UVA CS 4501: Machine Learning

Lecture 5: Non-Linear Regression Models

Dr. Yanjun Qi

University of Virginia
Department of Computer Science

Where are we ? → Five major sections of this course

- ❑ Regression (supervised)
- ❑ Classification (supervised)
- ❑ Unsupervised models
- ❑ Learning theory
- ❑ Graphical models

Today → Regression (supervised)

- ❑ Four ways to train / perform optimization for linear regression models
  - ❑ Normal Equation
  - ❑ Gradient Descent (GD)
  - ❑ Stochastic GD
  - ❑ Newton's method

- ❑ Supervised regression models
  - ❑ Linear regression (LR)
  - ❑ LR with non-linear basis functions
  - ❑ Locally weighted LR
  - ❑ LR with Regularizations

Today

- Regression Models Beyond Linear
  - LR with non-linear basis functions
  - Instance-based Regression: K-Nearest Neighbors
  - Locally weighted linear regression
  - Regression trees and Multilinear Interpolation (later)

LR with non-linear basis functions

- LR does not mean we can only deal with linear relationships

$$\hat{y} = \theta^T \mathbf{x} \quad \Rightarrow \quad \hat{y} = \theta_0 + \sum_{j=1}^{m} \theta_j \varphi_j(\mathbf{x}) = \theta^T \varphi(\mathbf{x})$$

LR with non-linear basis functions

- We are free to design basis functions (e.g., non-linear features:

Here $\varphi_j(x)$ are fixed basis functions (also define $\varphi_0(x)=1$)

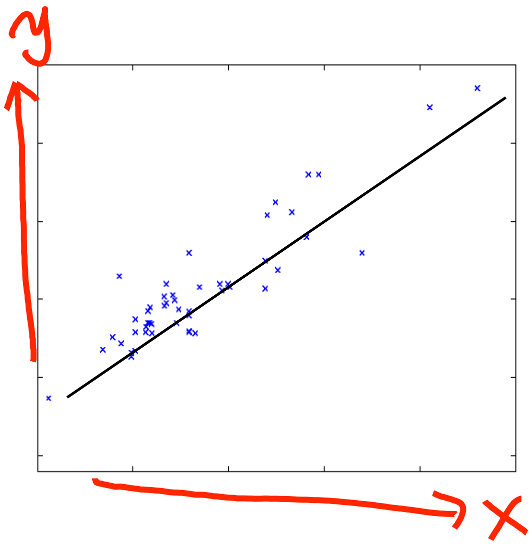
- E.g.: polynomial regression:

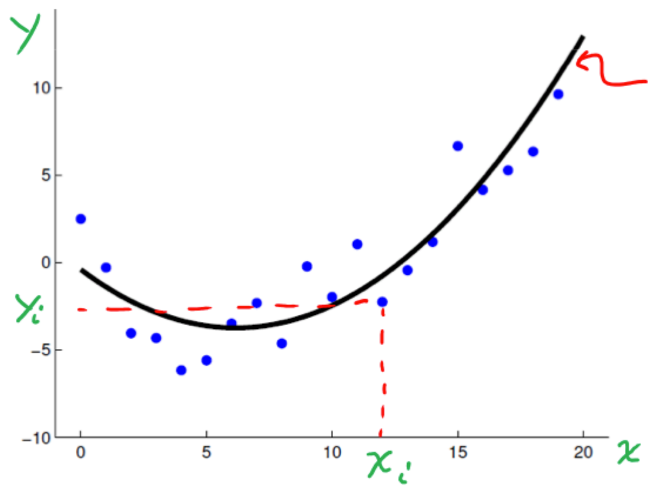
$$\varphi(x) := \left[1, x, x^2\right]^T$$

e.g. (1) polynomial regression

$$\hat{y} = \theta^T \mathbf{x}$$

$$\hat{y} = \theta^T \varphi(\mathbf{x})$$





$= \theta_0 + x\theta_1 + x^2\theta_2$

$$\theta^* = \left(X^T X\right)^{-1} X^T \vec{y}$$

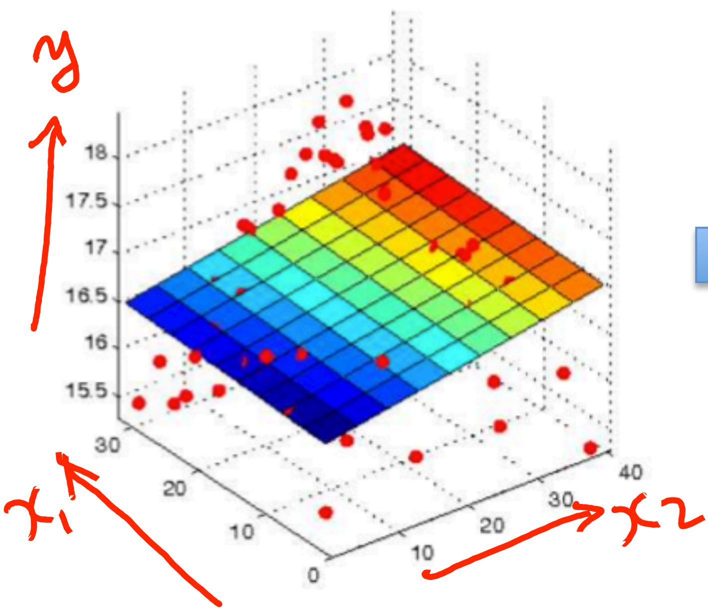
$$\theta^* = \left(\varphi^T \varphi\right)^{-1} \varphi^T \vec{y}$$

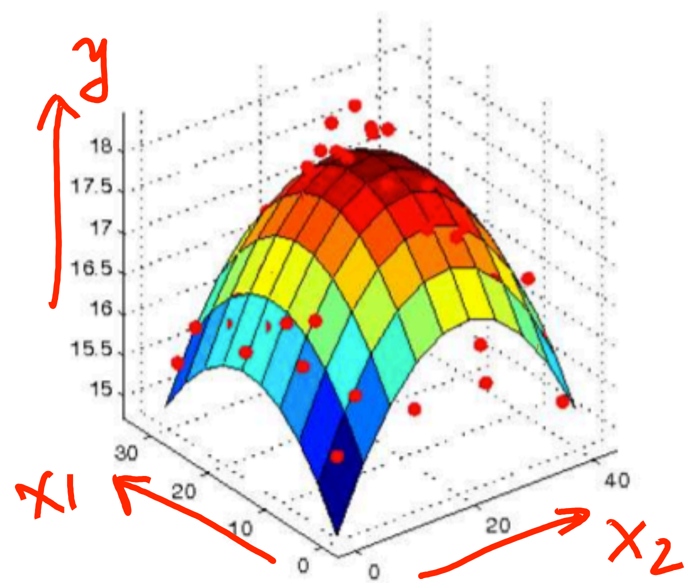
$$\varphi(x) := \left[1, x, x^2\right]^T$$

e.g. (1) **polynomial regression**

$$\hat{y} = \theta^T \mathbf{x} \quad \Rightarrow \quad \hat{y} = \theta^T \varphi(\mathbf{x})$$

$$\phi(\mathbf{x}) = [1, x_1, x_2, x_1^2, x_2^2]$$



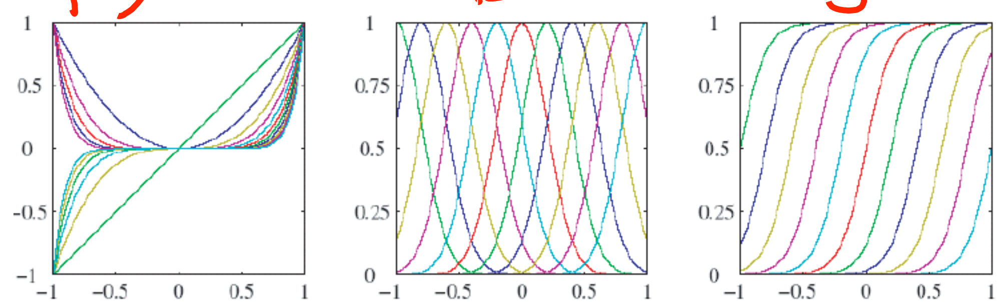


KEY: if the bases are given, the problem of learning the parameters is still linear.

