

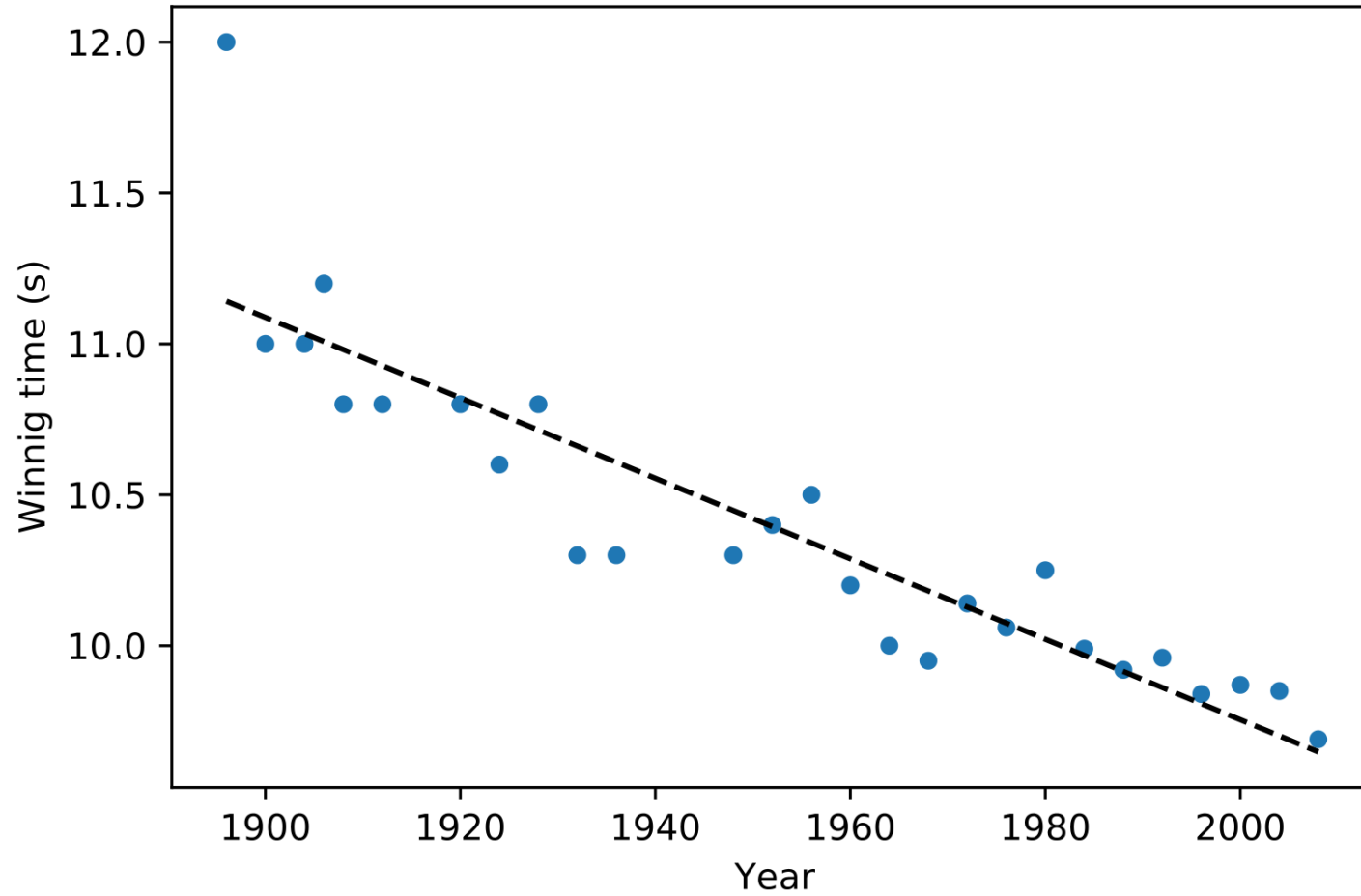
Linear regression

Polynomial regression and basis functions

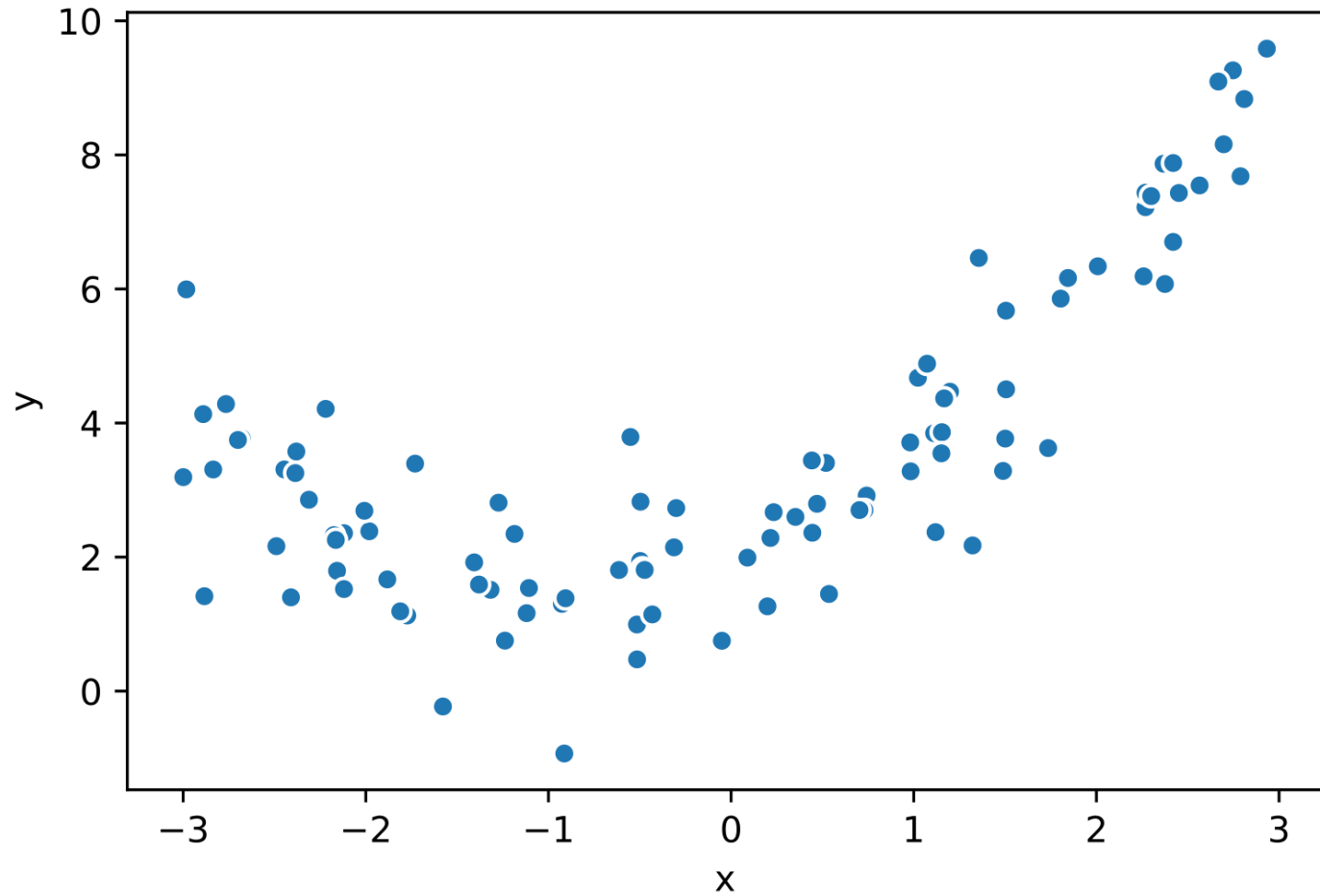
Herman Kamper

<http://www.kamperh.com/>

Linear regression



Non-linear relationship



Polynomial regression

Multiple linear regression recap:

$$f(\underline{x}; \underline{w}) = w_0 + w_1 x_1 + \dots + w_D x_D = \underline{w}^T \underline{x}$$

