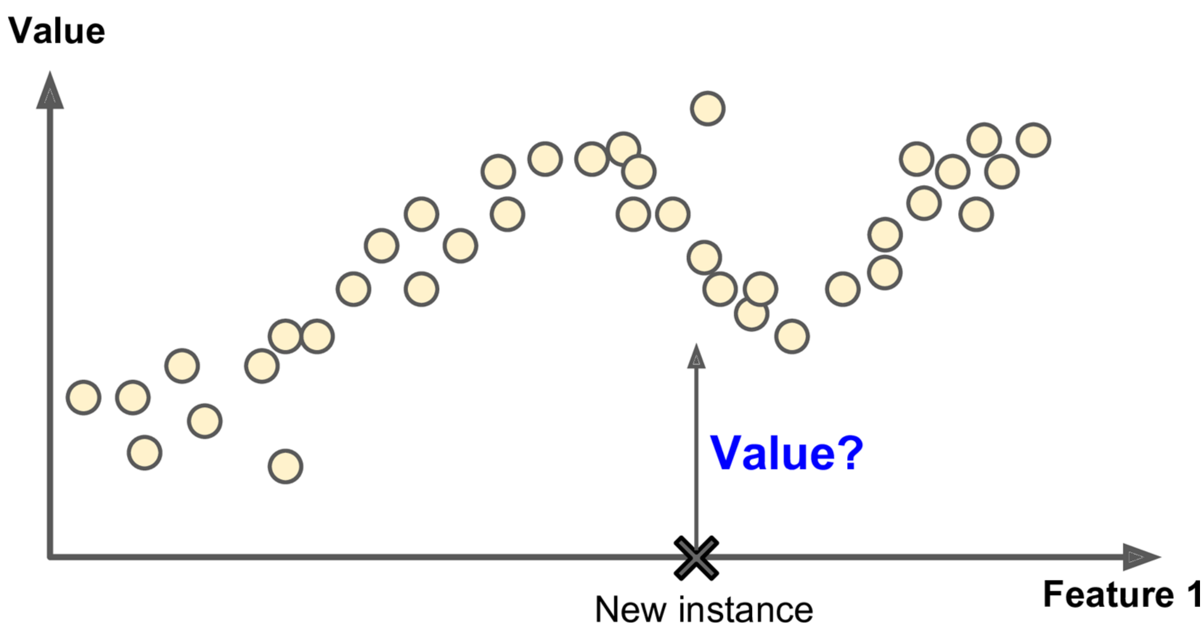
CSI 436/536
Introduction to Machine Learning

Regression and LLSE

Professor Siwei Lyu
Computer Science
University at Albany, State University of New York

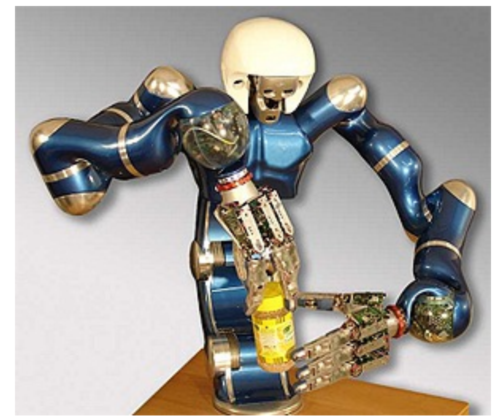
Regression problem

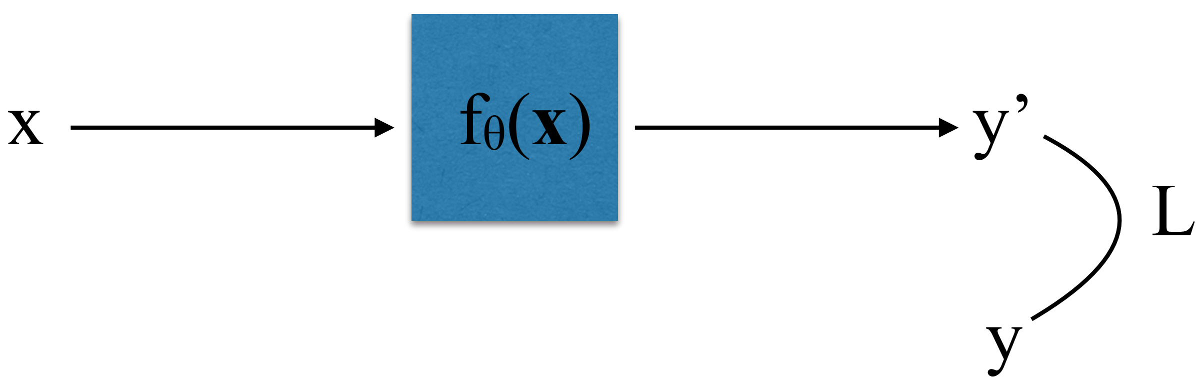
- Use input to estimate a target variable that takes continuous values
- It is an example of **supervised machine learning** problem: in training, the target variables together with the inputs are given
  - In testing, we only have input and need to estimate the target



