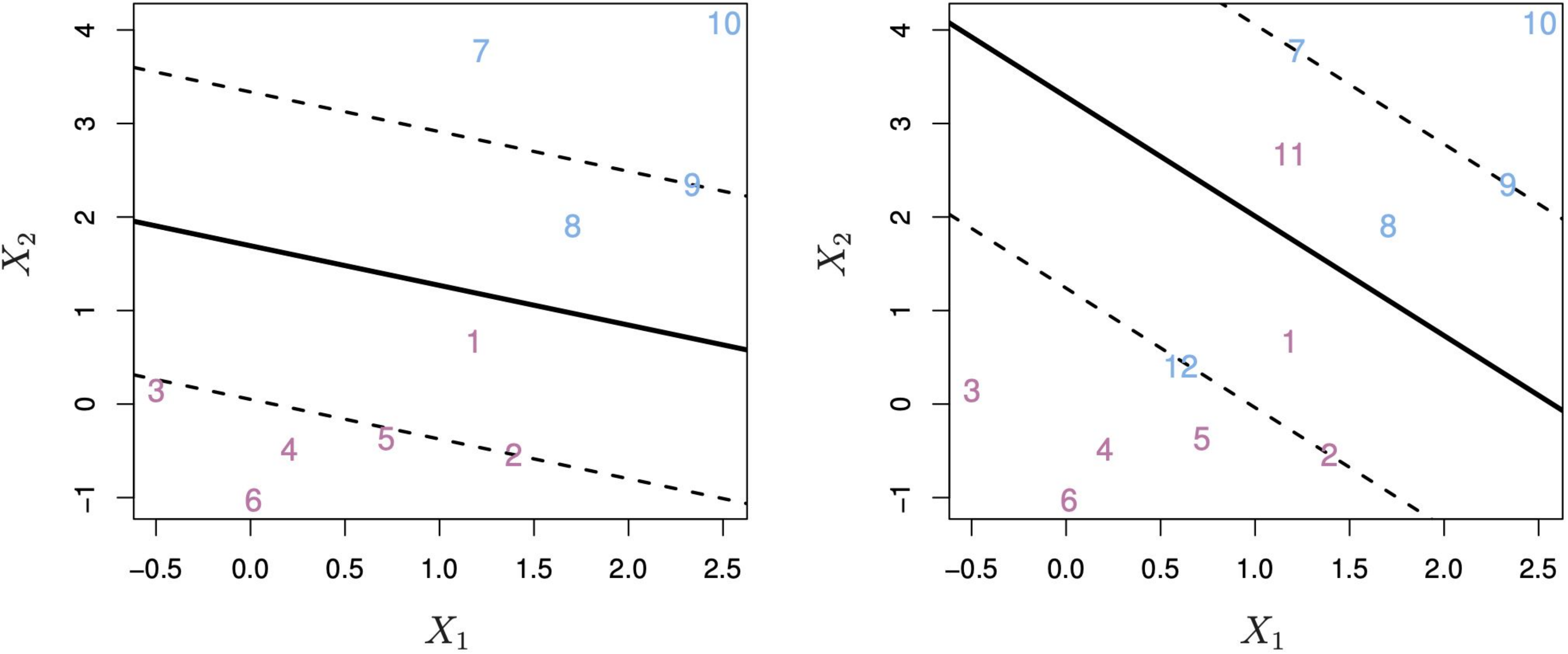
Support Vector Classifier



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Support Vector Classifier

Before:

$$\text{minimize } \frac{1}{2}\|\mathbf{w}\|^2$$

After:

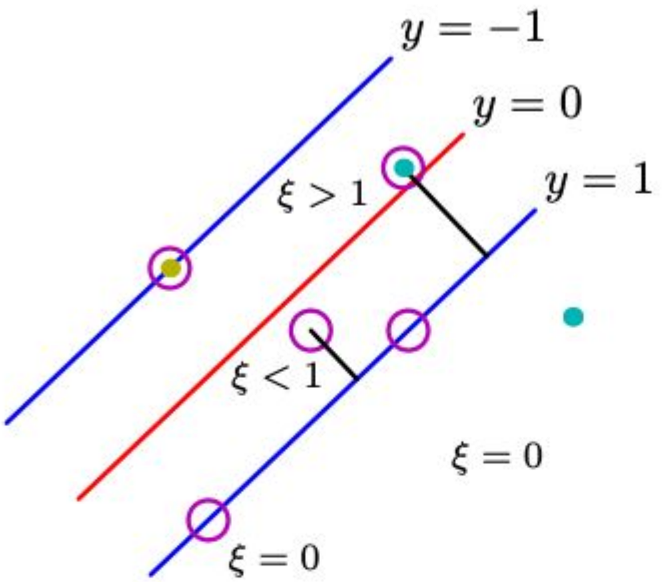
$$\text{minimize } C\sum_{n=1}^{N}\xi_n + \frac{1}{2}\|\mathbf{w}\|^2$$

Before:

$$t_n(w^T x_n + b) \geq 1$$

After:

$$t_n(w^T x_n + b) \geq 1 - \xi_n$$

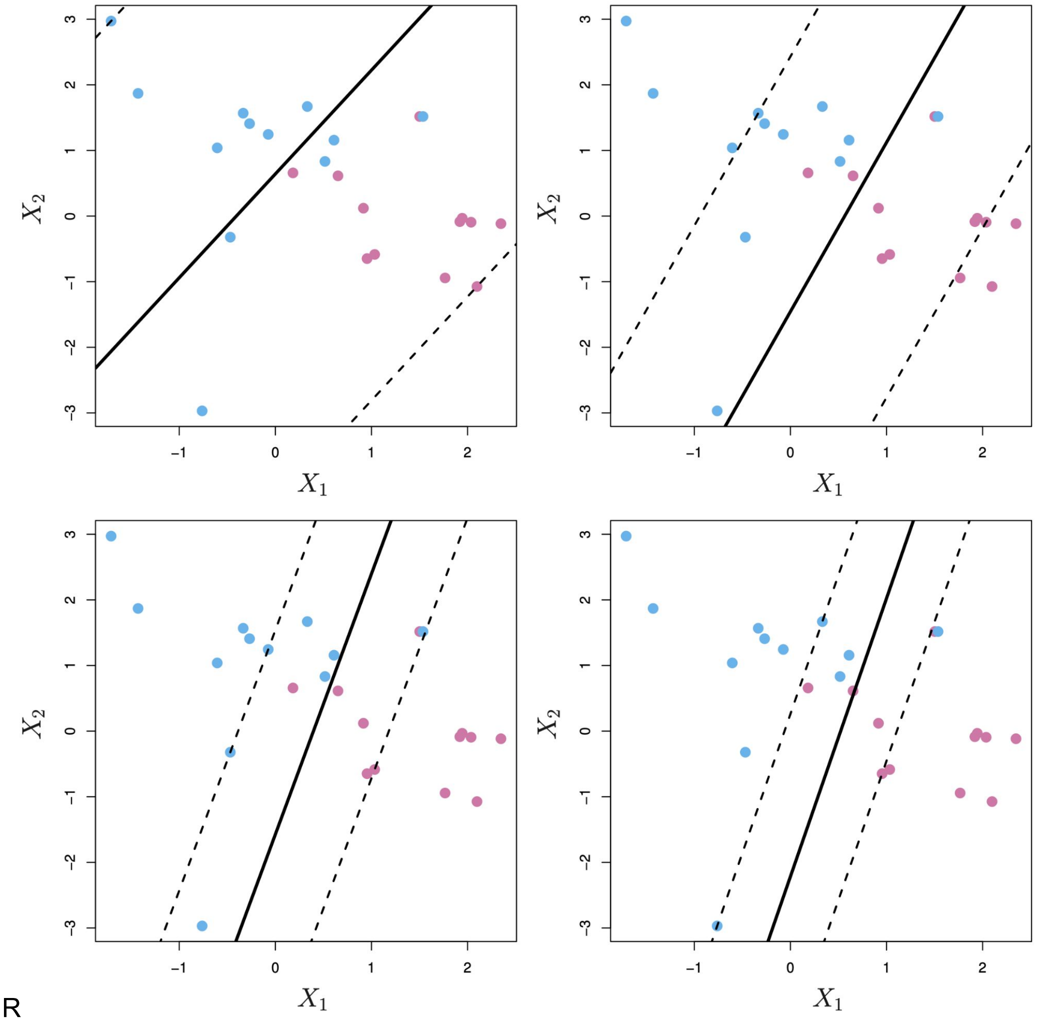


Support Vector Classifier

C: How much error to allow

Lower C: prone to overfitting

Higher C: prone to underfitting



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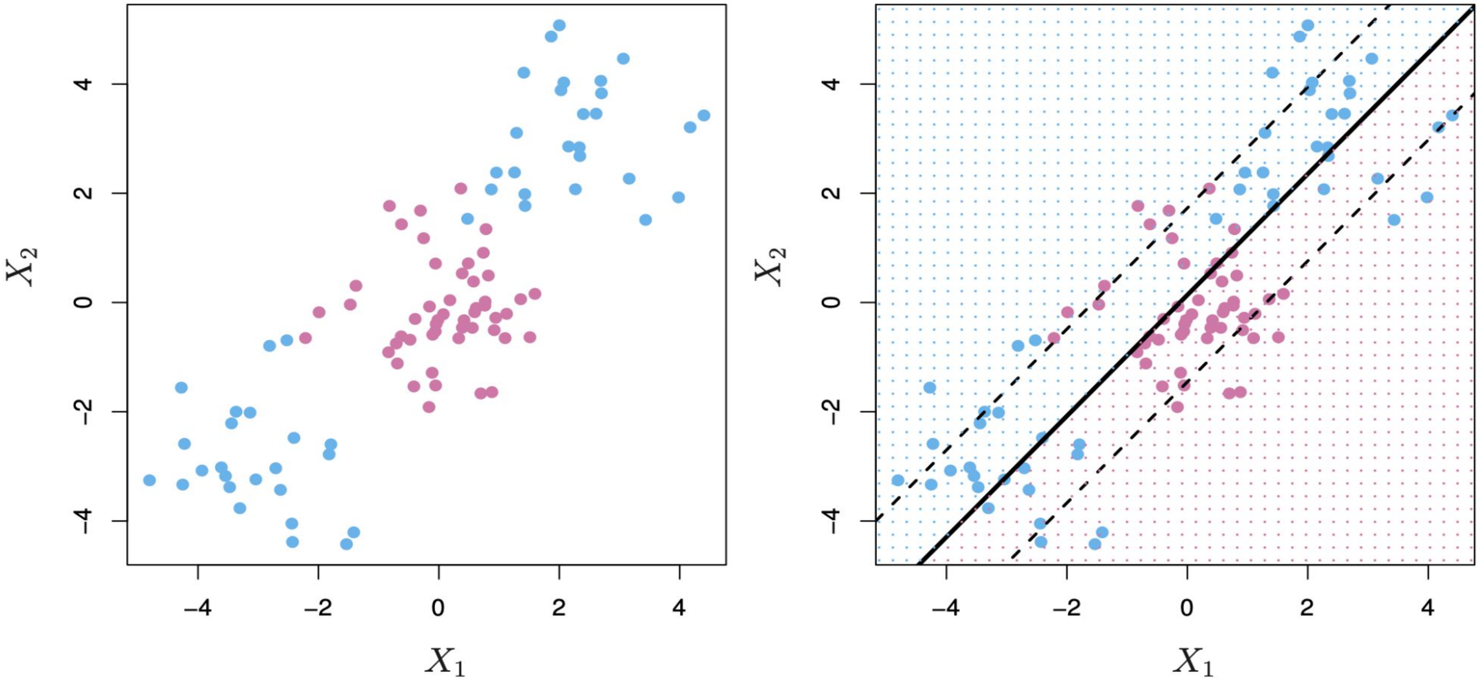
Support Vector Machines II