Fit on data $\{(\underline{x}^{(n)}, y^{(n)})\}_{n=1}^N$ using:

$$\begin{aligned} J(\underline{w}) &= \sum_{n=1}^N (y^{(n)} - f(\underline{x}^{(n)}; \underline{w}))^2 \\ &= (\underline{y} - \underline{X} \underline{w})^T (\underline{y} - \underline{X} \underline{w}), \text{ with} \\ \underline{X} &= \begin{bmatrix} - (\underline{x}^{(1)})^T - \\ - (\underline{x}^{(2)})^T - \\ \vdots \\ - (\underline{x}^{(N)})^T - \end{bmatrix}; \quad \underline{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(N)} \end{bmatrix} \end{aligned}$$

↑ Design matrix

Solution: $\hat{\underline{w}} = (\underline{X}^T \underline{X})^{-1} \underline{X}^T \underline{y}$ Normal equations

Polynomial regression:

What do we do if we want to fit $f(x; w_0, w_1, w_2) = w_0 + w_1 x + w_2 x^2$?

Let's define

$$\underline{\phi}(x) = \begin{bmatrix} 1 \\ x \\ x^2 \end{bmatrix}$$

" $\underline{w}^T \underline{x}$ " ↘

We can then write $f(x; \underline{w}) = \underline{w}^T \underline{\phi}(x)$
Now we can solve the problem exactly as for multiple linear regression by "pretending" that $\underline{\phi}(x)$ is \underline{x} .

Our design matrix would now become:

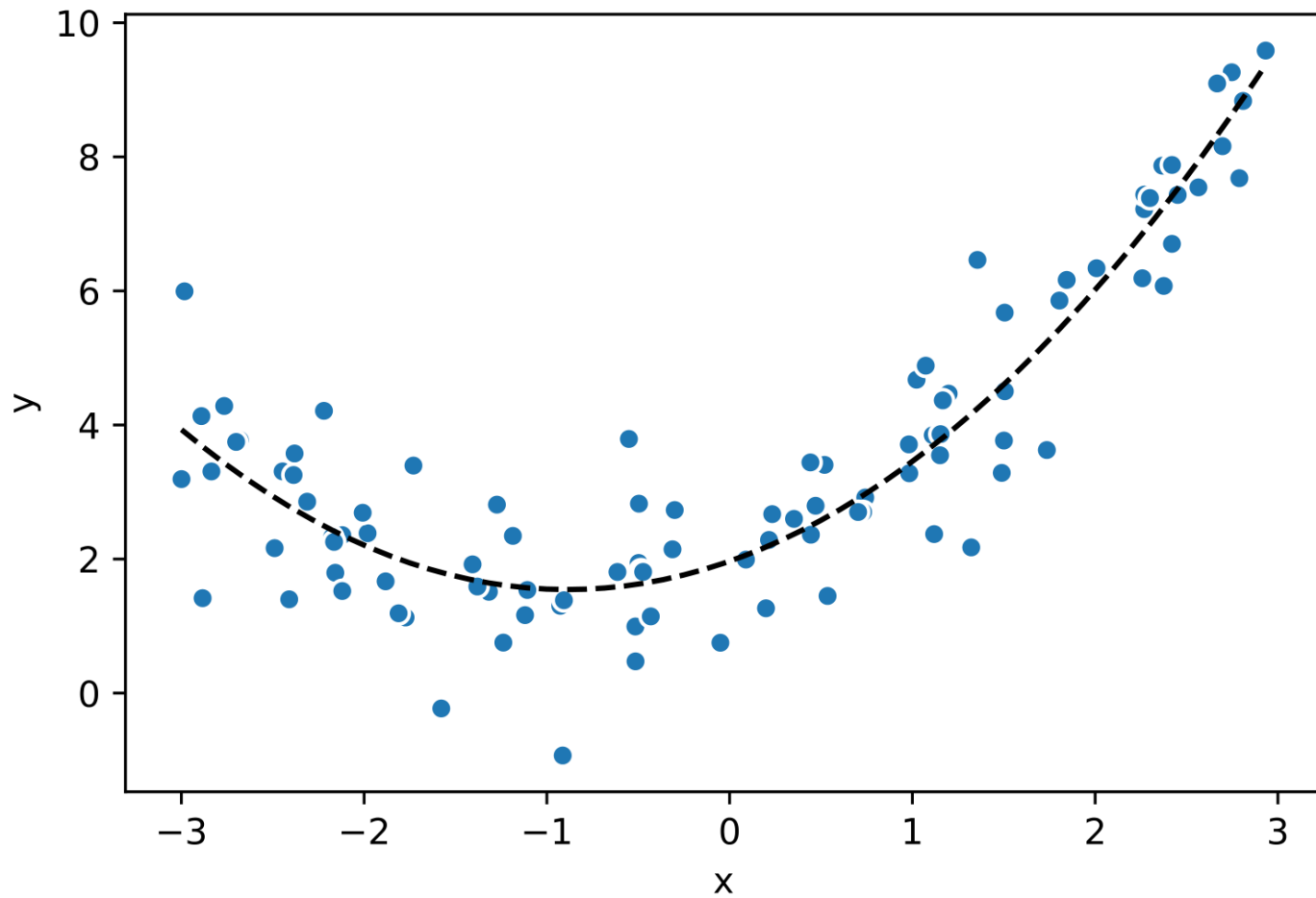
$$\underline{\Phi} = \begin{bmatrix} - \underline{\phi}(x^{(1)})^T - \\ - \underline{\phi}(x^{(2)})^T - \\ \vdots \\ - \underline{\phi}(x^{(N)})^T - \end{bmatrix} = \begin{bmatrix} 1 & x^{(1)} & (x^{(1)})^2 \\ 1 & x^{(2)} & (x^{(2)})^2 \\ \vdots & \vdots & \vdots \\ 1 & x^{(N)} & (x^{(N)})^2 \end{bmatrix}$$