Many Possible Basis functions

- There are many basis functions, e.g.:
  - Polynomial $\varphi_j(x) = x^{j-1}$ $1, x, x^2, x^3, \ldots, x^d$
  - Radial basis functions $\phi_j(x) = \exp\left(-\frac{(x-\mu_j)^2}{2s^2}\right)$
  - Sigmoidal $\phi_j(x) = \sigma\left(\frac{x-\mu_j}{s}\right)$
  - Splines,
  - Fourier,
  - Wavelets, etc

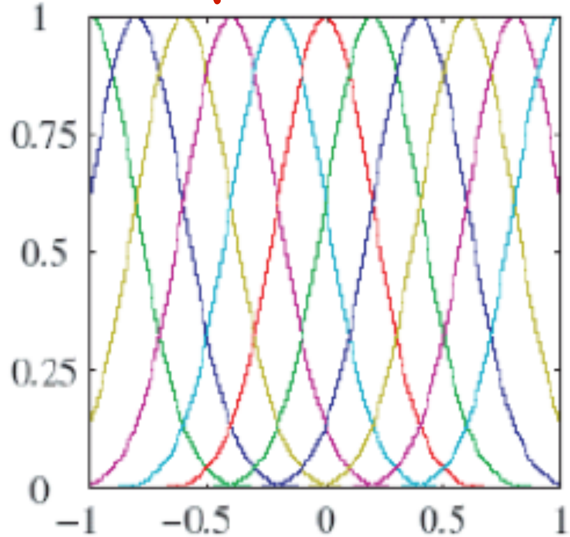
Poly RBF Sigmoid

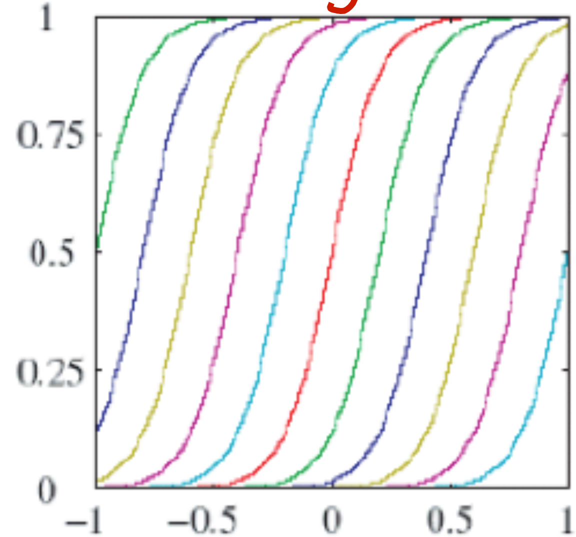


Many Possible Basis functions

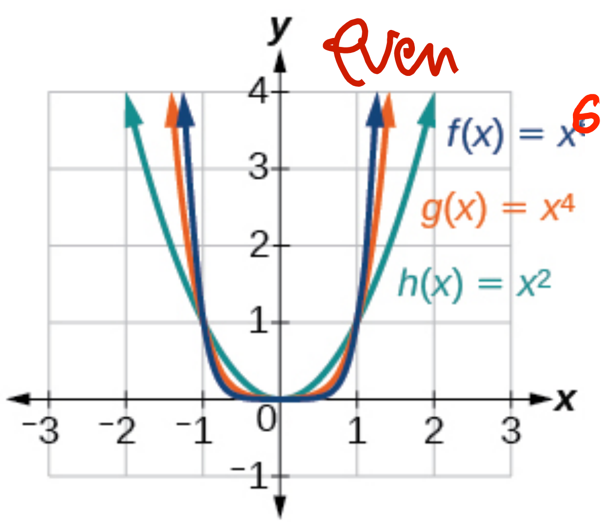
RBF

Sigmoid

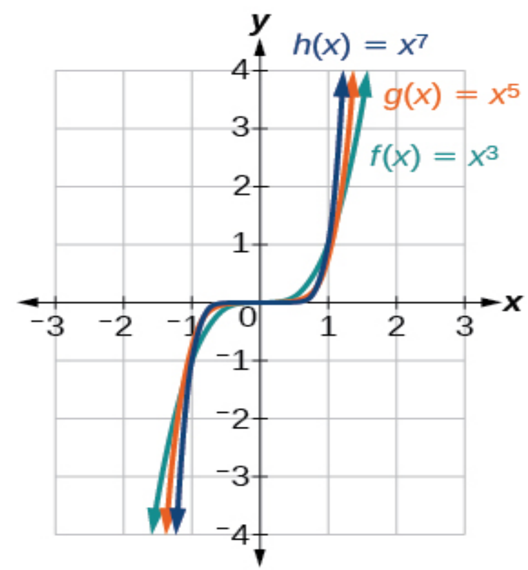




even



odd



e.g. (2) LR with radial-basis functions

- E.g.: LR with RBF regression:

$$\hat{y} = \theta_0 + \sum_{j=1}^{m} \theta_j \varphi_j(x) = \varphi(x)^T \theta$$

$$\varphi(x) := \left[1, K_{\lambda_1}(x, r_1), K_{\lambda 2}(x, r_2), K_{\lambda_3}(x, r_3), K_{\lambda 4}(x, r_4)\right]^T$$

$$\vec{\theta} = [\theta_0, \theta_1, \theta_2, \theta_3, \theta_4]^T$$

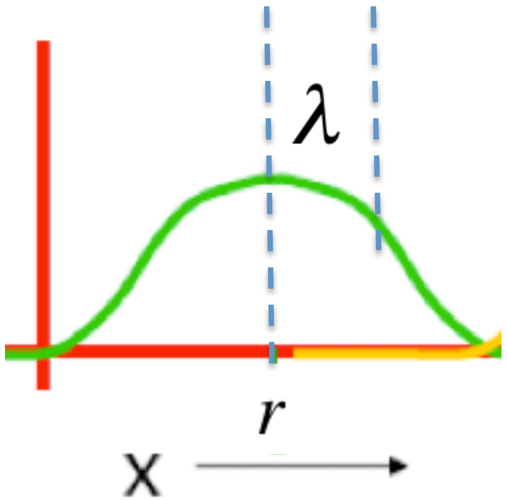
$$\theta^* = \left(\varphi^T \varphi\right)^{-1} \varphi^T \vec{y}$$

RBF = radial-basis function: a function which depends only on the radial distance from a centre point

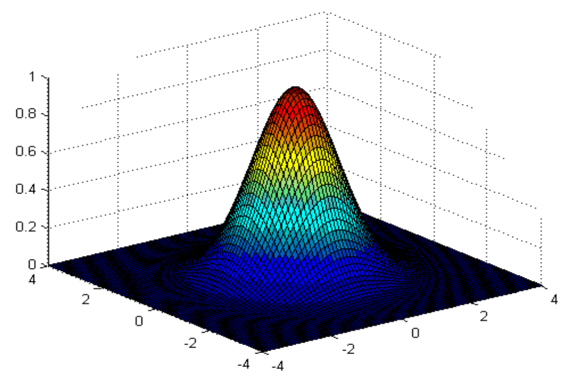
Gaussian RBF ➔

$$K_\lambda(x,r) = \exp\left(-\frac{(x-r)^2}{2\lambda^2}\right)$$

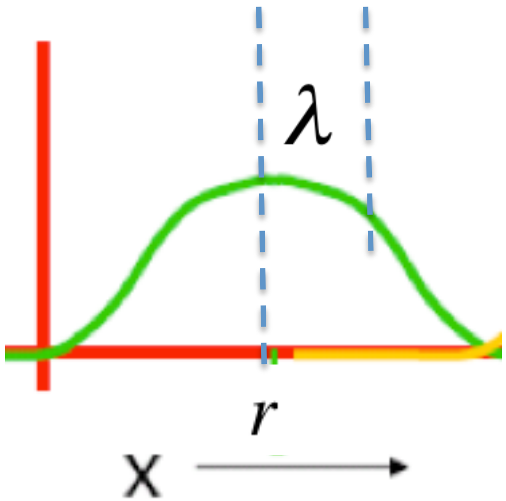
as distance from the center r increases, the output of the RBF decreases