Dr. Chelsea Parlett-Pelleriti

Support Vector **Machines**

Support Vector Machines

New problem: not linearly separable even with error



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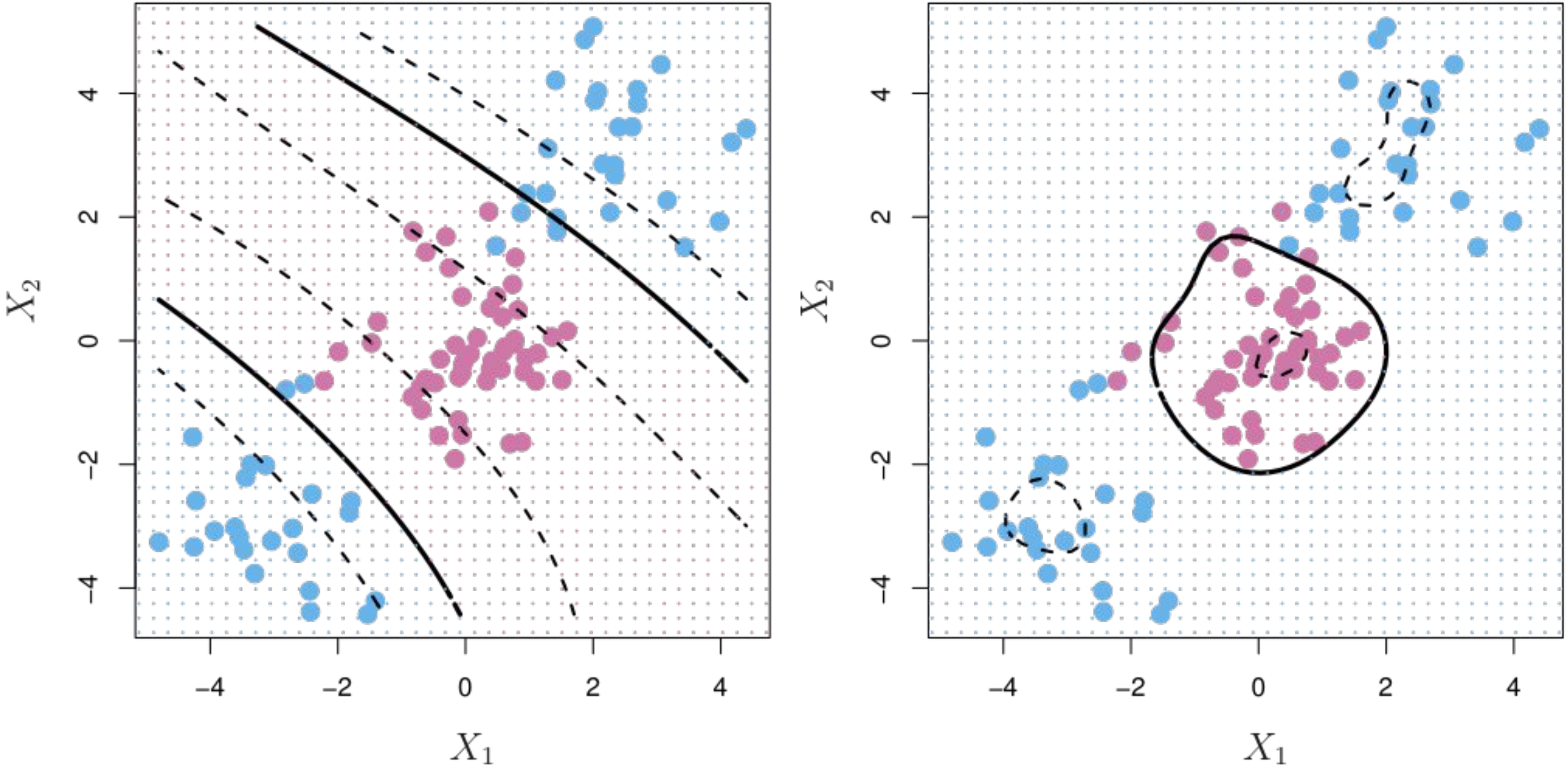
The Kernel Trick



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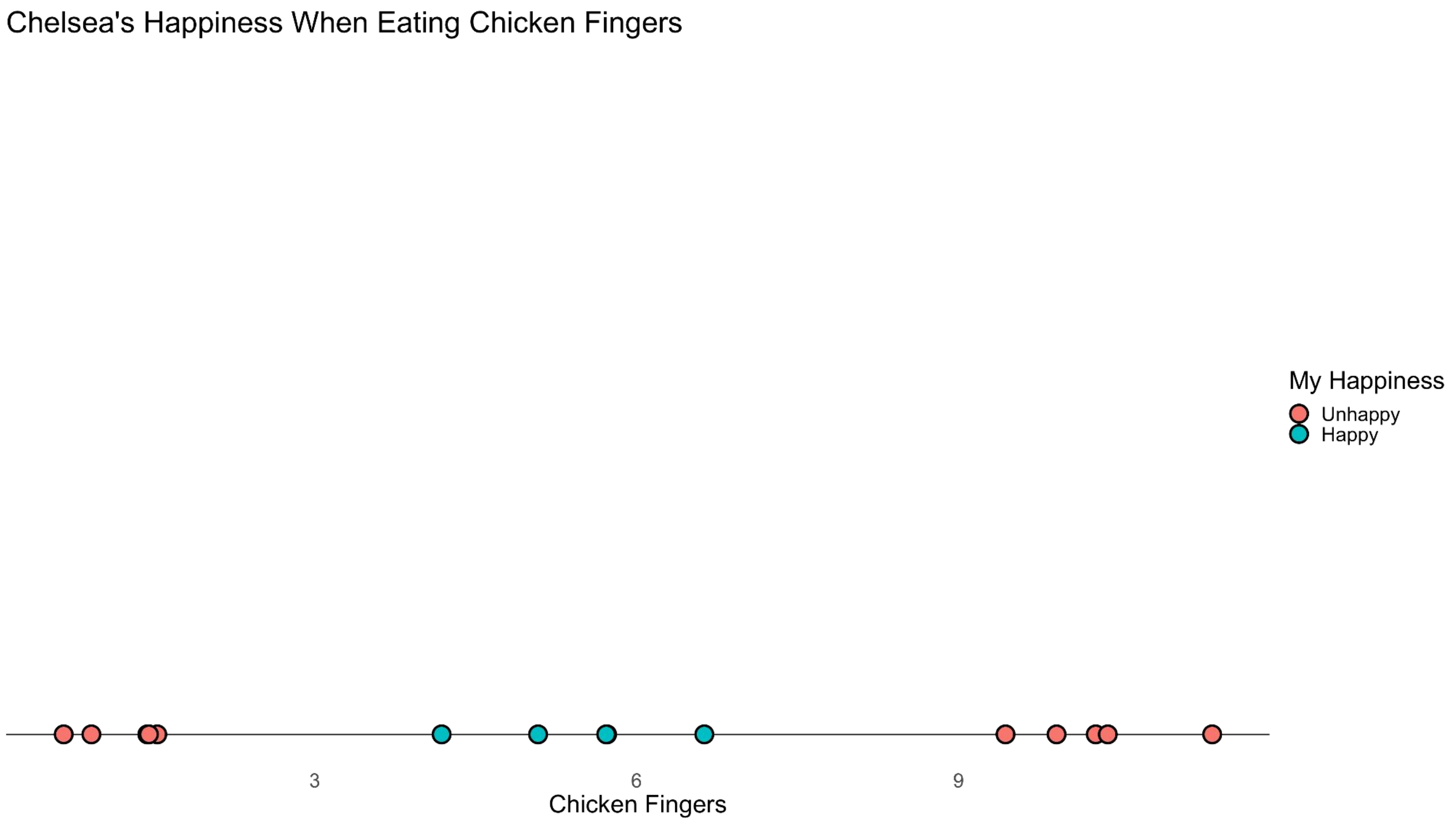

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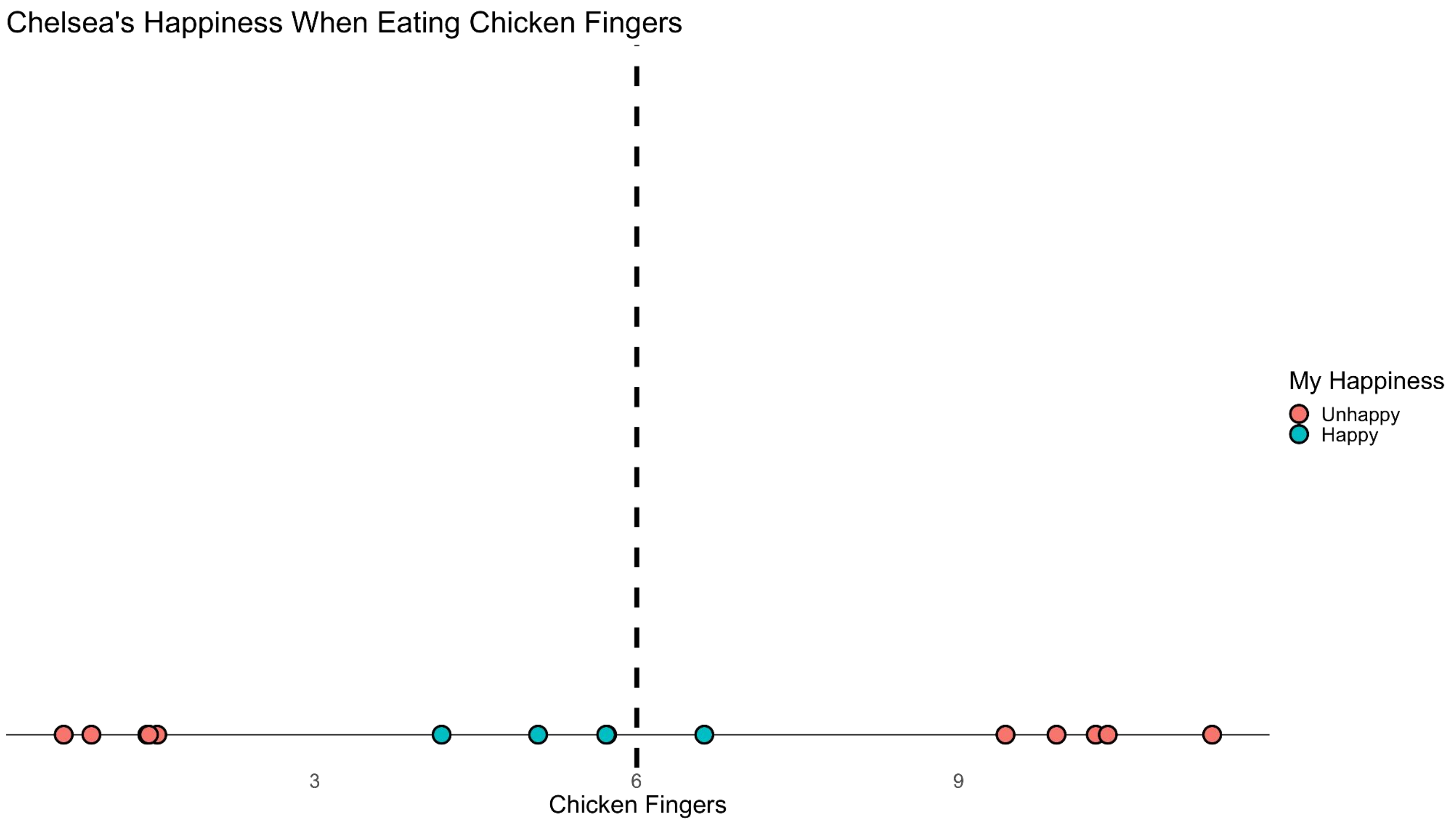