Other example:

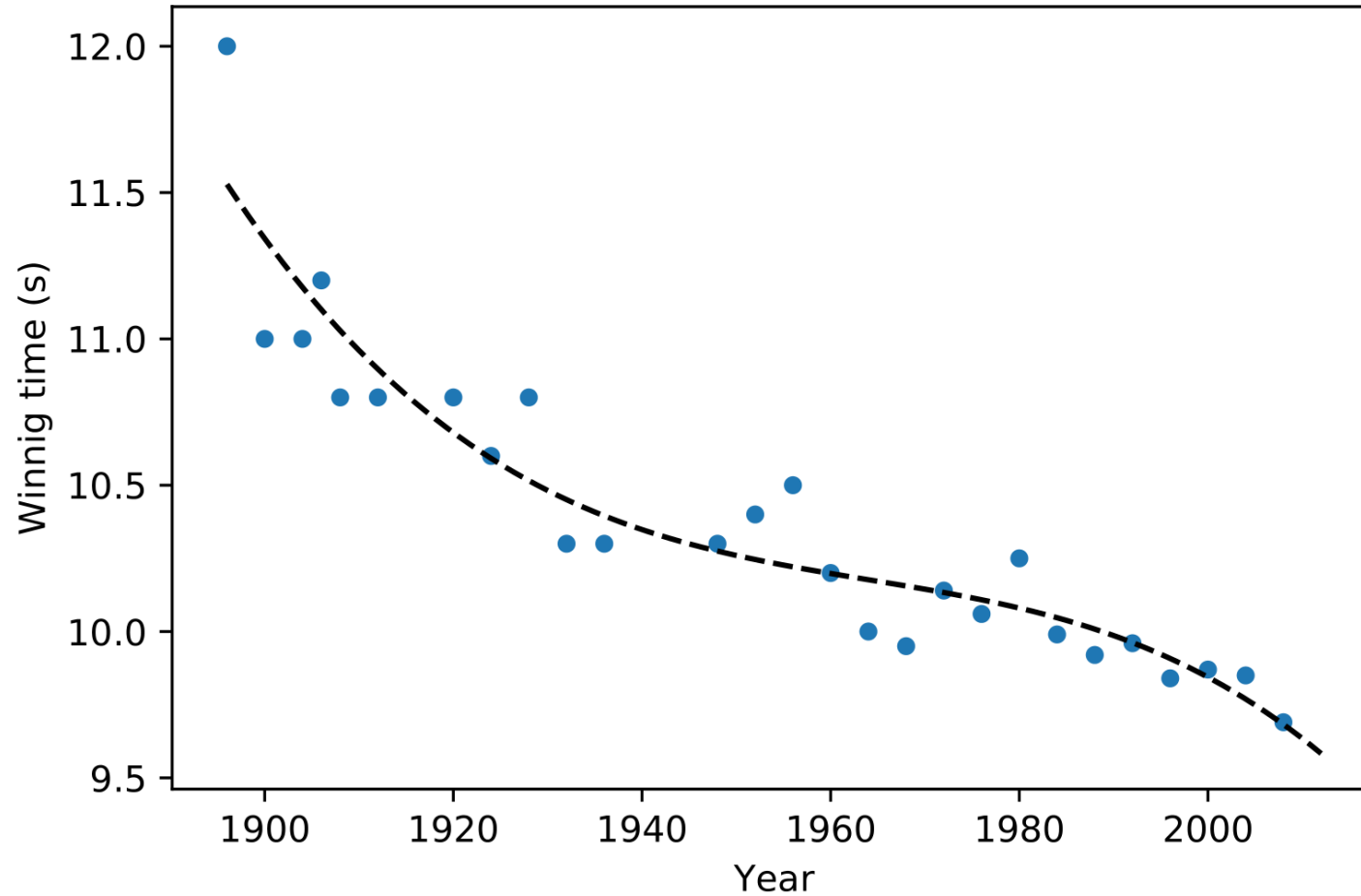
$$f(\underline{x}; \underline{w}) = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1 x_2 + w_4 x_1^2 + w_5 x_2^2$$