1D case



2D case



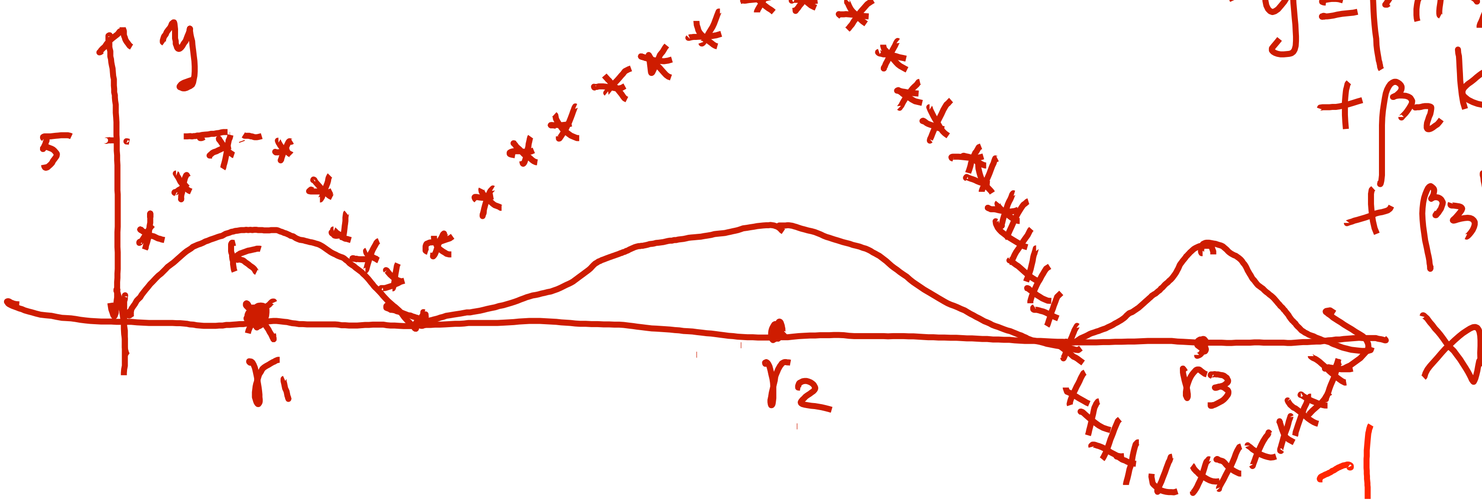
$$K_\lambda(x,r) = \exp\left(-\frac{(x-r)^2}{2\lambda^2}\right)$$

X =	$K_\lambda(x,r) =$
r	1
$r+\lambda$	0.6065307
$r+2\lambda$	0.1353353
$r+3\lambda$	0.0001234098

e.g. another Linear regression with 1D RBF basis functions (assuming 3 predefined centres and width)

$$\varphi(x) := \left[1, K_{\lambda_1}(x, r_1), K_{\lambda 2}(x, r_2), K_{\lambda_3}(x, r_3)\right]^T$$

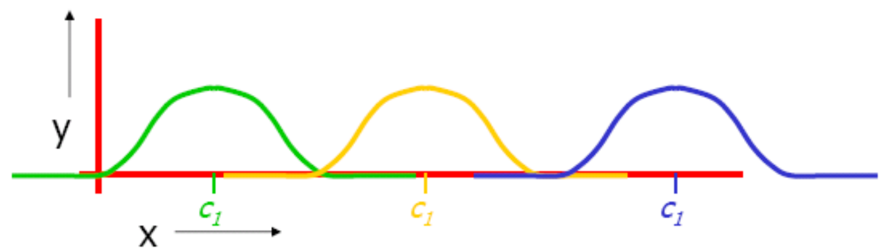
$$\theta^* = \left(\varphi^T \varphi\right)^{-1} \varphi^T \vec{y}$$



$y = \beta_1 K_{\lambda_1}(x, r_1) + \beta_2 K_{\lambda_2}(x, r_2) + \beta_3 K_{\lambda_3}(x, r_3)$

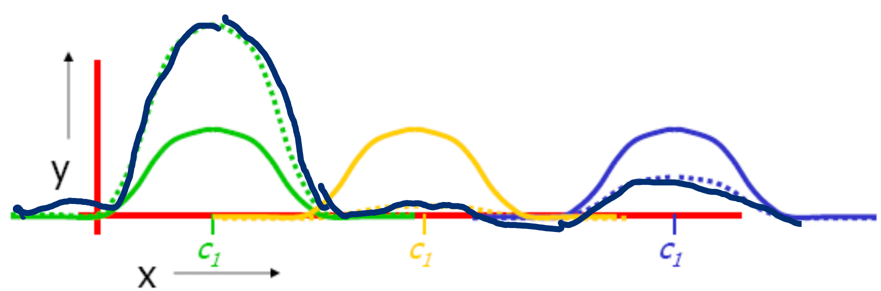
e.g. a LR with 1D RBFs (3 predefined centres and width)

- 1D RBF



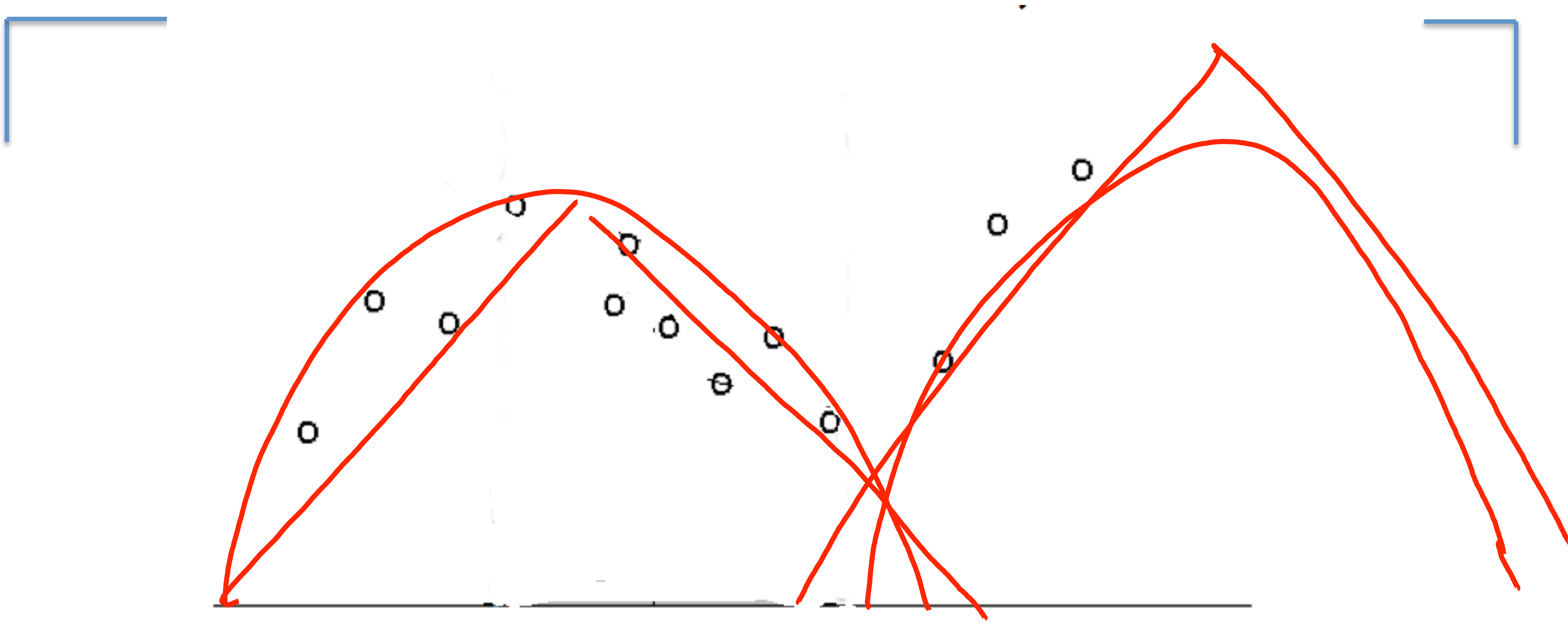
$$y^{est} = \beta_1 \phi_1(x) + \beta_2 \phi_2(x) + \beta_3 \phi_3(x)$$

- After fit:



$$y^{est} = 2\phi_1(x) + 0.05\phi_2(x) + 0.5\phi_3(x)$$

e.g. Even more possible Basis Func?