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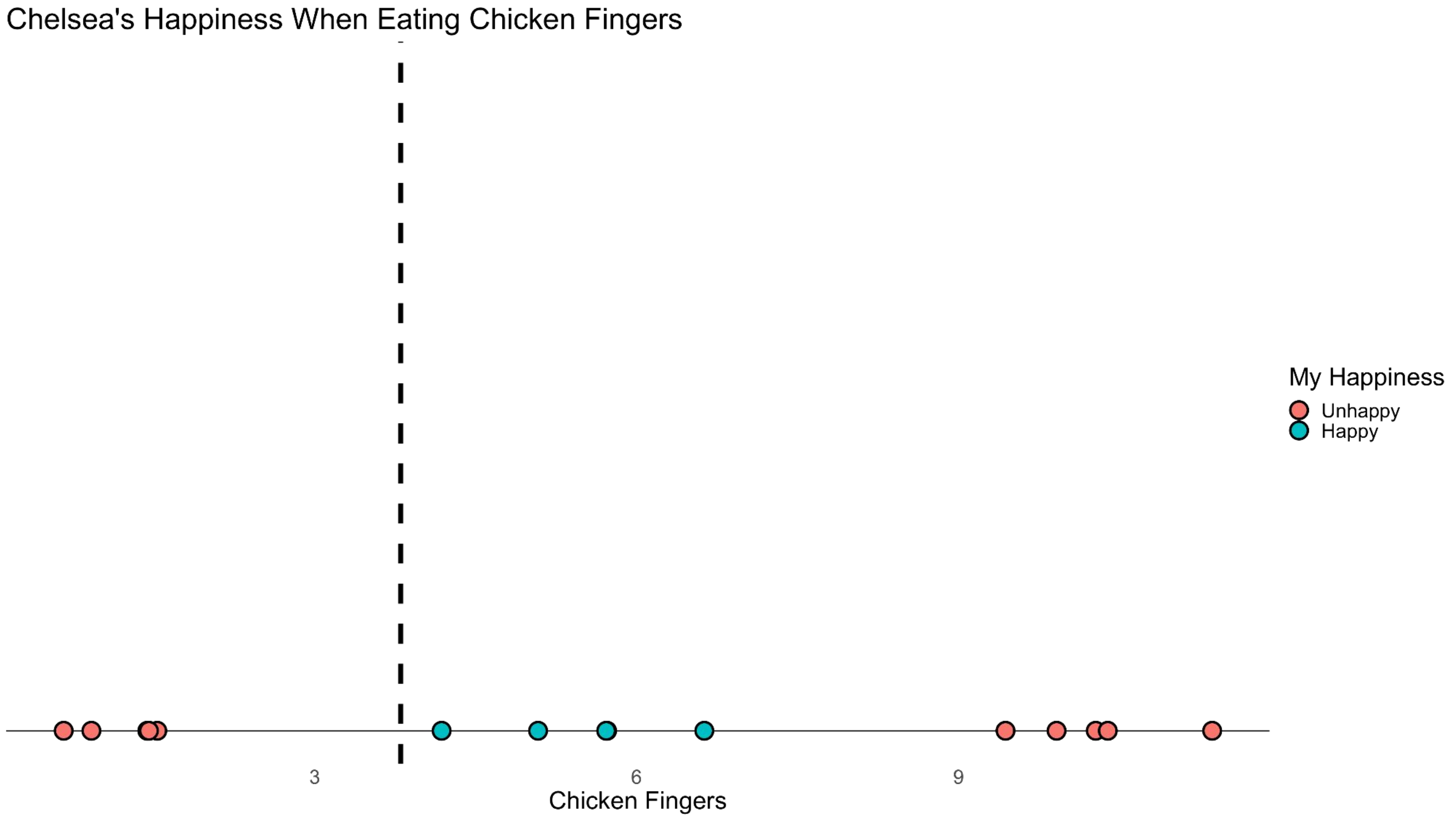

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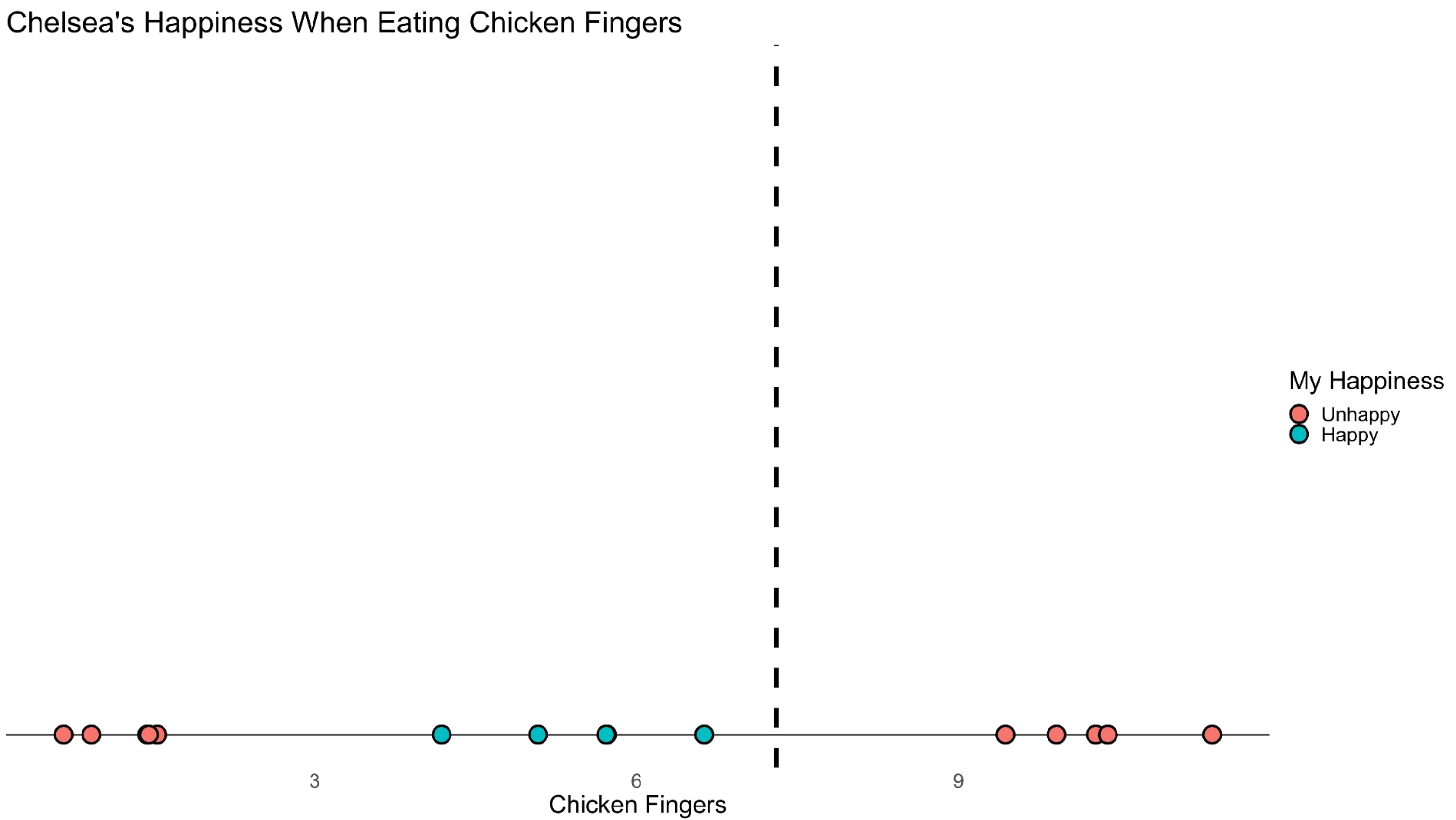

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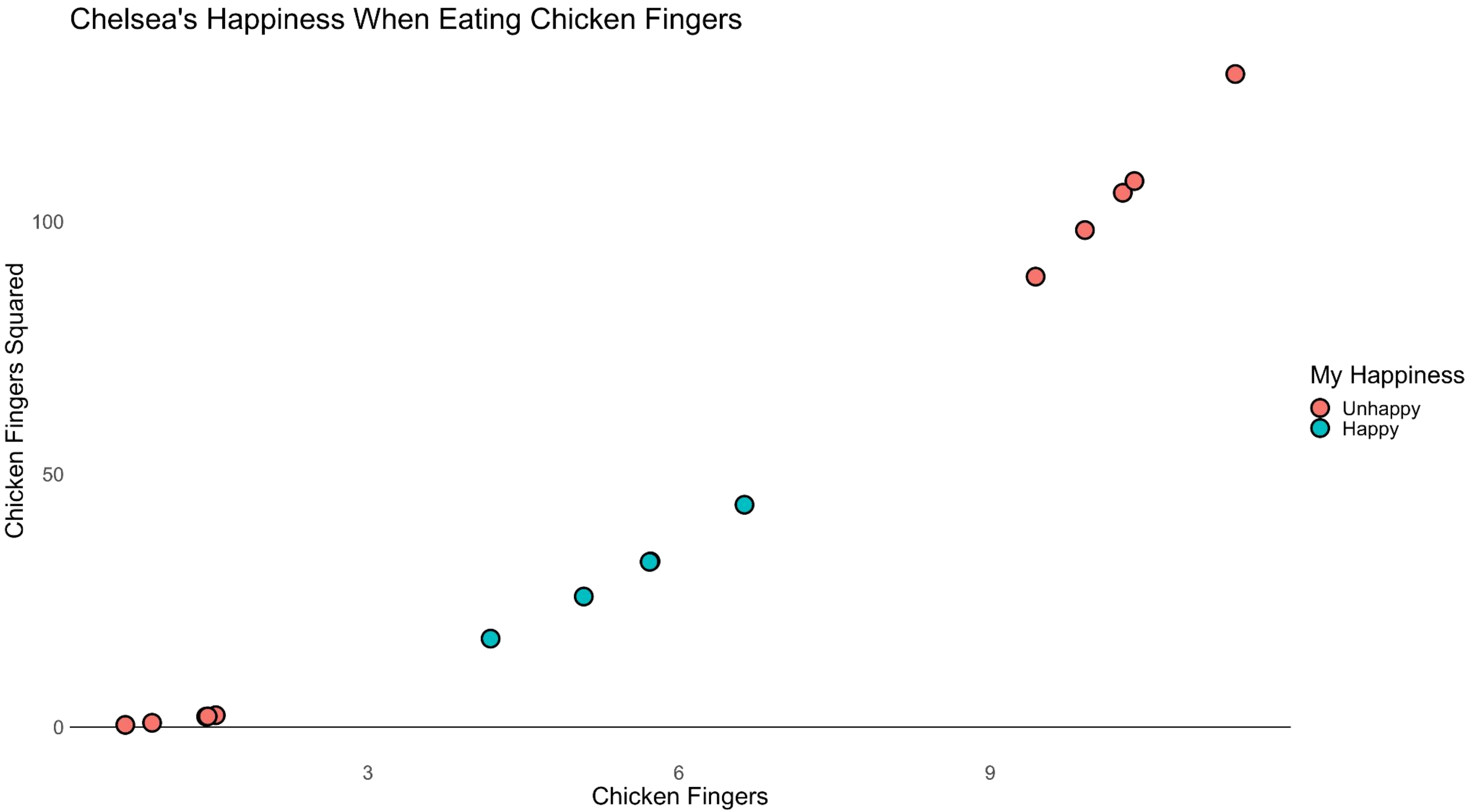