with $\underline{\phi}(\underline{x}) = [1 \quad x_1 \quad x_2 \quad x_1 x_2 \quad x_1^2 \quad x_2^2]^T$

Polynomial regression



3rd-order polynomial regression



Basis functions

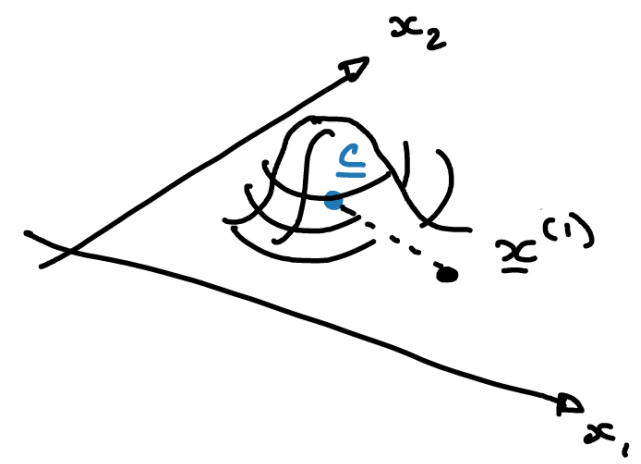
Instead of just polynomials, we can actually put any function in

$$\underline{\phi}(\underline{x}) = [\phi_1(\underline{x}) \quad \phi_2(\underline{x}) \quad \dots \quad \phi_k(\underline{x})]^T$$

e.g. sin, cos, log, exp, FFT, etc.

This can be quite useful if we have some inside domain knowledge of the data and problem.

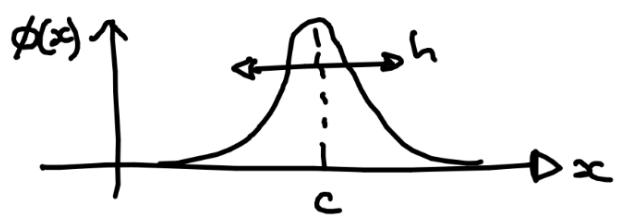
RBF in 2 dimensions:



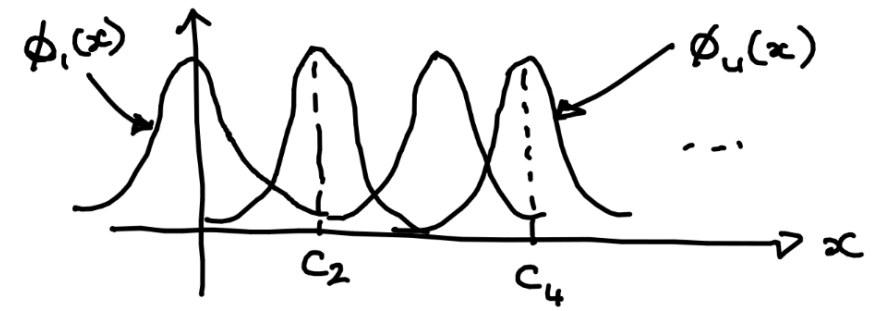
One possible choice as a basis function is the radial basis function (RBF):

$$\phi(\underline{x}) = \exp \left\{ - \frac{(\underline{x} - \underline{c})^T (\underline{x} - \underline{c})}{h^2} \right\}$$