Two main issues:

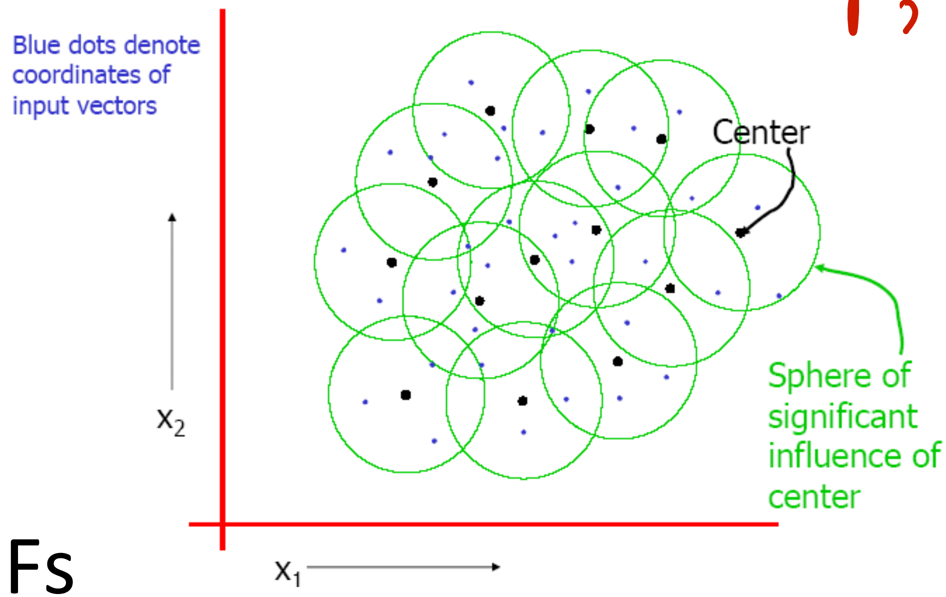
- To Learn the parameter θ^*
  - Almost the same as LR, just ➔ X to $\varphi(x)$
  - Linear combination of basis functions (that can be non-linear)

- How to choose the model order,
  - E.g. what polynomial degree for polynomial regression
  - E.g., where to put the centers for the RBF kernels? How wide?

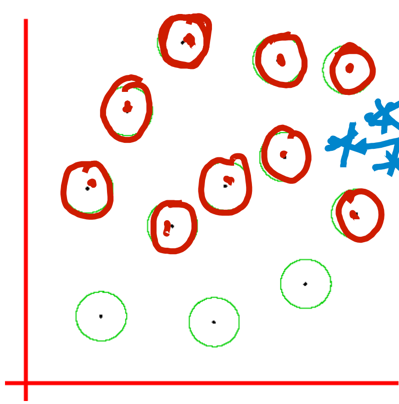
e.g. 2D Good and Bad RBF Basis

γ, λ

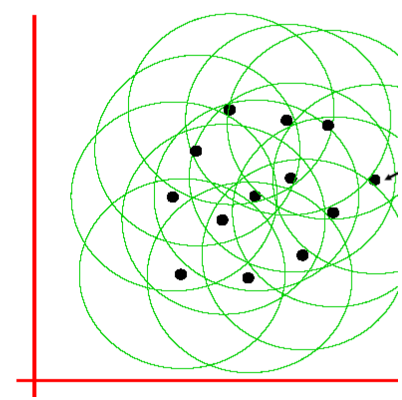
- A good 2D RBF



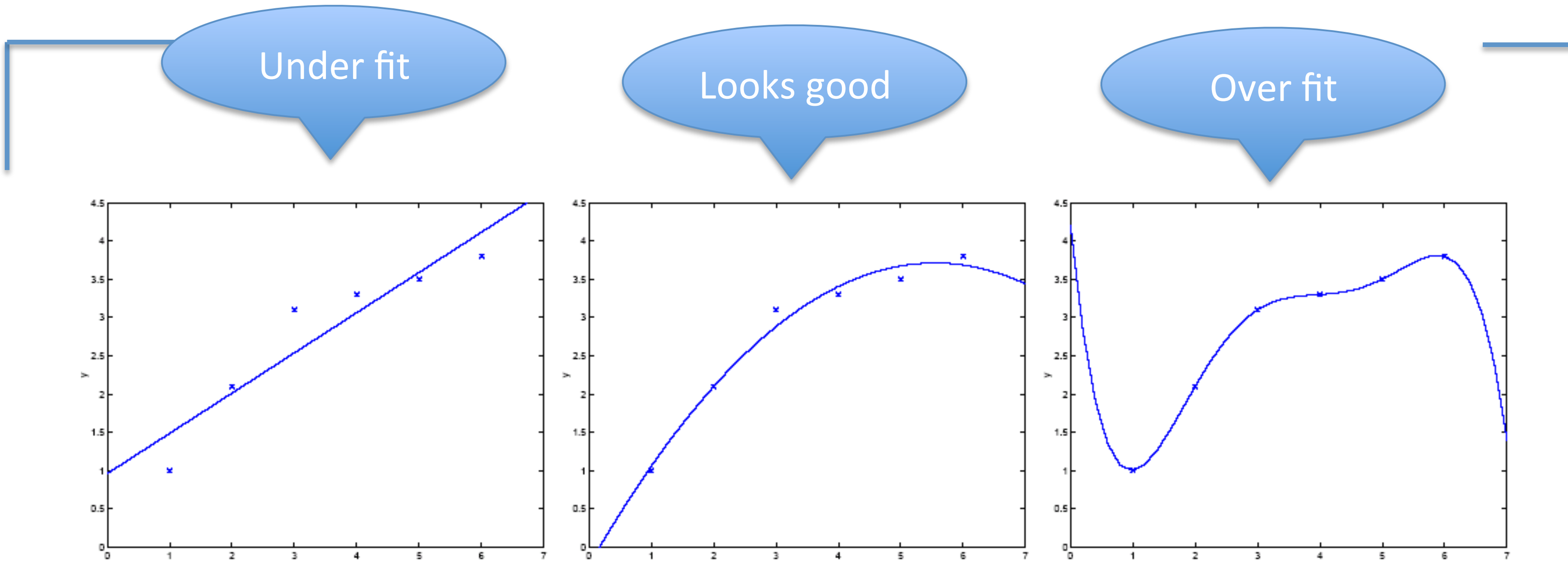
- Two bad 2D RBFs



no Basis can cover these points



Issue: Overfitting and underfitting



$$y = \theta_0 + \theta_1 x \qquad y = \theta_0 + \theta_1 x + \theta_2 x^2 \qquad y = \sum_{j=0}^{5} \theta_j x^j$$

Generalisation: learn function / hypothesis from past data in order to "explain", "predict", "model" or "control" new data examples

K-fold Cross Validation !!!!

(2) Multivariate Linear Regression with basis Expansion

Task → Representation → Score Function → Search/Optimization → Models, Parameters

Regression → Y = Weighted linear sum of (X basis expansion) → SSE → Linear algebra /GD /SGD → Regression coefficients

$$\hat{y} = \theta_0 + \sum_{j=1}^{m} \theta_j \varphi_j(x) = \varphi(x)^T \theta$$