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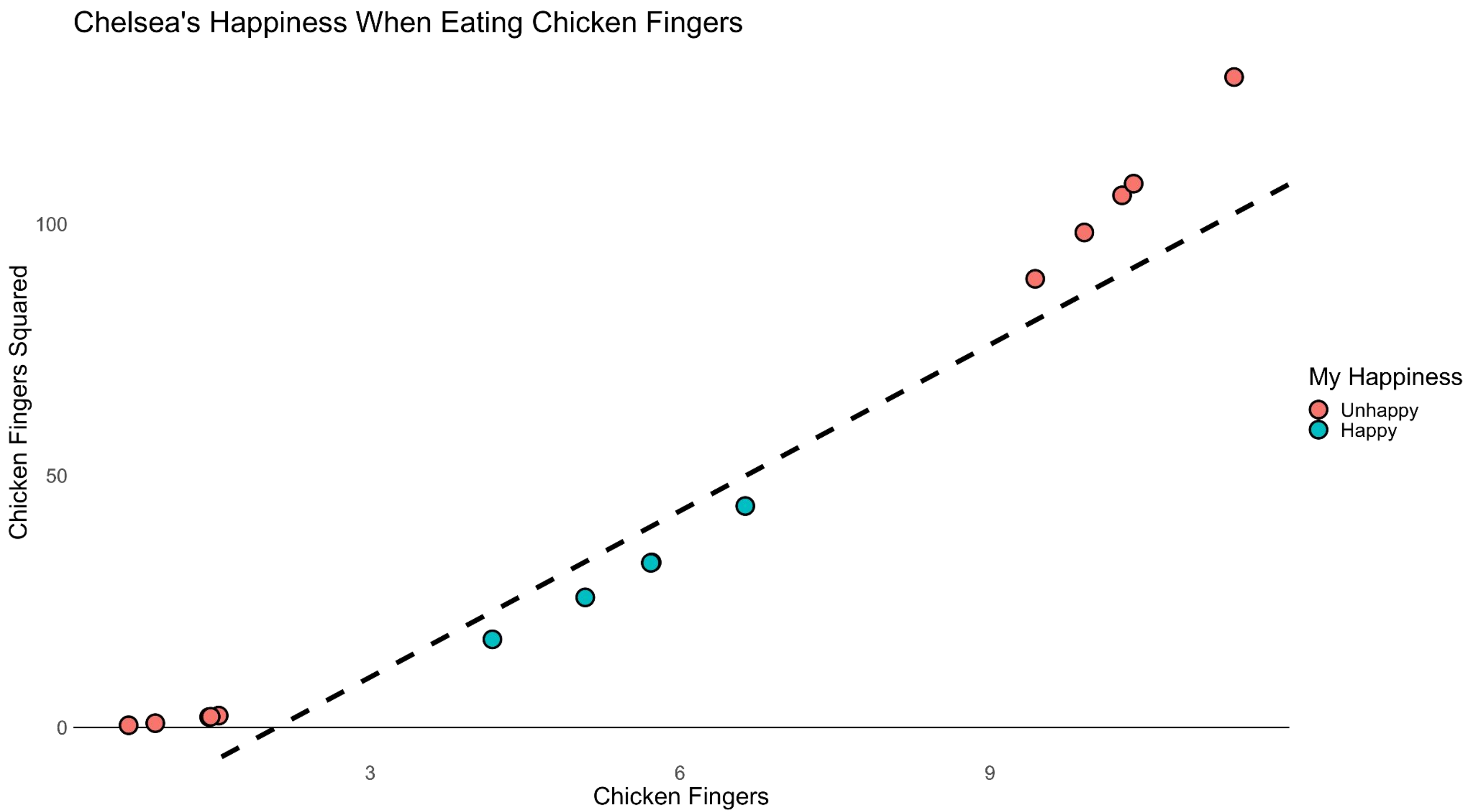


The Kernel Trick

What is a Kernel (in SVMs)?

A function that calculates the the relationship between two vectors in multiple dimensions (without *actually* having to calculate the coordinates for those dimensions)

The Kernel Trick

$$\underbrace{K(x, y)}_{\text{kernel}} = (x * y + r)^d$$

- We used a Polynomial Kernel with **r** (coefficient) and **d** (degree)

The Kernel Trick

$$\underbrace{K(x, y)}_{\text{kernel}} = (x * y + r)^d$$

A point Another point

- We used a Polynomial Kernel with **r** (coefficient) and **d** (degree)
- Let’s try d = 2, r = ½

The Kernel Trick

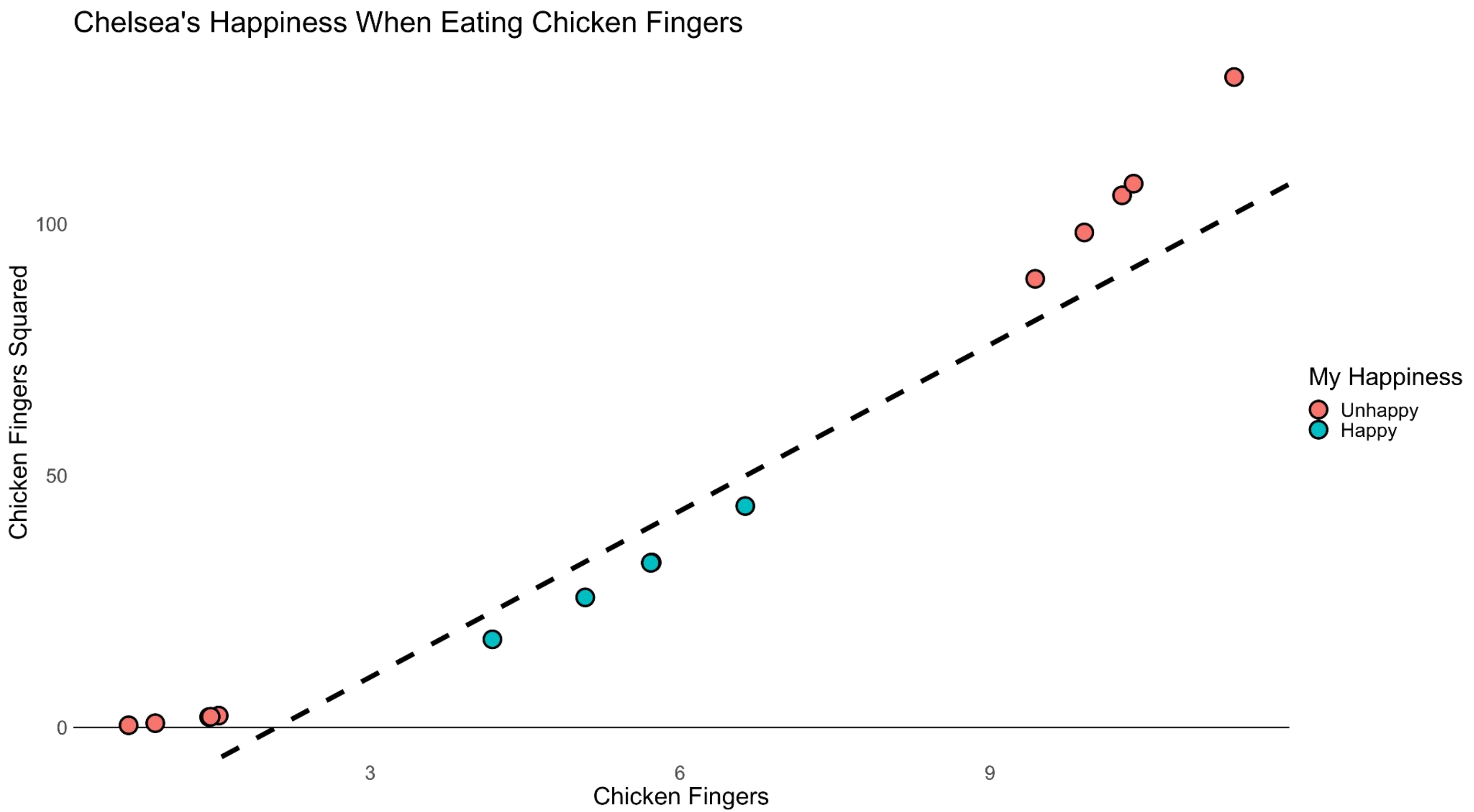
$$\underbrace{K(x, y)}_{\text{kernel}} = (x * y + r)^d$$

- We used a Polynomial Kernel with **r** (coefficient) and **d** (degree)
- Let's try d = 2, r = ½