Regression problem

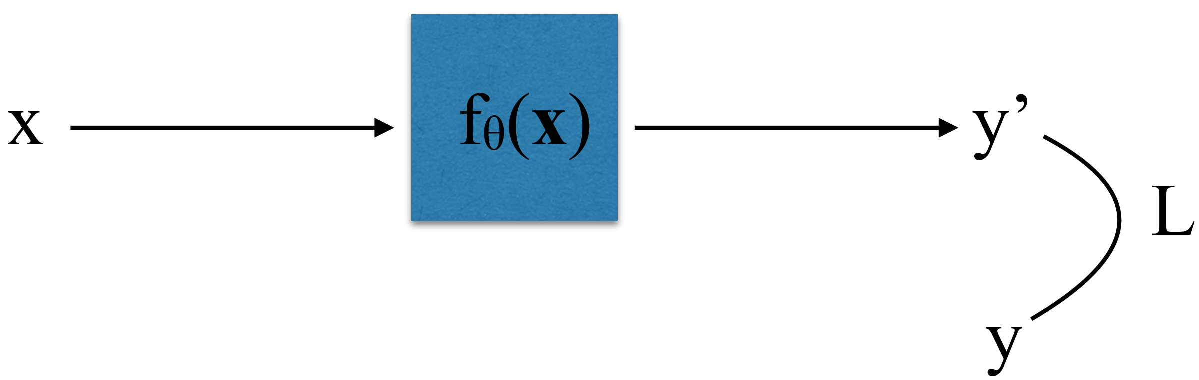
- robotic control/automatic driving
  - input: internal parameters of robotic arm (force at angle)
  - output: end effector location
  - treat input-output as going through a black box transform
  - use training data to figure out best control function





Regression problem

- High-frequency stock trading (algorithmic trading)
  - input: historic stock prices & trading records
  - output: new trading action
  - treat input-output as going through a black box transform
  - use training data to figure out best control function



Notations

- Data matrix can include processed data, i.e., g is a function on raw x
$$X = \begin{pmatrix} | & | & & | \\ g(x_1) & g(x_2) & \cdots & g(x_N) \\ | & | & & | \end{pmatrix}$$
- Mean and centering
  - introduce N-dim all one vectors 1_N, the (arithmetic) mean of data is computed as $m = \frac{1}{N} X 1_N$
  - The (column) centering operation is expressed as
  $$\tilde{X} = X - m1_N^T = X - \frac{1}{N} X 1_N 1_N^T = X\left(I - \frac{1}{N} 1_N 1_N^T\right)$$
  the final matrix is the column centering operation
- ***Correlation*** and ***covariance*** matrices are defined as XX^T and $\tilde{X}\tilde{X}^T$, respectively

Kernel matrix

- Definition: $G = X^T X \succeq 0$, $G_{ij} = x_i^T x_j$, element is the pairwise inner product of two points
  - This matrix is known as the inner product matrix, the Gram matrix, or the ***kernel*** matrix
  - It is in a sense the ***dual*** of the correlation matrix XX^T, when X is full ranked, then at least one of them is invertible
  - Kernel matrix plays a central role in the subsequent nonlinear extension of linear machine learning algorithms

General regression

- Training
  - Training data matrix
    data points are column vectors
    $$X = \begin{pmatrix} | & | & & | \\ x_1 & x_2 & \cdots & x_N \\ | & | & & | \end{pmatrix}$$
  - Training targets, assuming scalar
    $$y = (y_1, y_2, \cdots, y_N)^T$$
  - parametric function $f_w(\,\cdot\,) : R^d \mapsto R$
  - **loss function** $L(y - f_w(x)) \geq 0$
  - Numerical procedure to find optimal w to minimize
    the learning objective $\sum_{i=1}^{n} L(y_i - f_w(x_i))$
- In testing, for input x and generate prediction $f_w(x)$
  - **metric function** $m(y - f_w(x)) \geq 0$ on a validation
    dataset, may be different from the loss