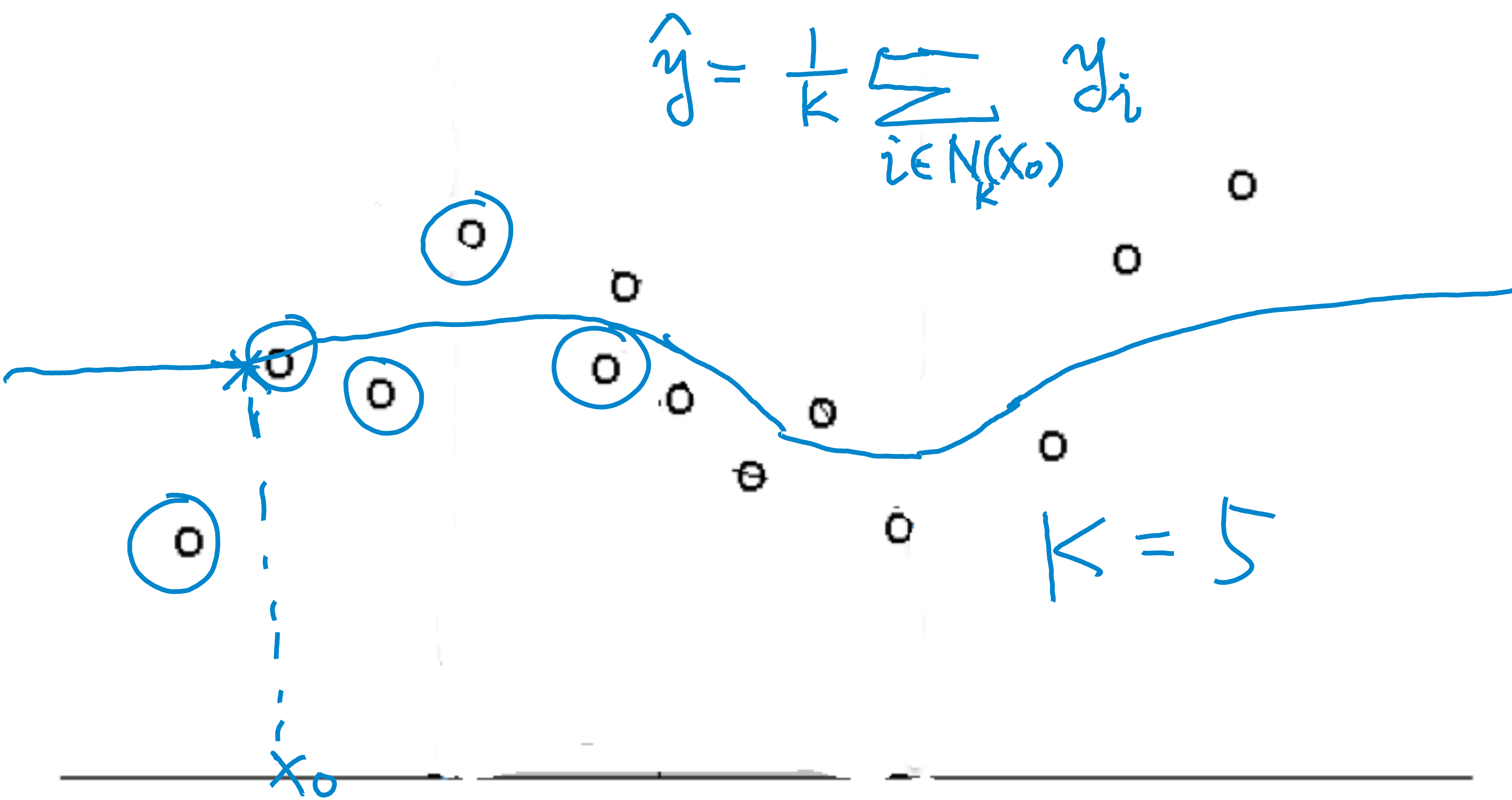
Today

- ❑ Regression Models Beyond Linear
  - – LR with non-linear basis functions
  - – Instance-based Regression: K-Nearest Neighbors
  - – Locally weighted linear regression
  - – Regression trees and Multilinear Interpolation (later)

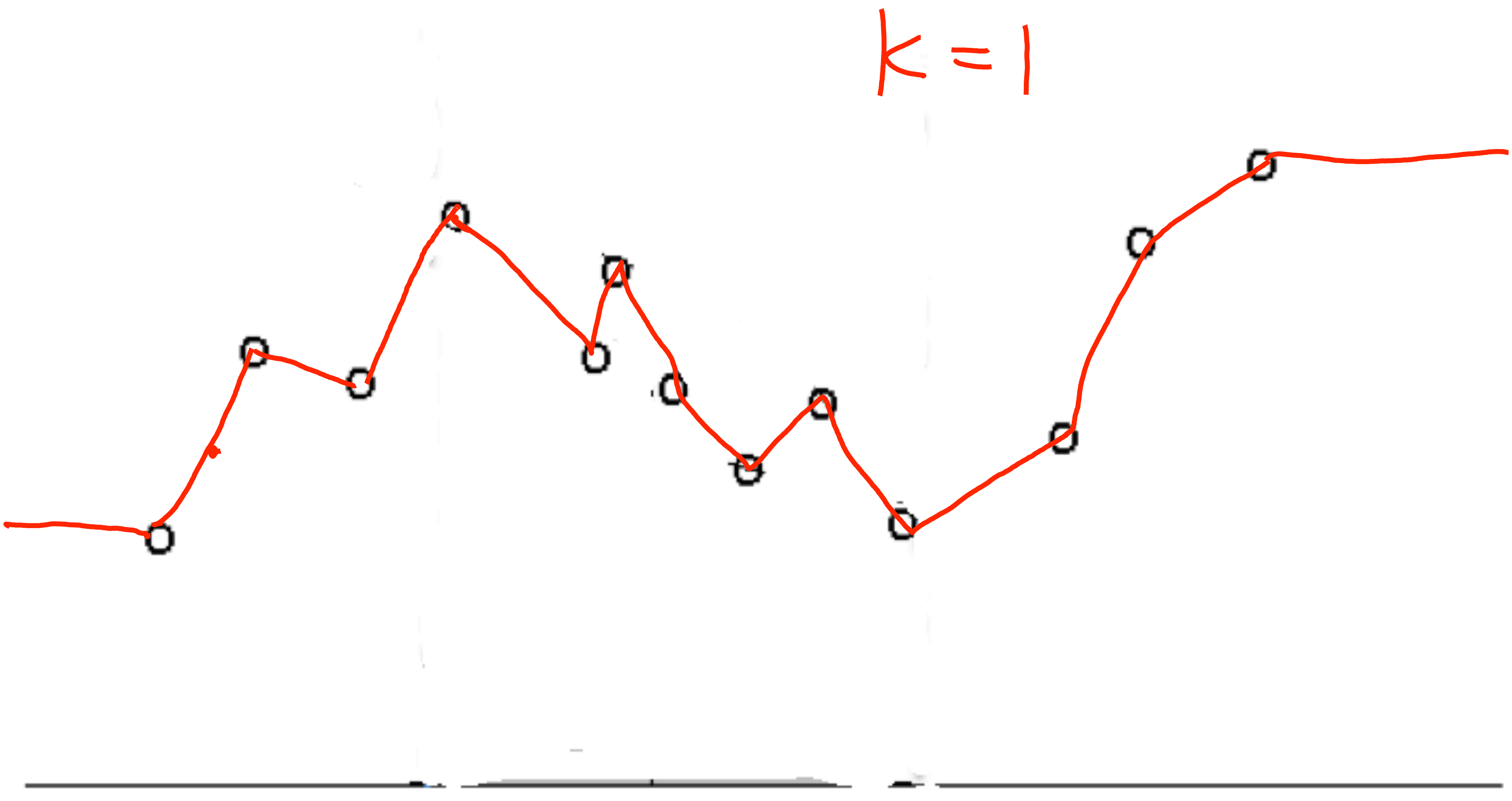
K-Nearest Neighbor

- Features
  - All instances correspond to points in an p-dimensional Euclidean space
  - Regression is delayed till a new instance arrives
  - Regression is done by comparing feature vectors of the different points
  - Target function may be discrete or real-valued
    - When target is continuous, the prediction is the mean value of the k nearest training examples

K=5-Nearest Neighbor (1D input)



K=1-Nearest Neighbor (1D input)



K-Nearest Neighbor

Task	Regression/ classification
Representation	Local Smoothness
Score Function	NA
Search/Optimization	NA
Models, Parameters	Training Samples

Variants: Distance-Weighted k-Nearest Neighbor Algorithm

- Assign weights to the neighbors based on their "distance" from the query point
  - Weight "may" be inverse square of the distances

- All training points may influence a particular instance
  - E.g., Shepard's method/ Modified Shepard, … by Geospatial Analysis

e.g. $\hat{y} = \frac{1}{K} \sum_{i \in N_k(x_0)} W_i y_i$

$W_i \rightarrow$ RBF

$K_\lambda(x_i, x_0)$

Instance-based Regression vs. Linear Regression

- Linear Regression Learning
  - Explicit description of target function on the whole training set