Polynomial Kernel

$$\underbrace{K(x, y)}_{\text{kernel}} = (x * y + r)^d$$

The Kernel Trick

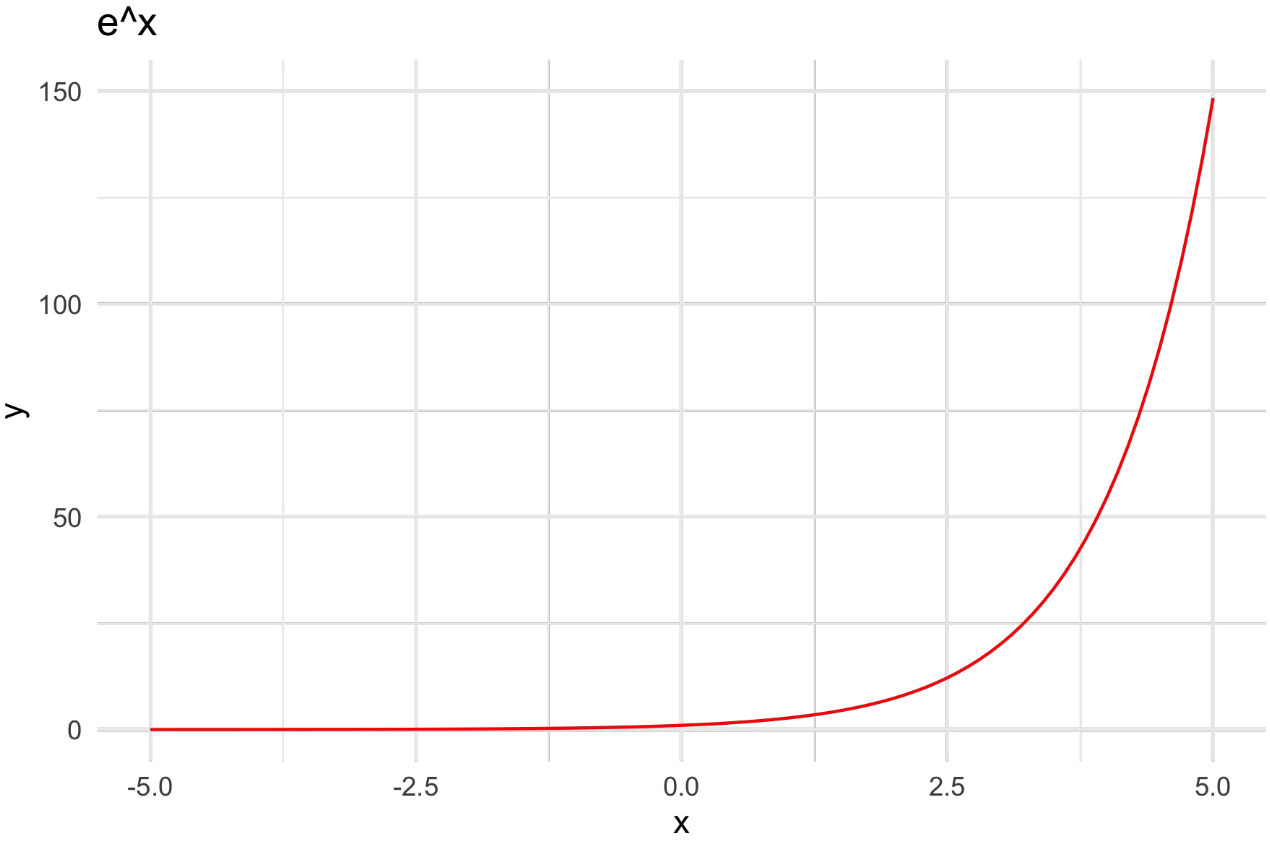


Radial Kernel (RBF)

$$\underbrace{K(x, y)}_{\text{kernel}} = e^{-\gamma(x-y)^2}$$

- Projects to *infinite dimensional* space
- Similar to a nearest neighbors classifier (points that are far away have less influence)

Taylor Series (visually)



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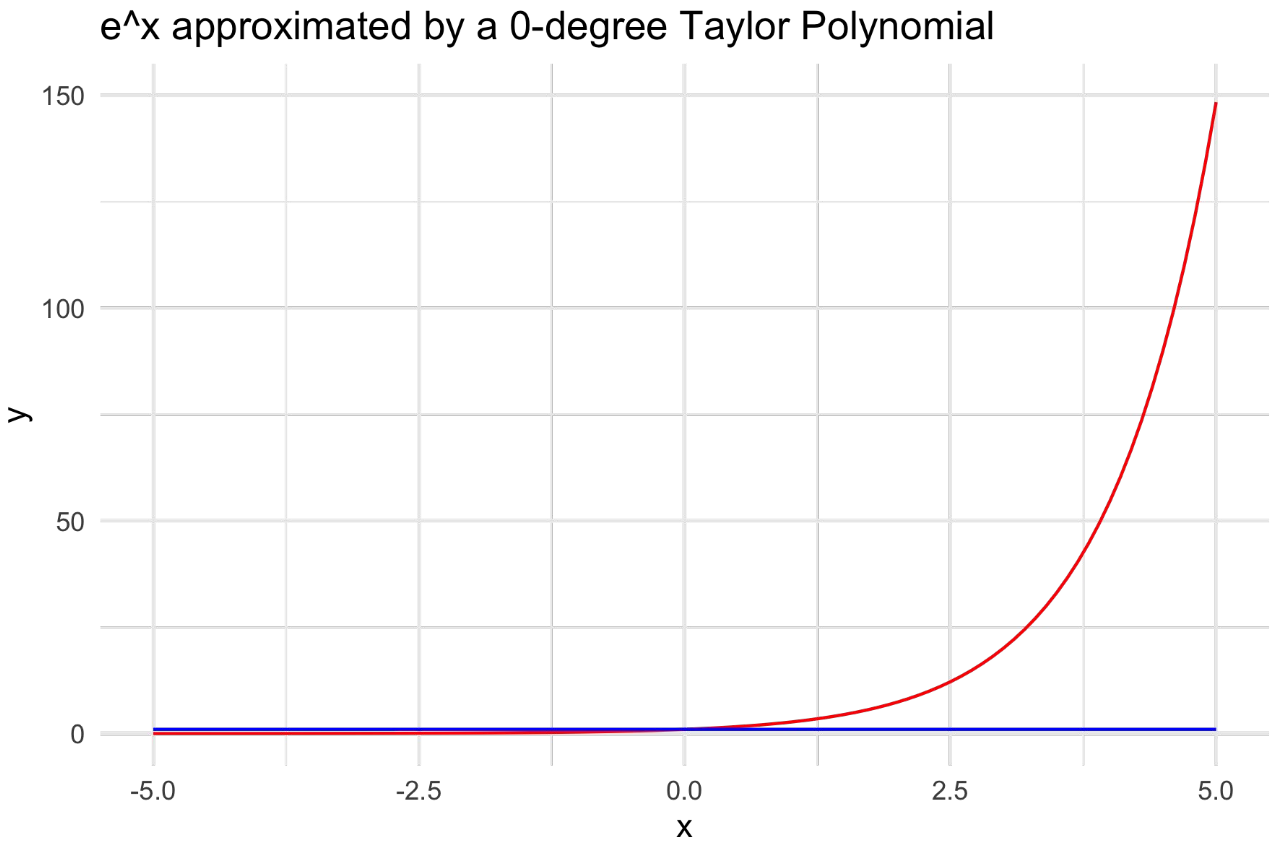

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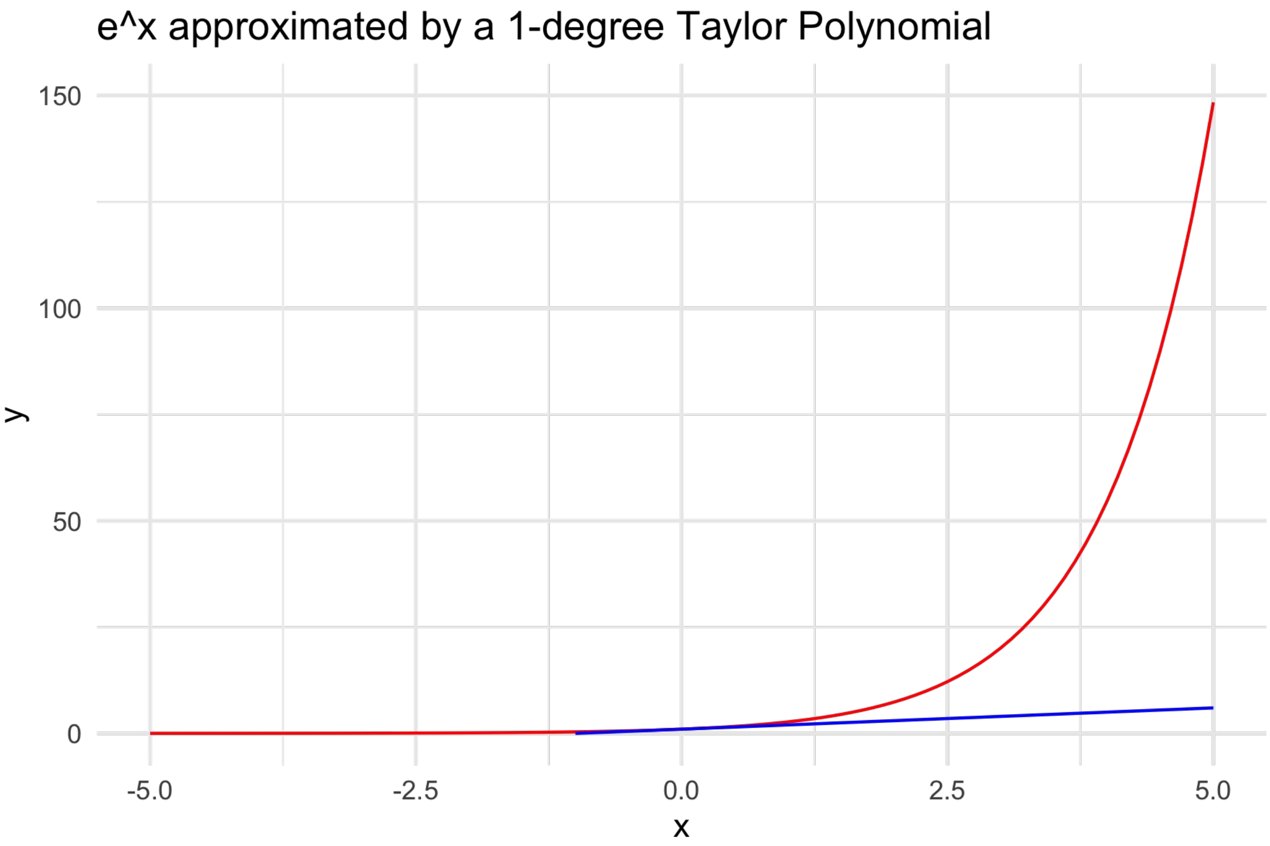