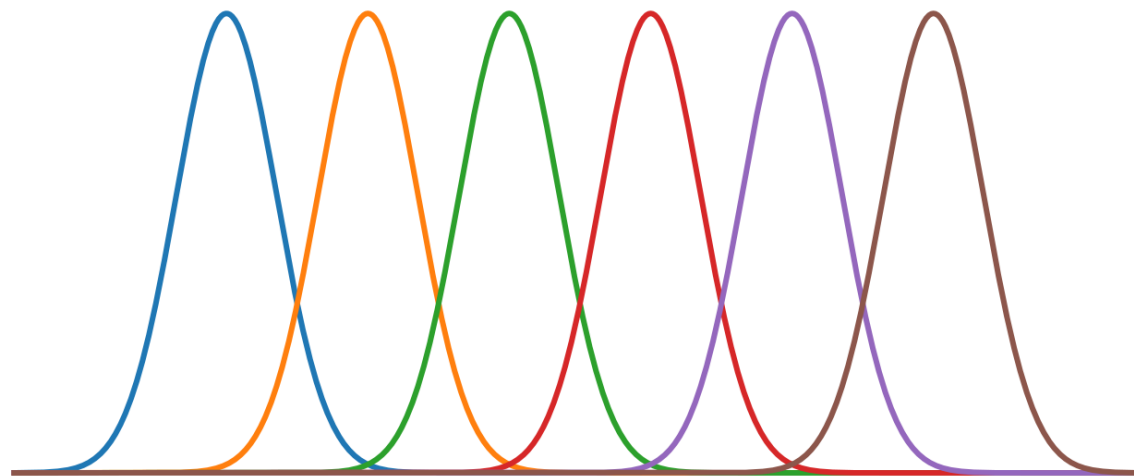
In the 1-D case:



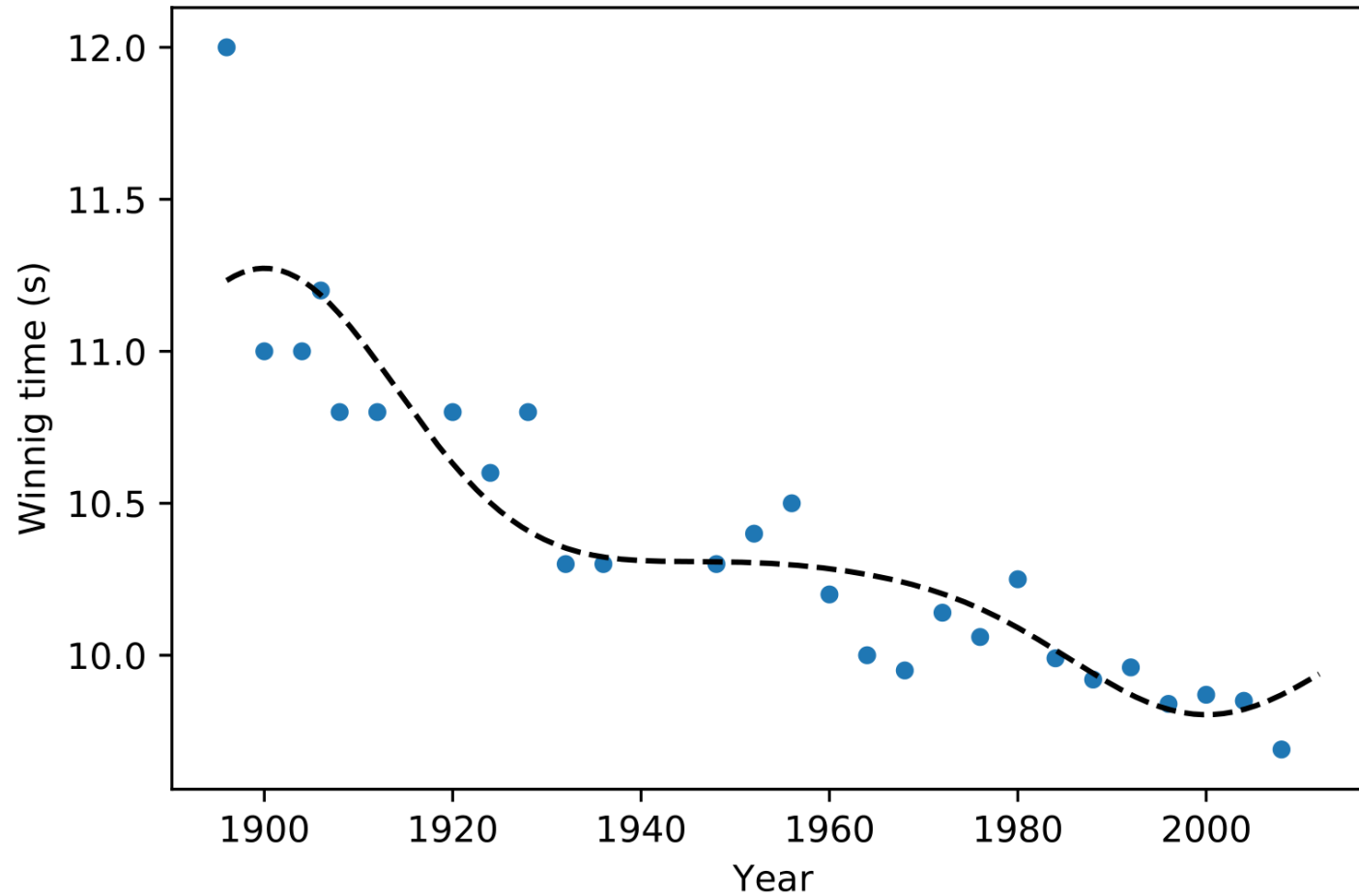
Can even have a family of RBFs:



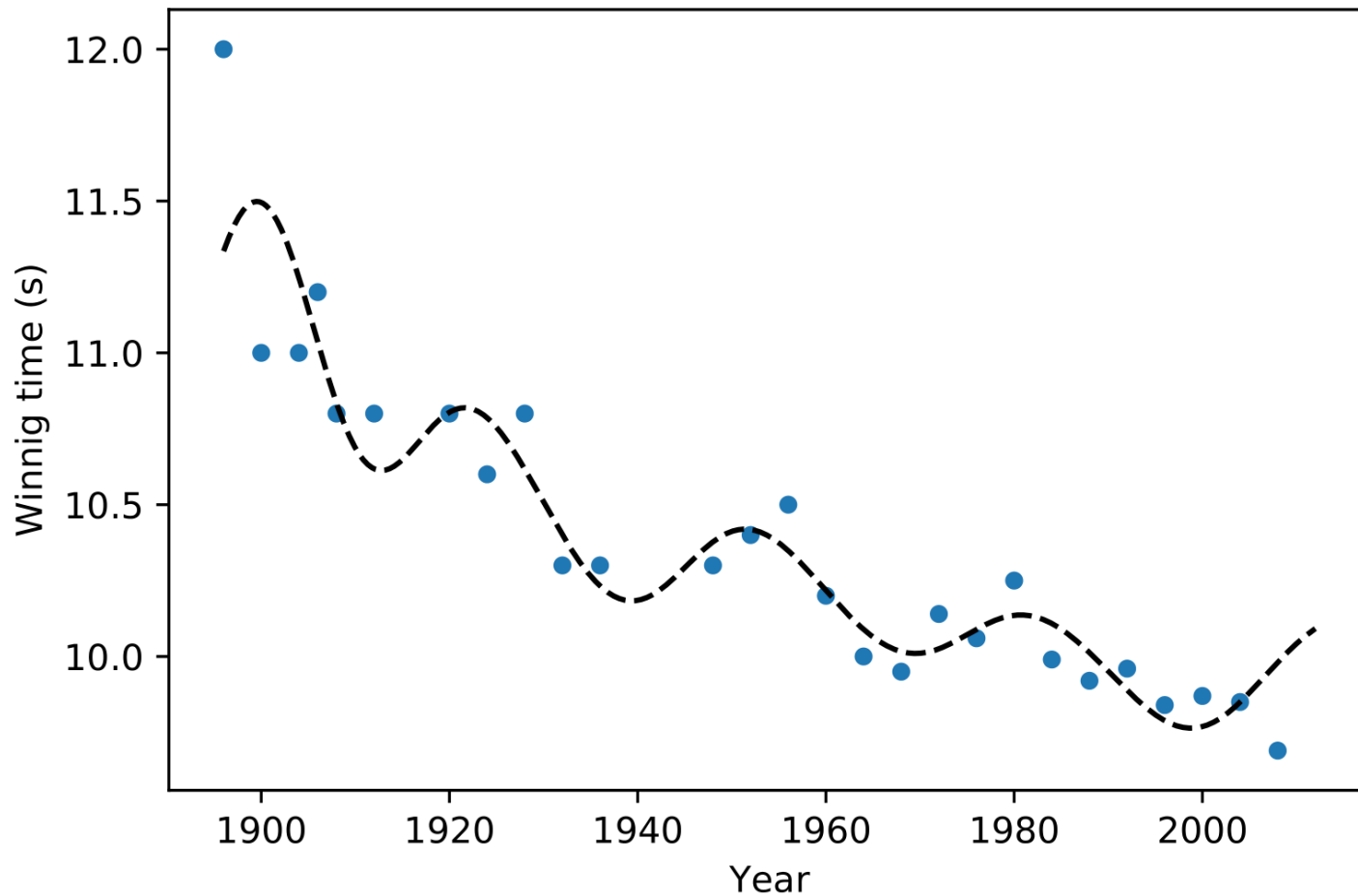
Basis functions: RBF



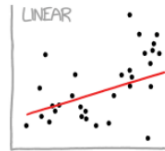
RBF with $c = [1900, 1950, 2000]$ and $h = 20$



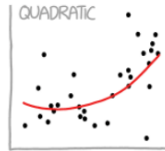
RBF with $c = [1900, 1910, \dots, 2000]$ and $h = 10$



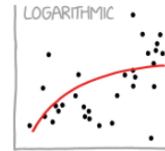
CURVE-FITTING METHODS AND THE MESSAGES THEY SEND



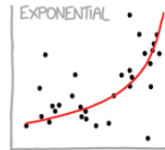
"HEY, I DID A
REGRESSION!"



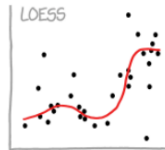
"I WANTED A CURVED
LINE, SO I MADE ONE
WITH MATH!"



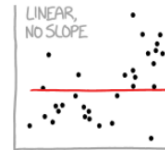
"LOOK, IT'S
TAPERING OFF!"



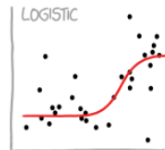
"LOOK, IT'S GROWING
UNCONTROLLABLY!"



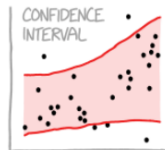