- Instance-based Learning
  - Learning=storing all training instances
  - Referred to as "Lazy" learning

Today

- Regression Models Beyond Linear
  - LR with non-linear basis functions
  - Instance-based Regression: K-Nearest Neighbors
  - Locally weighted linear regression
  - Regression trees and Multilinear Interpolation (later)

Locally weighted regression

- *aka* locally weighted regression, local linear regression, LOESS, …
  - A combination of kNN and Linear regression

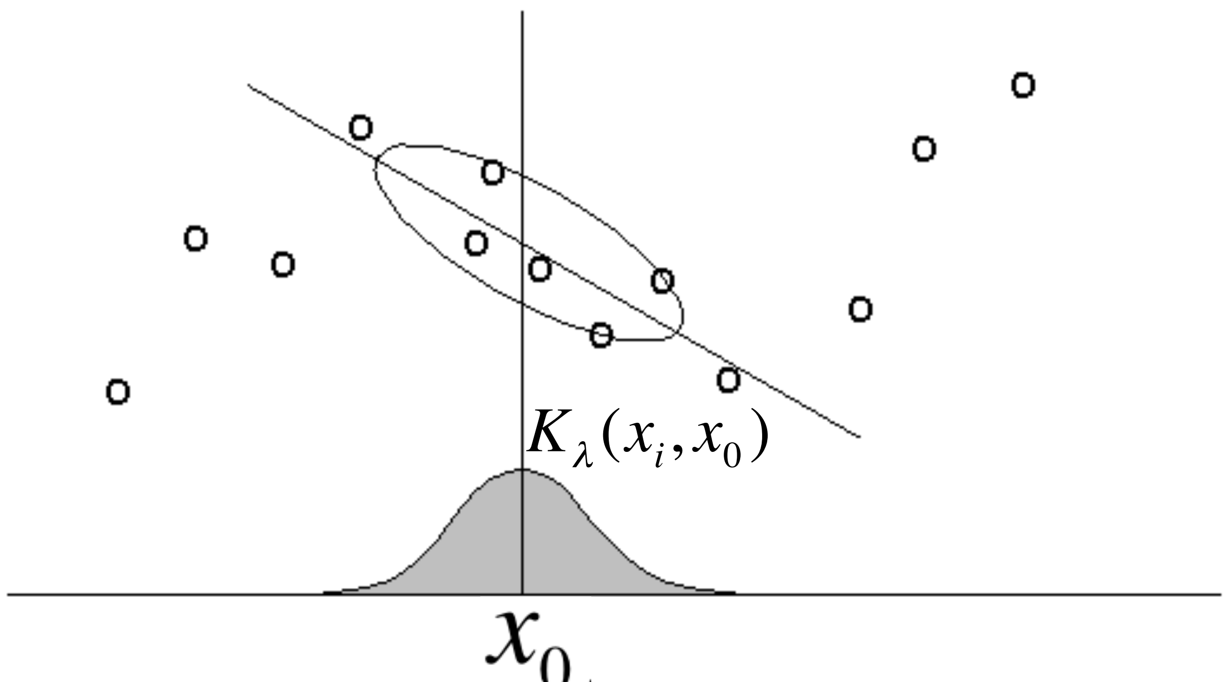


Figure 2: In locally weighted regression, points are weighted by proximity to the current **x** in question using a kernel. A regression is then computed using the weighted points.

Locally weighted regression

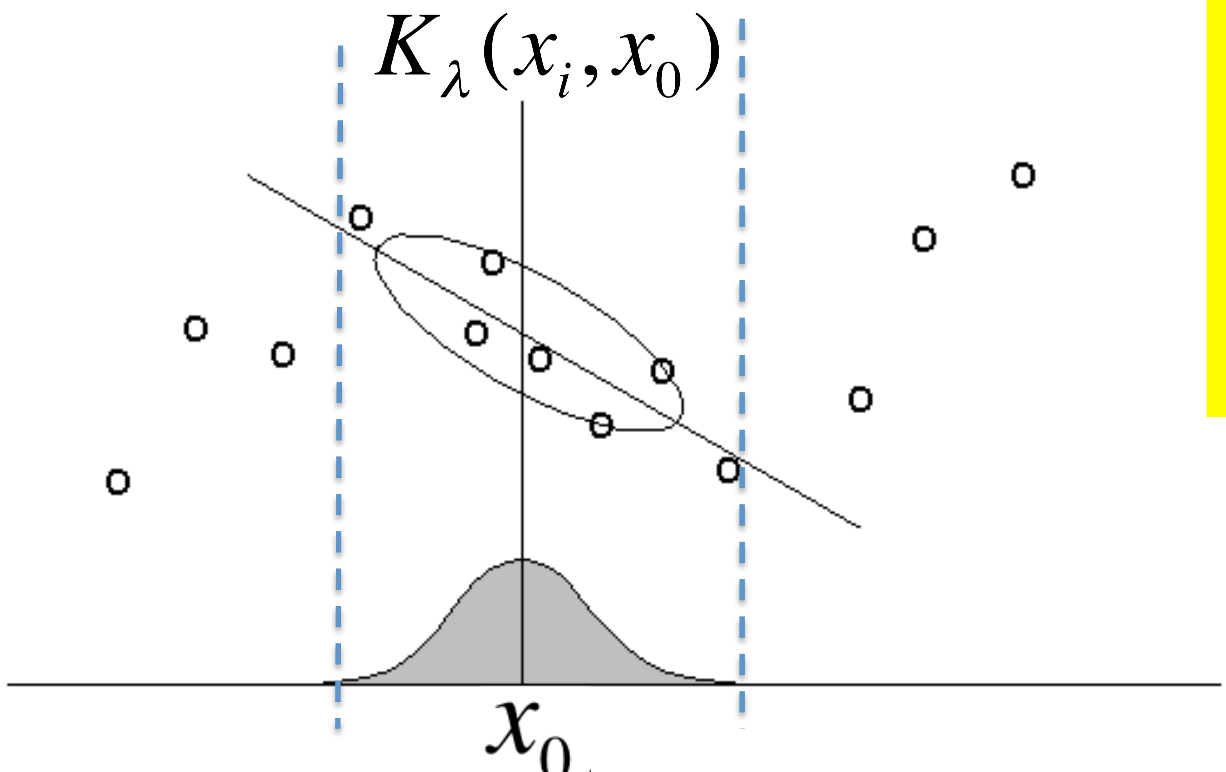
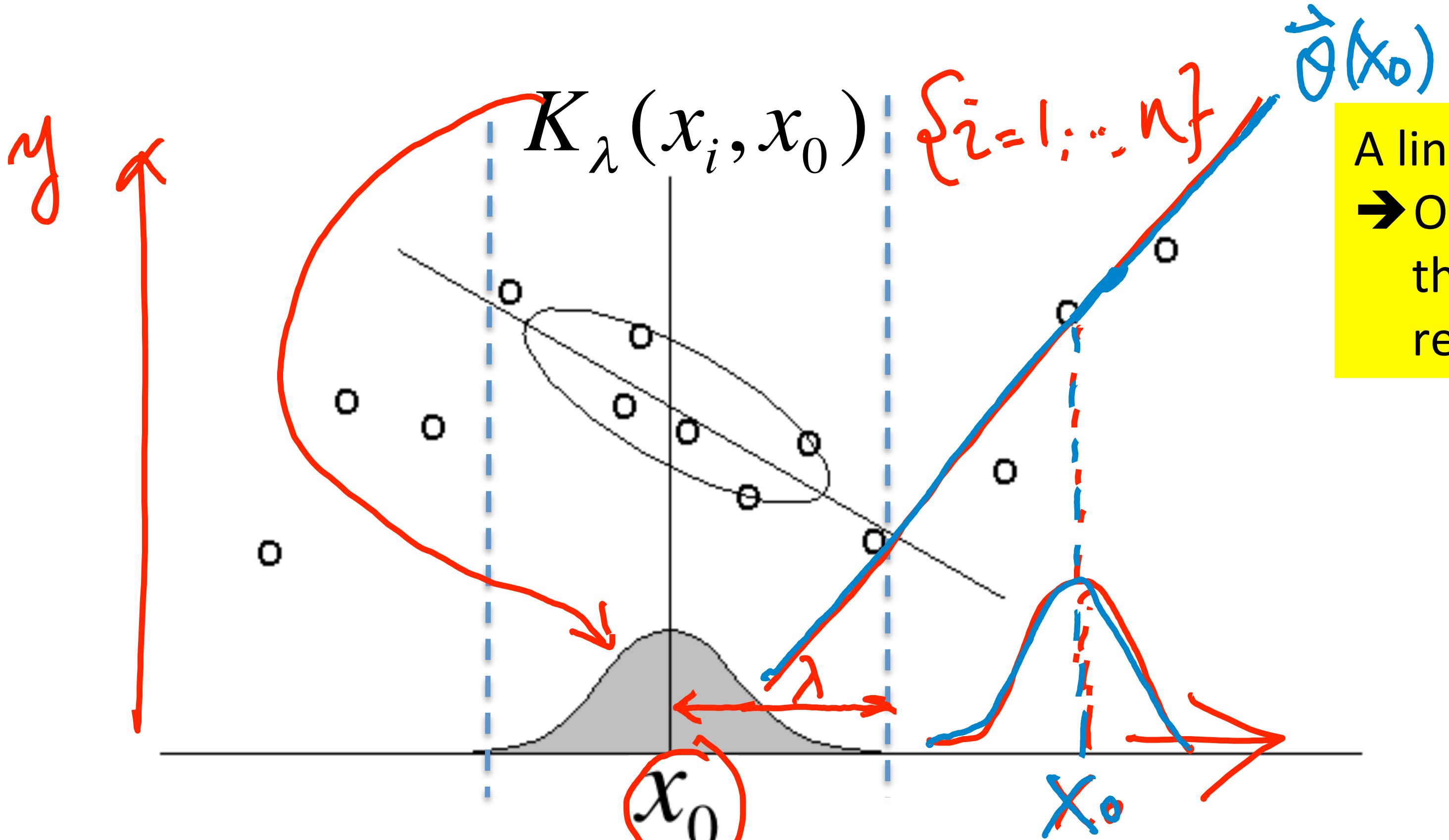