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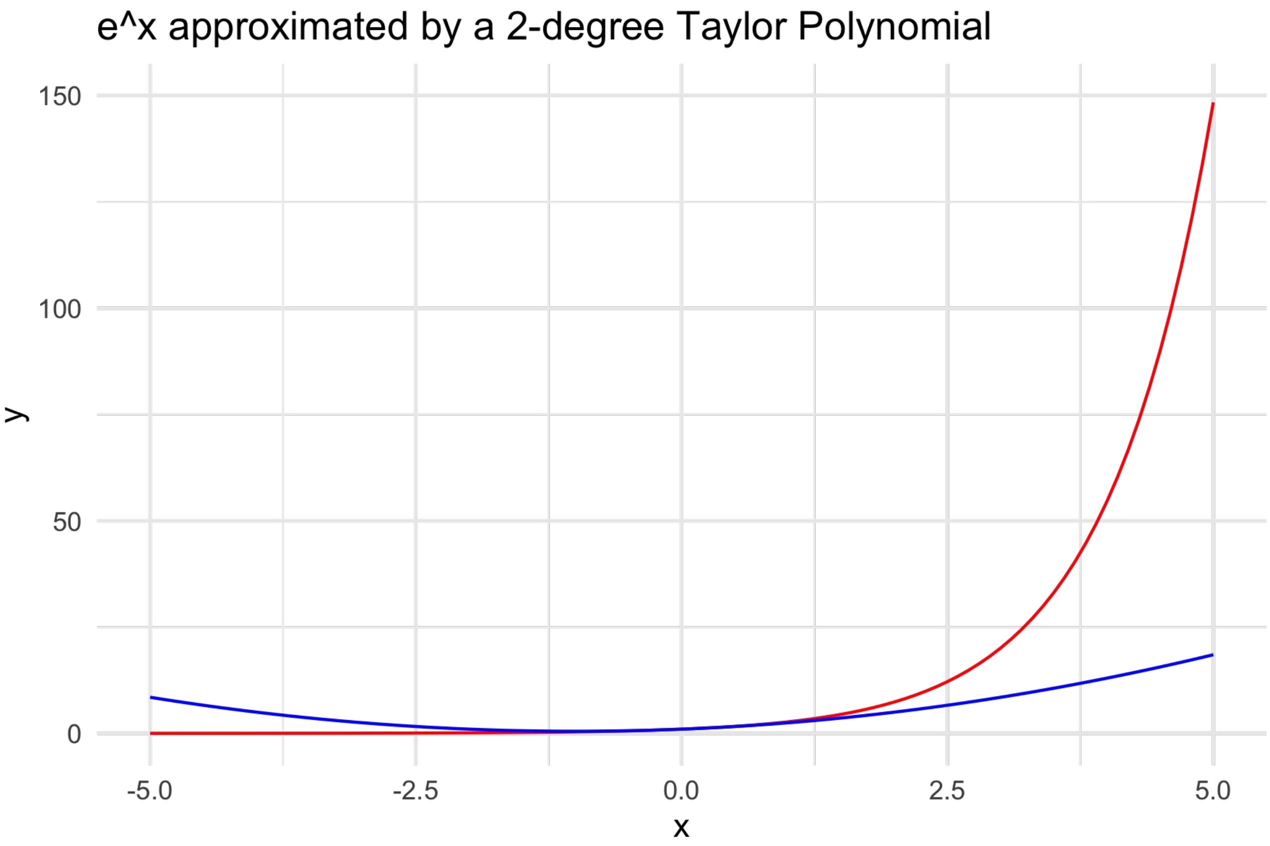

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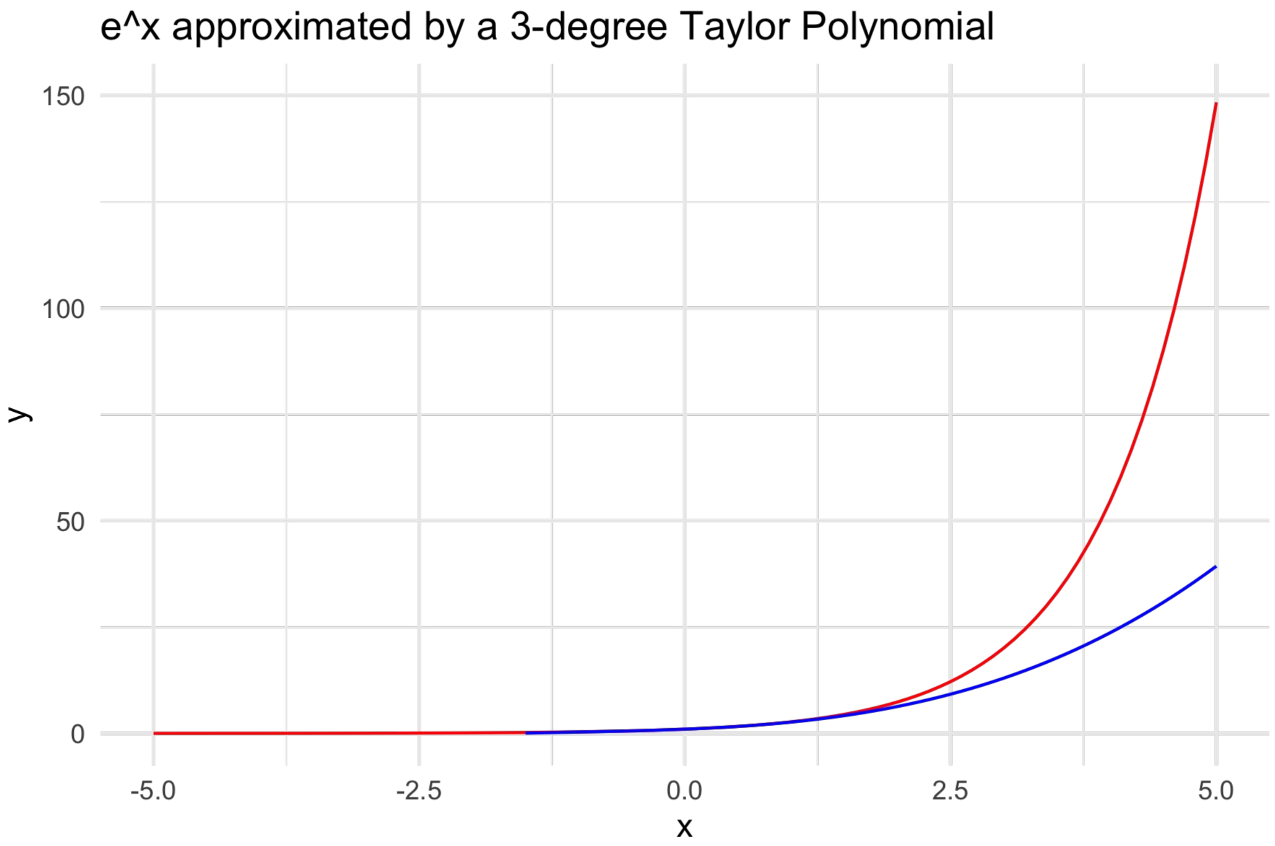
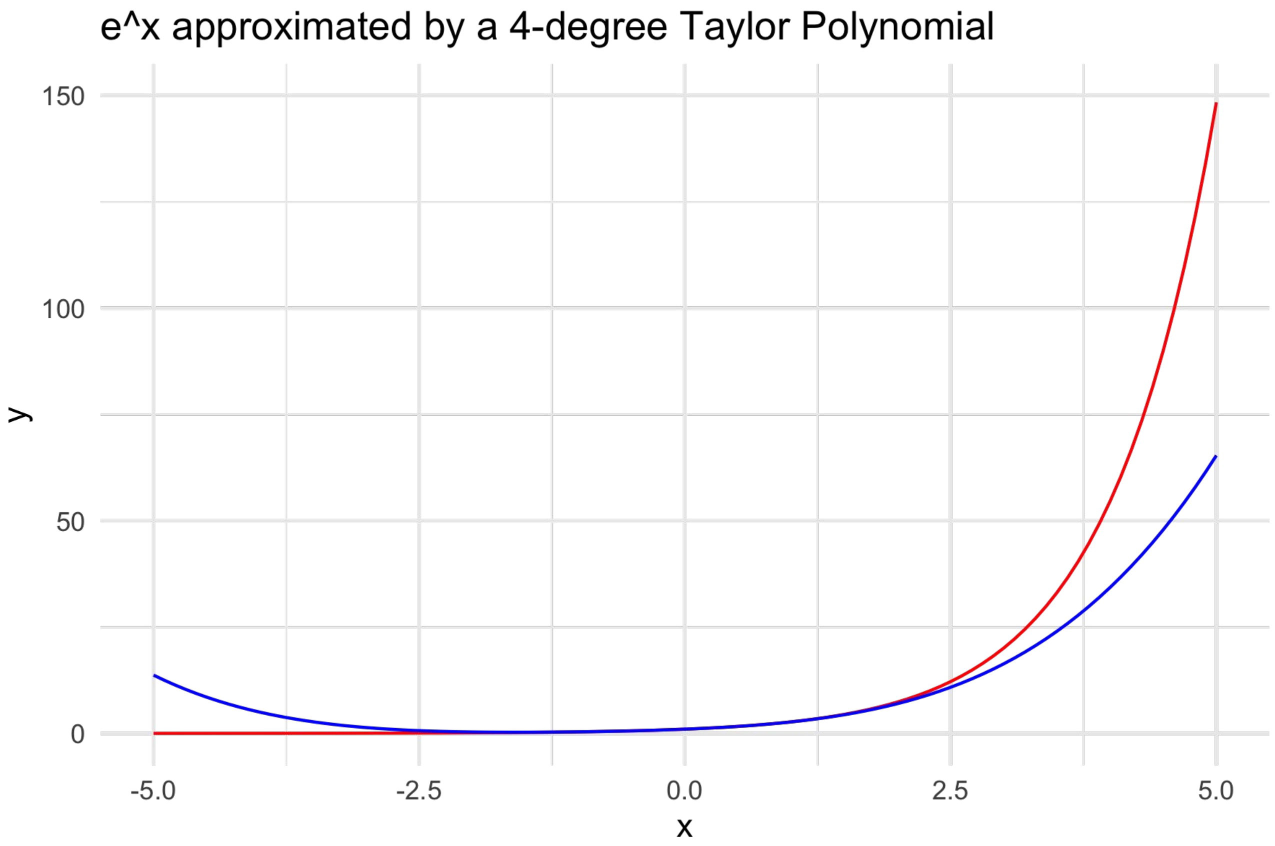
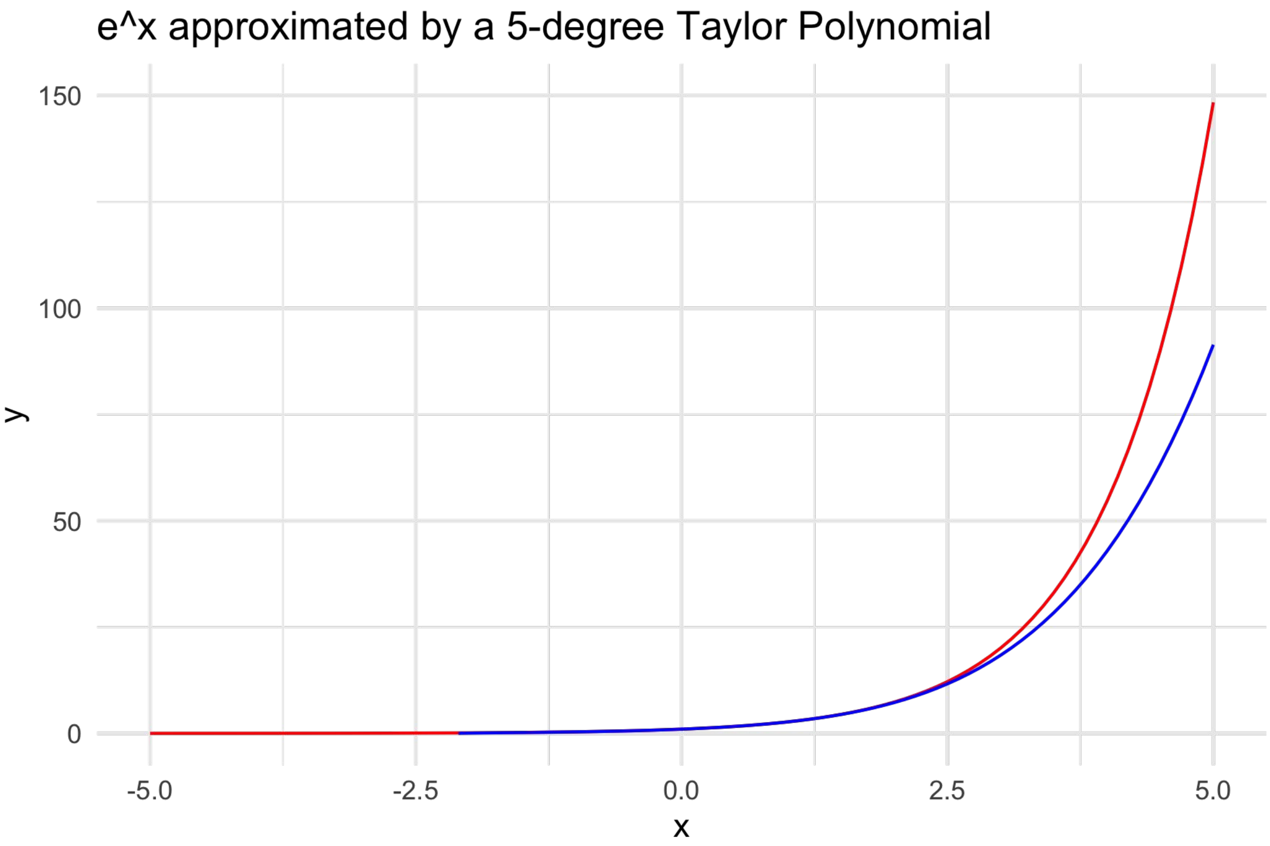