"I'M SOPHISTICATED, NOT
LIKE THOSE BUMBLING
POLYNOMIAL PEOPLE!"



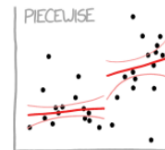
"I'M MAKING A
SCATTER PLOT BUT
I DON'T WANT TO."



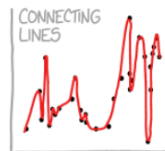
"I NEED TO CONNECT THESE
TWO LINES, BUT MY FIRST IDEA
DIDN'T HAVE ENOUGH MATH!"



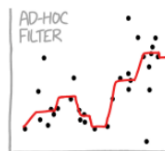
"LISTEN, SCIENCE IS HARD,
BUT I'M A SERIOUS
PERSON DOING MY BEST."



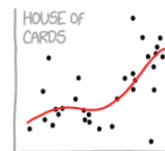
"I HAVE A THEORY,
AND THIS IS THE ONLY
DATA I COULD FIND."



"I CLICKED 'SMOOTH
LINES' IN EXCEL."



"I HAD AN IDEA FOR HOW
TO CLEAN UP THE DATA.
WHAT DO YOU THINK?"



"AS YOU CAN SEE, THIS
MODEL SMOOTHLY FITS
THE- WAIT NO NO DON'T
EXTEND IT AAAAAA!!"