Figure 2: In locally weighted regression, points are weighted by proximity to the current **x** in question using a kernel. A regression is then computed using the weighted points.

Use RBF function to pick out/emphasize the neighbor region of x_0
➔ $K_\lambda(x_i, x_0)$

Locally weighted regression

$$\hat{f}(x_0) = \widehat{\theta_0}(x_0) + \widehat{\theta_1}(x_0)x_0$$



A linear_func(x)->y
➔ Only to represent the neighbor region of x_0

Figure 2: In locally weighted regression, points are weighted by proximity to the current **x** in question using a kernel. A regression is then computed using the weighted points.

Locally weighted linear regression

Instead of minimizing

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{n}(\mathbf{x}_i^T\theta - y_i)^2$$

SSE

↓

now we fit to minimize

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{n} w_i(\mathbf{x}_i^T\theta - y_i)^2$$

WSSE

$$w_i = K_\lambda(\mathbf{x}_i, \mathbf{x}_0) = \exp\left(-\frac{(\mathbf{x}_i - \mathbf{x}_0)^2}{2\lambda^2}\right)$$

where $\mathbf{x\_0}$ is the query point for which we'd like to know its corresponding $\mathbf{y}$

Locally weighted linear regression

We fit \theta to minimize $$J(\theta) = \frac{1}{2}\sum_{i=1}^{n} w_i(\mathbf{x}_i^T\theta - y_i)^2$$

w_i comes from:

$$w_i = K_\lambda(\mathbf{x}_i, \mathbf{x}_0) = \exp\left(-\frac{(\mathbf{x}_i - \mathbf{x}_0)^2}{2\lambda^2}\right)$$

- **x_0** is the query point for which we'd like to know its corresponding **y**

Essentially we put higher weights on training examples that are close to the query point x_0 (than those that are further away from the query point x_0)

Locally weighted linear regression

- The width of RBF matters !

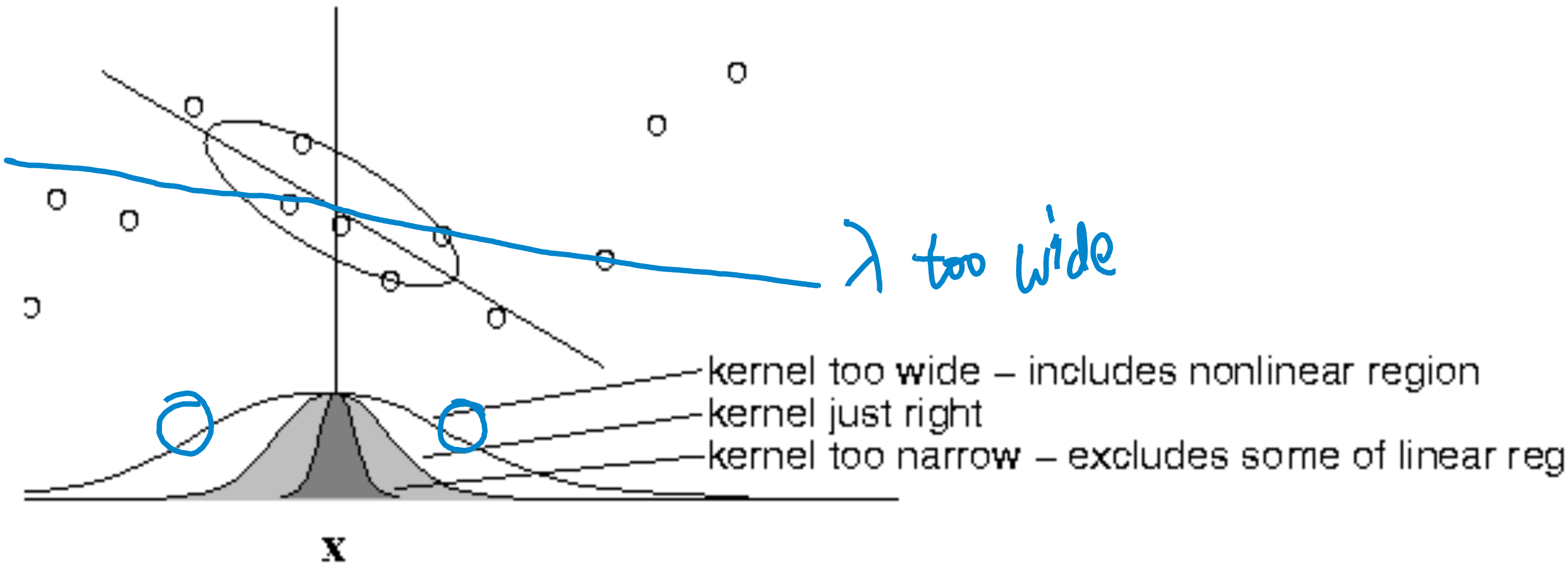
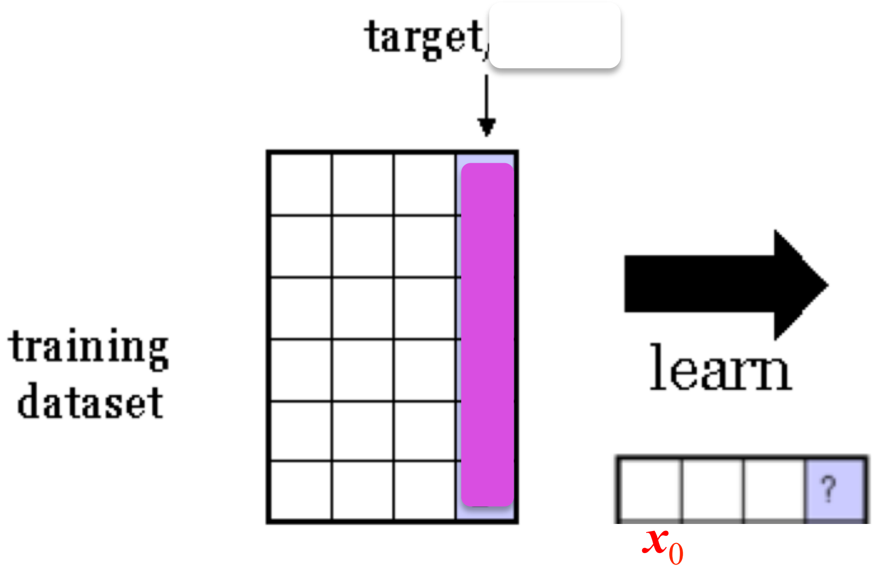


Figure 3: The estimator variance is minimized when the kernel includes as many training points as can be accommodated by the model. Here the linear LOESS model is shown. Too large a kernel includes points that degrade the fit; too small a kernel neglects points that increase confidence in the fit.