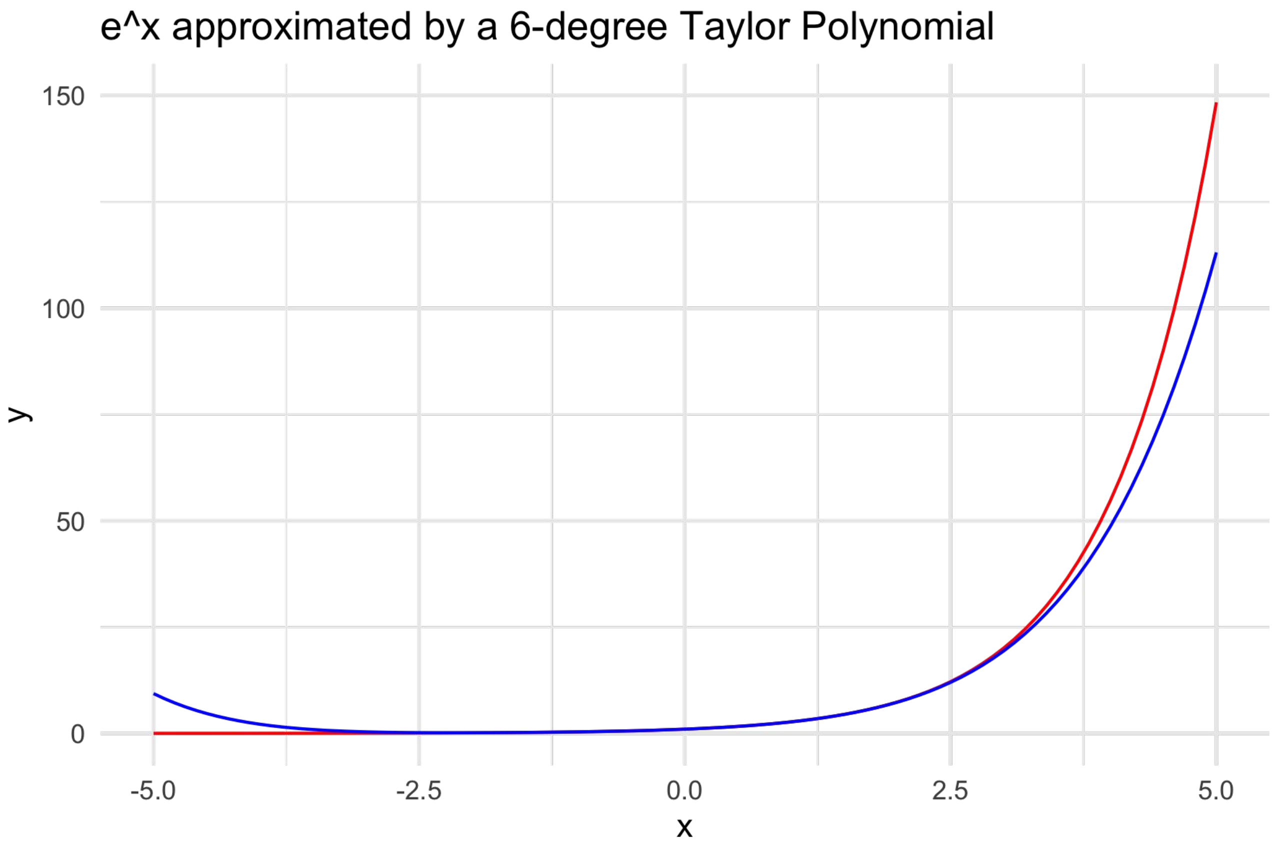
Taylor Series (visually)



Taylor Series (visually)



Taylor Series (visually)



Taylor Series

$$\sum_{n=0}^{\infty} \frac{f^n(a)}{n!}(x-a)^n = f(a) + \frac{f'(a)}{1}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \ldots + \frac{f^\infty(a)}{\infty!}(x-a)^\infty$$

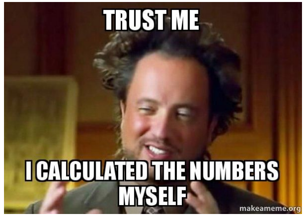
$$\sum_{n=0}^{\infty} \frac{f^n(a)}{n!}(x-a)^n = \boxed{\underbrace{f(a) + \frac{f'(a)}{1}(x-a) + \frac{f''(a)}{2!}(x-a)^2}_{\text{use just this for approximation of f(x))}}} + \ldots + \frac{f^\infty(a)}{\infty!}(x-a)^\infty$$

Radial Kernel (Taylor's Version)

$$\underbrace{K(x, y)}_{\text{kernel}} = e^{-\gamma(x-y)^2}$$

$$\underbrace{K(x, y)}_{\text{kernel}} = (x * y + r)^d$$

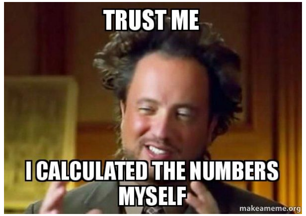
Radial Kernel (Taylor's Version)



$$K(x, y) = (x * y)^1 = x^1 y^1 = x^1 \cdot y^1$$

$$K(x, y) = (x * y)^2 = x^2 y^2 = x^2 \cdot y^2$$

Radial Kernel (Taylor's Version)



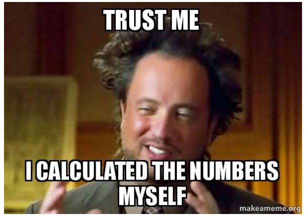
$$K(x, y) = (x * y)^1 = x^1 y^1 = x^1 \cdot y^1$$

$$K(x, y) = (x * y)^2 = x^2 y^2 = x^2 \cdot y^2$$

$$x^1 y^1 + x^2 y^2 = (x^1, x^2) \cdot (y^1, y^2)$$

$$x^1 y^1 + x^2 y^2 + x^3 y^3 = (x^1, x^2, x^3) \cdot (y^1, y^2, y^3)$$

Radial Kernel (Taylor's Version)



$$K(x, y) = (x * y)^1 = x^1 y^1 = x^1 \cdot y^1$$

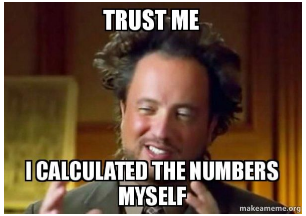
$$K(x, y) = (x * y)^2 = x^2 y^2 = x^2 \cdot y^2$$

$$x^1 y^1 + x^2 y^2 = (x^1, x^2) \cdot (y^1, y^2)$$

$$x^1 y^1 + x^2 y^2 + x^3 y^3 = (x^1, x^2, x^3) \cdot (y^1, y^2, y^3)$$

$$x^1 y^1 + x^2 y^2 + x^3 y^3 + \ldots + x^\infty y^\infty = (x^1, x^2, x^3, \ldots, x^\infty) \cdot (y^1, y^2, y^3, \ldots, y^\infty)$$

Radial Kernel (Taylor's Version)



$$K(x,y) = (x * y)^1 = x^1 y^1 = x^1 \cdot y^1$$

$$K(x,y) = (x * y)^2 = x^2 y^2 = x^2 \cdot y^2$$

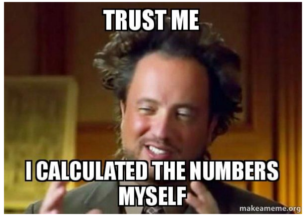
$$\underbrace{K(x,y)}_{\text{kernel}} = e^{-\gamma(x-y)^2}$$

$$x^1 y^1 + x^2 y^2 = (x^1, x^2) \cdot (y^1, y^2)$$

$$x^1 y^1 + x^2 y^2 + x^3 y^3 = (x^1, x^2, x^3) \cdot (y^1, y^2, y^3)$$

$$x^1 y^1 + x^2 y^2 + x^3 y^3 + \ldots + x^\infty y^\infty = (x^1, x^2, x^3, \ldots, x^\infty) \cdot (y^1, y^2, y^3, \ldots, y^\infty)$$

Radial Kernel (Taylor's Version)



$$\underbrace{K(x, y)}_{\text{kernel}} = e^{-\gamma(x-y)^2}$$

$$e^{-\gamma(x-y)^2} = e^{-\gamma(x^2+y^2-2xy)}$$

$$e^{-\gamma(x^2+y^2)}e^{\gamma 2xy}$$

Radial Kernel (Taylor's Version)

$$\underbrace{K(x,y)}_{\text{kernel}} = e^{-\gamma(x-y)^2}$$

$$e^{-\gamma(x-y)^2} = e^{-\gamma(x^2+y^2-2xy)}$$

$$e^{-\gamma(x^2+y^2)}e^{\gamma 2xy}$$

$$e^{-\frac{1}{2}(x^2+y^2)}e^{xy}$$

Radial Kernel (Taylor's Version)

$$\underbrace{K(x,y)}_{\text{kernel}} = e^{-\gamma(x-y)^2}$$

$$e^{-\gamma(x-y)^2} = e^{-\gamma(x^2+y^2-2xy)}$$

$$e^{-\gamma(x^2+y^2)}e^{\gamma 2xy}$$

$$e^{-\frac{1}{2}(x^2+y^2)}\boxed{e^{xy}}$$

Radial Kernel (Taylor's Version)

$$e^x = e^a + \frac{e^a}{1!}(x-a) + \frac{e^a}{2!}(x-a)^2 + \frac{e^a}{3!}(x-a)^3 + \ldots + \frac{e^\infty}{\infty!}(x-a)^\infty$$

$$e^x = e^0 + \frac{e^0}{1!}(x-0) + \frac{e^0}{2!}(x-0)^2 + \frac{e^0}{3!}(x-0)^3 + \ldots + \frac{e^0}{\infty!}(x-0)^\infty$$

$$e^x = 1 + \frac{1}{1!}(x) + \frac{1}{2!}(x)^2 + \frac{1}{3!}(x)^3 + \ldots + \frac{1}{\infty!}(x)^\infty$$

$$\underbrace{K(x, y)}_{\text{kernel}} = e^{-\gamma(x-y)^2}$$

$$e^{xy} = 1 + \frac{1}{1!}(xy) + \frac{1}{2!}(xy)^2 + \frac{1}{3!}(xy)^3 + \ldots + \frac{1}{\infty!}(xy)^\infty$$

$$x^0y^0 + x^1y^1 + x^2y^2 + \ldots + x^\infty y^\infty = (1, x, x^2, \ldots, x^\infty) \cdot (1, y, y^2, \ldots, y^\infty)$$