Linear least squares regression

- Training
  - Training data matrix
    data points are column vectors
  - Training targets, assuming scalar
  - **Linear** function $f_w(x) = w^T \phi(x)$
  - **Least squares loss function**
    $L(y, f_w(x)) = \|y - f_w(x)\|^2$
  - Optimal solution to the learning objective
    $\sum_{i=1}^{n} L(y_i - f_w(x_i))$ satisfies the normal equation

$$X = \begin{pmatrix} | & | & & | \\ x_1 & x_2 & \cdots & x_N \\ | & | & & | \end{pmatrix}$$

$$y = (y_1, y_2, \cdots, y_N)^T$$

- Testing
  - Metric function is also the least squares loss

LLSE: the Swiss army knife in ML

- Learning tasks
  - Supervised learning
    - Regression: basic LLSE and weighted LLSE
    - Classification: discriminative LLSE
  - Unsupervised learning
    - Clustering: multi-modal LLSE
    - Dimension reduction: total LLSE
- Learning paradigms
  - Batch learning: all other LLSE methods
  - Online learning: recursive LLSE
  - Dynamic programming: segmented LLSE
- Control of overfitting
  - Model selection: model selection LLSE
  - cross-validation: LOO LLSE
  - Regularization: ridge LLSE & LASSO

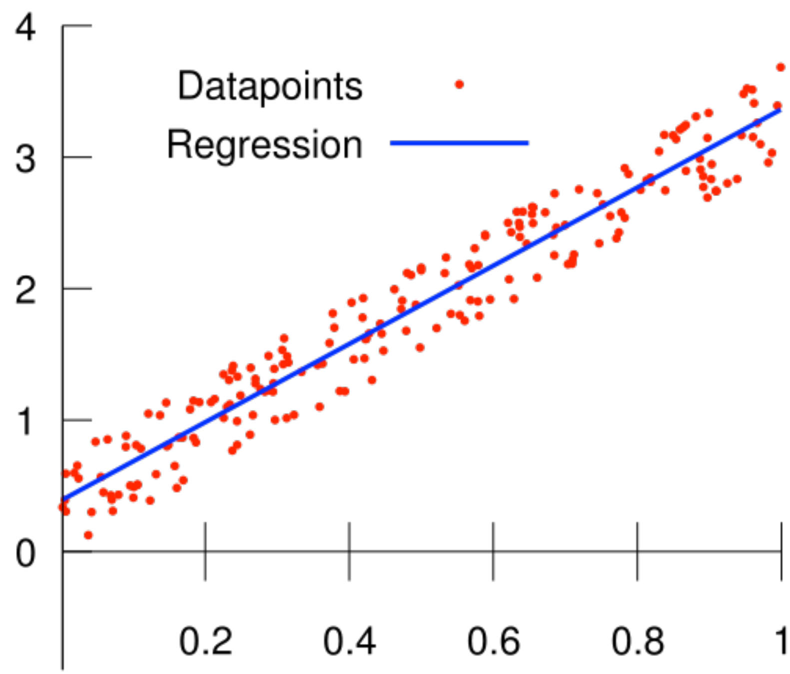
LLSE — linear function

- finding linear relation between input/output

$$f(x) = ax + b$$

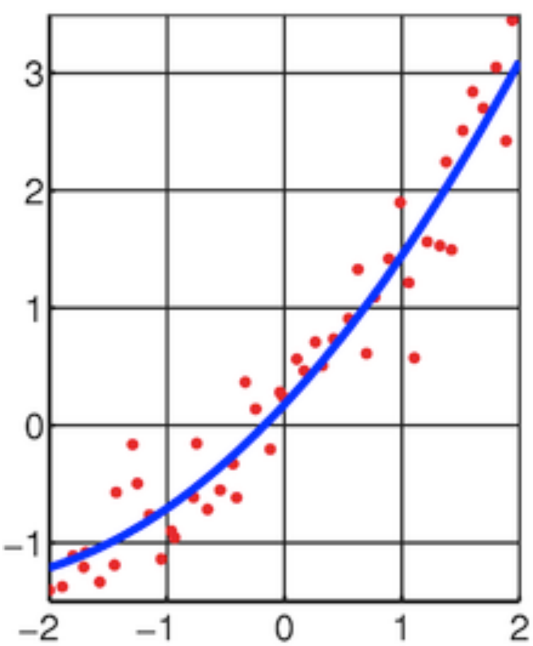
- solving an optimization problem

$$\min_{w=(a,b)^T} \sum_{i=1}^{N} (y_i - ax_i - b)^2$$



LLSE — quadratic function

- finding quadratic relation between input/output
$$f(x) = ax^2 + bx + c$$
- solving an optimization problem
$$\min_{w=(a,b,c)^T} \sum_{i=1}^{N} (y_i - ax_i^2 - bx_i^2 - c)^2$$