LEARNING of Locally weighted linear regression



$$\hat{f}(x_0) = \widehat{\theta_0}(x_0) + \widehat{\theta_1}(x_0)x_0$$

- Separate weighted least squares training and inference **at each target point x_0**

Locally weighted linear regression

- ➔Separate weighted least square error minimization **at each target point x_0:**

$$\theta^*(\mathbf{x}_0) = \arg\min \frac{1}{2}\sum_{i=1}^{n} w_i (\mathbf{x}_i^T \theta(\mathbf{x}_0) - y_i)^2$$

$$= \arg\min \frac{1}{2}\sum_{i=1}^{n} K_\lambda(x_i, x_0)(\mathbf{x}_i^T \theta(\mathbf{x}_0) - y_i)^2$$

$$\hat{f}(x_0) = \mathbf{x}_0^T \theta^*(\mathbf{x}_0)$$

e.g. $\hat{f}(x_0) =$

$$\hat{f}(x_0) = \hat{\alpha}(x_0) + \hat{\beta}(x_0) x_0$$

Extra: Solution of Locally weighted linear/NonLinearBasis regression

$$W_{N\times N}(x_0) = diag\left(K_\lambda(x_0, x_i)\right), i = 1, \ldots, N$$

Locally weighted LR : $(X^T W_{x_0} X)^{-1} X^T W_{x_0} \vec{y}$

LWR $\theta^*(\mathbf{x}_0) = (B^T W(x_0) B)^{-1} B^T W(x_0) y$

Locally weighted e.g. Polynomial Regression $X \to B$

versus

LR $\theta^* = \left(X^T X\right)^{-1} X^T \vec{y}$

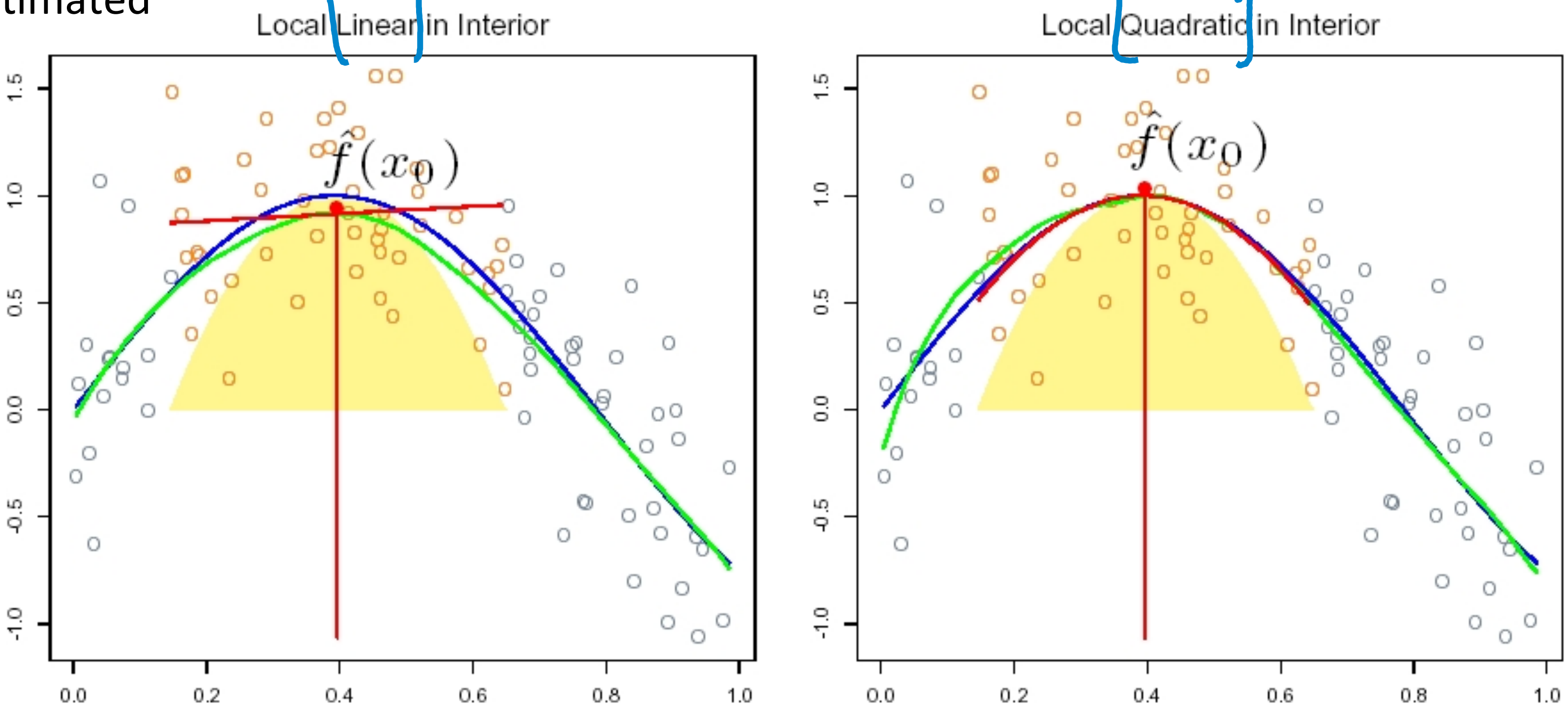
More ➔ Local Weighted Polynomial Regression

- Local polynomial fits of any degree d

$$\min_{\alpha(x_0),\beta_j(x_0),j=1,\dots,d} \sum_{i=1}^{N} K_\lambda(x_0,x_i)\left[y_i-\alpha(x_0)-\sum_{j=1}^{d}\beta_j(x_0)x_i^j\right]^2$$

$$\hat{f}(x_0)=\hat{\alpha}(x_0)+\sum_{j=1}^{d}\hat{\beta}_j(x_0)x_0^j$$

Blue: true
Green: estimated



Extra: Parametric vs. non-parametric

- Locally weighted linear regression is a **non-parametric** algorithm.

$f(x_i) = x_?^T \theta^*$

- The (unweighted) linear regression algorithm that we saw earlier is known as a **parametric** learning algorithm
  - because it has a fixed, finite number of parameters (the θ^*), which are fit to the data;
  - Once we've fit the *theta* and stored them away, we no longer need to keep the training data around to make future predictions.
  - In contrast, to make predictions using locally weighted linear regression, we need to keep the entire training set around.
- The term "non-parametric" (roughly) refers to the fact that the amount of knowledge we need to keep, in order to represent the hypothesis grows with linearly the size of the training set.

$f(x_?) = x_?^T \theta^*(x_?)$

(3) Locally Weighted / Kernel Linear Regression

Task → Representation → Score Function → Search/Optimization → Models, Parameters

Regression → Y = Weighted linear sum of X' s → Weighted SSE → Linear algebra → Local Regression coefficients (conditioned on each test point)

$$\boxed{\theta^*(\mathbf{x}_0) = (B^T W(x_0) B)^{-1} B^T W(x_0) y}$$

$$\min_{\alpha(x_0),\beta(x_0)} \sum_{i=1}^{N} K_\lambda(x_0, x_i)[y_i - \alpha(x_0) - \beta(x_0)x_i]^2$$

$$\hat{f}(x_0) = \hat{\alpha}(x_0) + \hat{\beta}(x_0)x_0$$

Today Recap

- Regression Models Beyond Linear
  - LR with non-linear basis functions
  - Instance-based Regression: K-Nearest Neighbors
  - Locally weighted linear regression
  - Regression trees and Multilinear Interpolation (later)

References

- Big thanks to Prof. Eric Xing @ CMU for allowing me to reuse some of his slides
- ❑ Prof. Nando de Freitas's tutorial slide