Radial Kernel (Taylor's Version)

$$\underbrace{K(x, y)}_{\text{kernel}} = e^{-\gamma(x-y)^2}$$

$$e^{xy} = \boxed{1} + \frac{1}{1!}(xy) + \frac{1}{2!}(xy)^2 + \frac{1}{3!}(xy)^3 + \ldots + \frac{1}{\infty!}(xy)^{\infty}$$

$$\boxed{x^0 y^0} + x^1 y^1 + x^2 y^2 + \ldots + x^{\infty} y^{\infty} = (1, x, x^2, \ldots, x^{\infty}) \cdot (1, y, y^2, \ldots, y^{\infty})$$

Radial Kernel (Taylor's Version)

$$\underbrace{K(x, y)}_{\text{kernel}} = e^{-\gamma(x-y)^2}$$

$$e^{xy} = \boxed{1} + \frac{1}{1!}\boxed{(xy)} + \frac{1}{2!}(xy)^2 + \frac{1}{3!}(xy)^3 + \ldots + \frac{1}{\infty!}(xy)^\infty$$

$$\boxed{x^0y^0} + \boxed{x^1y^1} + x^2y^2 + \ldots + x^\infty y^\infty = (1, x, x^2, \ldots, x^\infty) \cdot (1, y, y^2, \ldots, y^\infty)$$

Radial Kernel (Taylor's Version)

$$\underbrace{K(x, y)}_{\text{kernel}} = e^{-\gamma(x-y)^2}$$

$$e^{xy} = \boxed{1} + \frac{1}{1!}\boxed{(xy)} + \frac{1}{2!}\boxed{(xy)^2} + \frac{1}{3!}(xy)^3 + \ldots + \frac{1}{\infty!}(xy)^\infty$$

$$\boxed{x^0 y^0} + \boxed{x^1 y^1} + \boxed{x^2 y^2} + \ldots + x^\infty y^\infty = (1, x, x^2, \ldots, x^\infty) \cdot (1, y, y^2, \ldots, y^\infty)$$

Radial Kernel (Taylor's Version)

$$\underbrace{K(x, y)}_{\text{kernel}} = e^{-\gamma(x-y)^2}$$

$$e^{xy} = \boxed{1} + \frac{1}{1!}\boxed{(xy)} + \frac{1}{2!}\boxed{(xy)^2} + \frac{1}{3!}(xy)^3 + \ldots + \frac{1}{\infty!}\boxed{(xy)^\infty}$$

$$\boxed{x^0y^0} + \boxed{x^1y^1} + \boxed{x^2y^2} + \ldots + \boxed{x^\infty y^\infty} = (1, x, x^2, \ldots, x^\infty)\cdot(1, y, y^2, \ldots, y^\infty)$$

Radial Kernel (Taylor's Version)

$$\underbrace{K(x,y)}_{\text{kernel}} = e^{-\gamma(x-y)^2}$$

$e^{xy} = \boxed{1} + \frac{1}{1!}($ …

$\boxed{x^0y^0} + \boxed{x^1y^1} +$ … $, \ldots, y^\infty)$

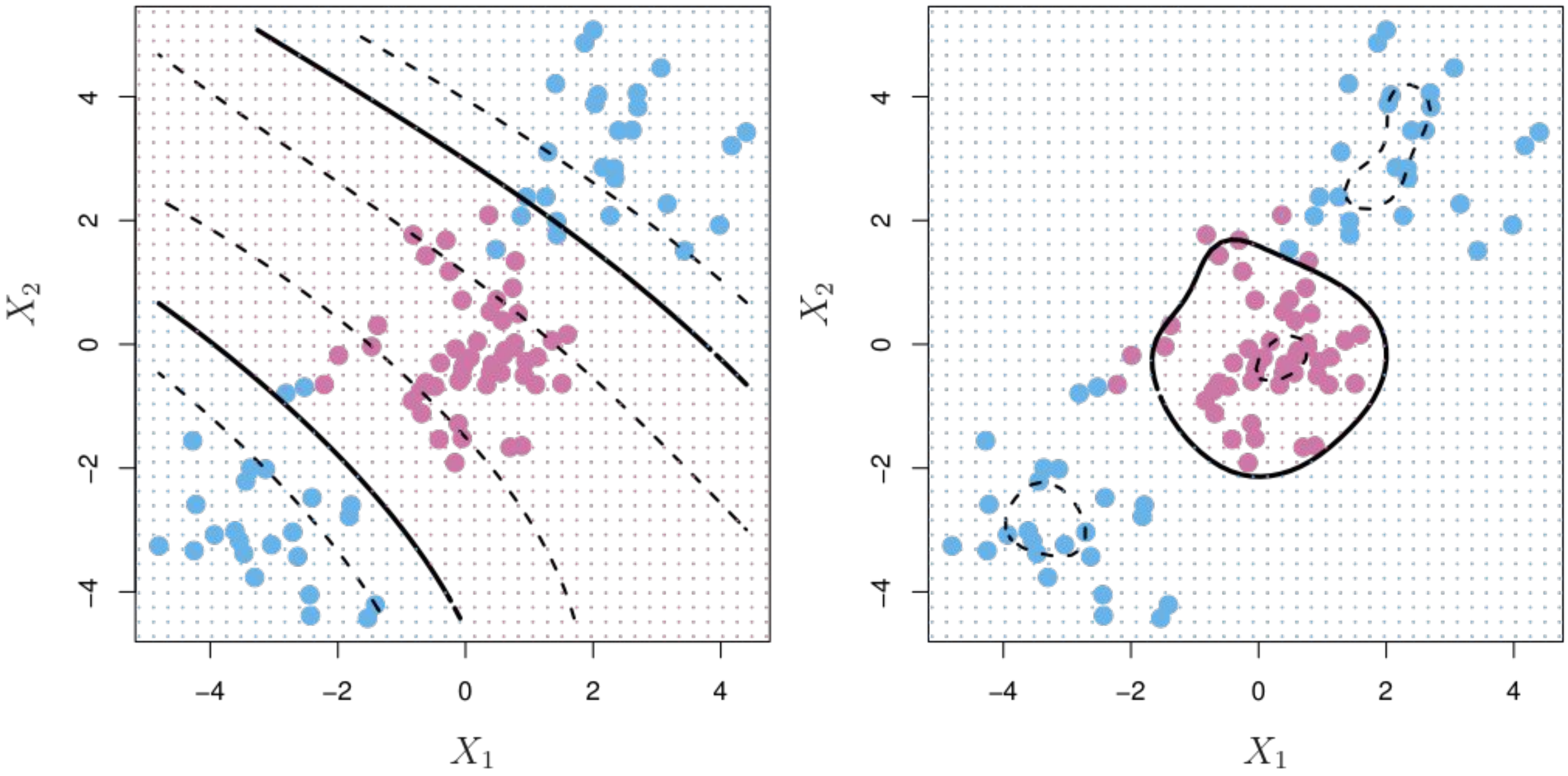
Radial Basis Kernels have coordinates for infinite dimensions!

Support Vector Machines Part 3:

$$e^{-\gamma(a-b)^2}$$

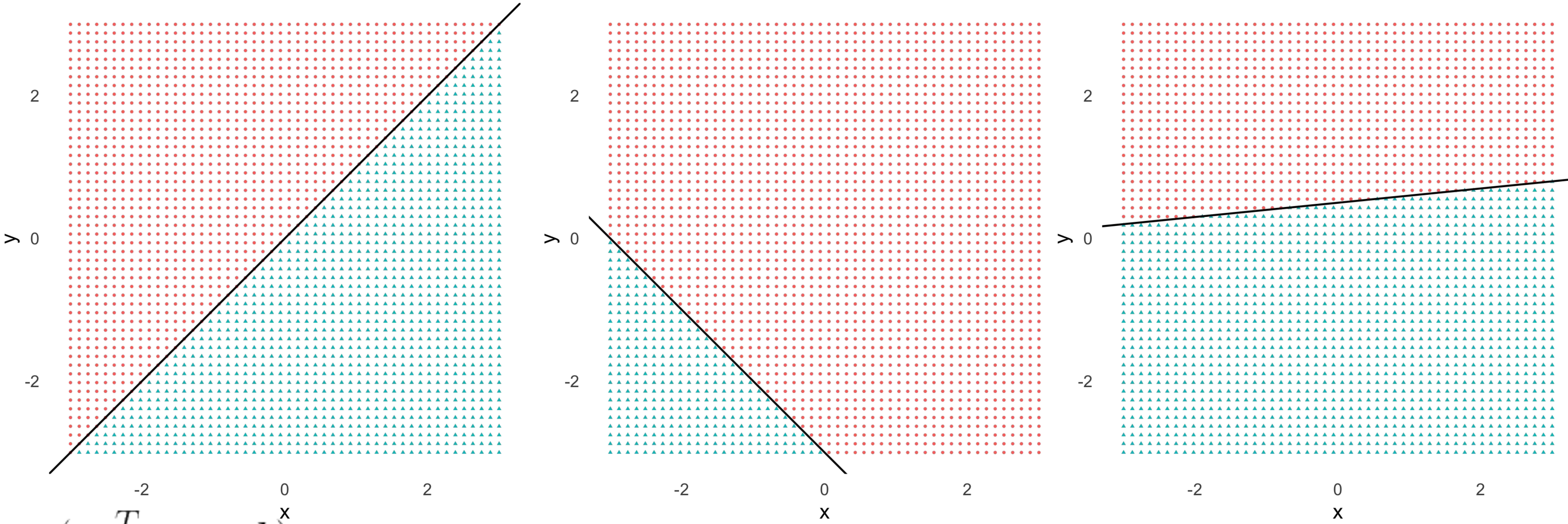
...The Radial Kernel!!!

Radial Basis Kernel Example



Images from an Introduction to Statistical Learning with applications in R

Kernels



$$t_n(\mathbf{w}^T x_n + b)$$

$$t_n(\mathbf{w}^T \phi(x_n) + b)$$

Kernels

$$\overbrace{y(\mathbf{w}) = \sum_{n=1}^{N} a_n t_n \;\; \phi(x) \cdot \phi(x_n) \;\; + b}^{\text{formula to classify new data point } x}$$

$$\overbrace{y(\mathbf{w}) = \sum_{n=1}^{N} a_n t_n \;\; \underbrace{K(x, y)}_{\text{kernel}} \;\; +b}^{\text{formula to classify new data point } x}$$