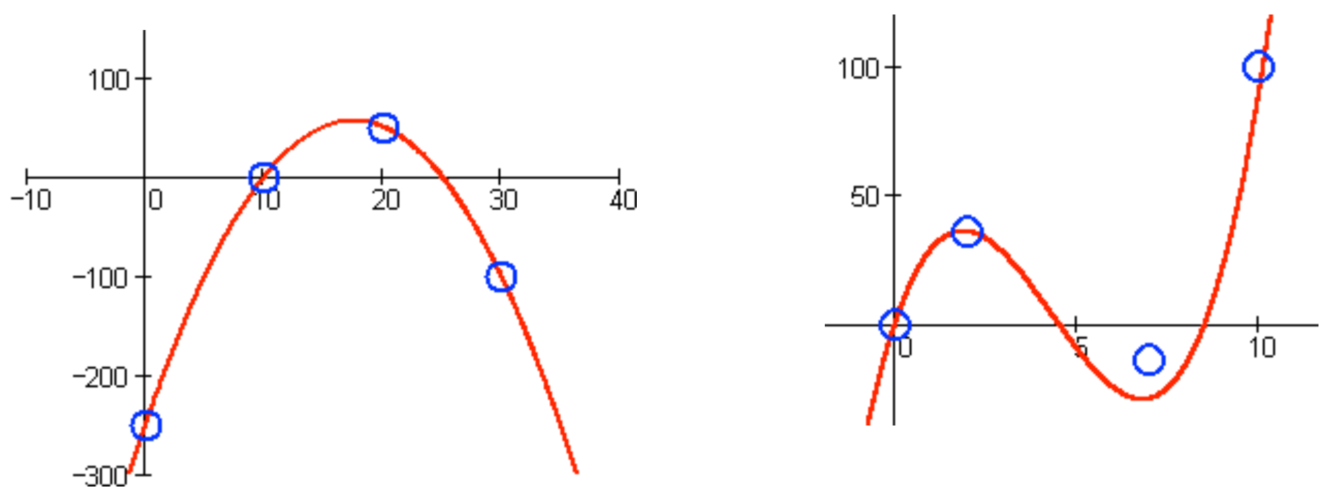
LLSE — polynomial function

- find d-degree polynomial

$$f(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_d x^d$$

as

$$\min_{w=(a_0,\cdots,a_d)^T} \sum_{i=1}^{N} (y_i - f(x_i))^2$$



LLSE — arbitrary basis functions

- find linear combinations of basis functions
  $f(x) = a_0 + a_1 g_1(x) + a_2 g_2(x) + \cdots + a_d g_d(x)$
  to $\min_{w=(a_0,\cdots,a_d)^T} \sum_{i=1}^{N} (y_i - f(x_i))^2$

  - monomials: $g_i(x) = x^i$ (polynomial fitting)
  - Chebychev (orthogonal) polynomials
  - Hermite polynomials: $g_i(x) = e^{x^2} \dfrac{d^i e^{-x^2}}{dx^i}$
  - complex exponentials (Fourier transform):
    $g_i(x) = e^{-\imath i x}$
  - radial basis functions (RBFs): $g_i(x) = e^{-a_i (x - b_i)^2}$

LLSE — general case

- Define the general problem as fitting $\sum_{i=1}^{m} a_i g_i(x_j)$ to target y by minimizing $\sum_{j=1}^{n} (y_j - \sum_{i=1}^{m} a_i g_i(x_j))^2$
- Rewrite using linear algebra notations

$$y = \begin{pmatrix} y_1 \\ y_2 \\ \cdots \\ y_N \end{pmatrix}, w = \begin{pmatrix} a_1 \\ a_2 \\ \cdots \\ a_m \end{pmatrix}, \text{objective is } \min_w \|y - X^T w\|^2 \text{data}$$

$$\text{matrix } X = \begin{pmatrix} g_1(x_1) & g_1(x_2) & \cdots & g_1(x_N) \\ g_2(x_1) & g_2(x_2) & \cdots & g_2(x_N) \\ \vdots & \vdots & \ddots & \vdots \\ g_m(x_1) & g_m(x_2) & \cdots & g_m(x_N) \end{pmatrix}$$

Solving LLSE

- Expand the terms
  $\|y - X^T w\|^2 = y^T y - 2y^T X^T w + w^T X X^T w$
  - Taking derivative on both sides w.r.t. w
    $\nabla_w \|y - X^T w\|^2 = 2(XX^T w - Xy) = 0$
    - The solution is given by $XX^T w = Xy$, which is known as the **normal equation**
  - Check Hessian matrix $\nabla \nabla_w^T \|y - X^T w\|^2 = 2XX^T \succeq 0$ (why?)
    so the solution is a minimum
- We will assume the data matrix is full ranked (no linearly dependent rows or columns)

Weighted LLSE

- Introducing a weight matrix W, usually diagonal with $W_{ii} \geq 0$, and to solve
$$\min_w (y - X^T w)^T W (y - X^T w)$$
- This is known as weighted LLSE
  - When W = I, WLLSE reduces to LLSE

$$(y - X^T w)^T W (y - X^T w) = \sum_{i=1}^{n} W_{ii} \left(y_i - \sum_{j=1}^{m} a_j g_j(x_i) \right)^2$$

- Solution
$\nabla_w (y - X^T w)^T W (y - X^T w) = 2(XWX^T w - XWy) = 0$
so $XWX^T w = XWy \Rightarrow w = (XWX^T)^{-1} XWy$

Weighted LLSE

- How to determine the weight
  - Larger weight => error has to be small
  - Smaller weight => more relaxed error
- Relation with the variance of the error
  - $W_{ii} = \dfrac{1}{\sigma_i^2}$, where σ_i^2 is the variance of the error in the corresponding component
  - Larger variance => less reliable estimation => smaller weight => more relaxed error
  - smaller variance => more reliable estimation => larger weight => error has to be small

Solving normal equation

- case 1: complete problem
  $N = m$, i.e., # of data = # of parameters
  $\Rightarrow$ matrix X is square
  $\Rightarrow$ correlation matrix XX^T, X and X^T are all invertible
- case 2: over-complete problem
  $N > m$, i.e., # of data > # of parameters
  $\Rightarrow$ matrix X is short & fat
  $\Rightarrow$ correlation matrix XX^T is $N \times N$ and invertible
- case 3: under-complete problem
  $N < m$, i.e., # of data < # of parameters
  $\Rightarrow$ matrix X is tall & thin
  $\Rightarrow$ correlation matrix XX^T is $m \times m$ and **not** invertible, but the Gram matrix X^TX is invertible

Complete case

- We can solve directly by matrix inversion
  $XX^T w = Xy \Rightarrow X^T w = y \Rightarrow w = X^{-T} y$
- Prediction error is zero: $y - X^T w = y - X^T X^{-T} y = 0$
  - Direct matrix inversion is usually not a good option
  - Solving Xp = y becomes LDUp = y, then two steps Lx = y (forward elimination), DUp = x (backward elimination)
    - This is known as Gaussian elimination
  - Solution time is O(n^2), and numerically it is very stable (caveat: if the pivots are chosen right)
  - It is numerically stable (only divide by pivot)

over-complete problem

- Correlation matrix XX^T is invertible and positive definite so LLSE objective function has unique global optimal solution, as $XX^T w = Xy \Rightarrow w = (XX^T)^{-1}Xy$
  - interpretation: projection of y in row space of X
  - Prediction is $X^T w = X^T(XX^T)^{-1}Xy$
  - Prediction error is $y - X^T w = y - X^T(XX^T)^{-1}Xy = (I_N - X^T(XX^T)^{-1}X)y$
- $(XX^T)^{-1}X$ is known as the **left Penrose-Moore** pseudo inverse of general matrix X^T, as $(XX^T)^{-1}XX^T = I_N$

under-complete problem

- X is not invertible, X^TX is invertible and p.d.
- Define the right Penrose-Moore pseudo inverse of general matrix X, $X^T(XX^T)^{-1}$, then $w = X^T(XX^T)^{-1}y$ is a solution to the normal equation
- solution is not unique
  - for any vector in the null space of X, $X\mathbf{h} = 0$, $\mathbf{p}+\mathbf{h}$ is also a solution
  - $\mathbf{p}$ is a solution, we have $X(\mathbf{p}+\mathbf{h}) = X\mathbf{p} = \mathbf{y}$
- there are infinite number of solutions that lead to zero least squares error (ill-posed problem)

under-complete problem

- Correlation matrix XX^T is not invertible, but Gram matrix X^TX is invertible and p.d.
- Define the right Penrose-Moore pseudo inverse of general matrix X, $X(X^TX)^{-1}$, then $w = X(X^TX)^{-1}y$ is a solution to the normal equation
- solution is not unique
    - for any vector in the row null space of X, $X^T\mathbf{h} = 0$, $\mathbf{w}+\mathbf{h}$ is also a solution
    - $\mathbf{w}$ is a solution, we have $X^T(\mathbf{w}+\mathbf{h}) = X^Tw = y$
- there are infinite number of solutions that lead to zero least squares error (ill-posed problem)

Solving normal equation

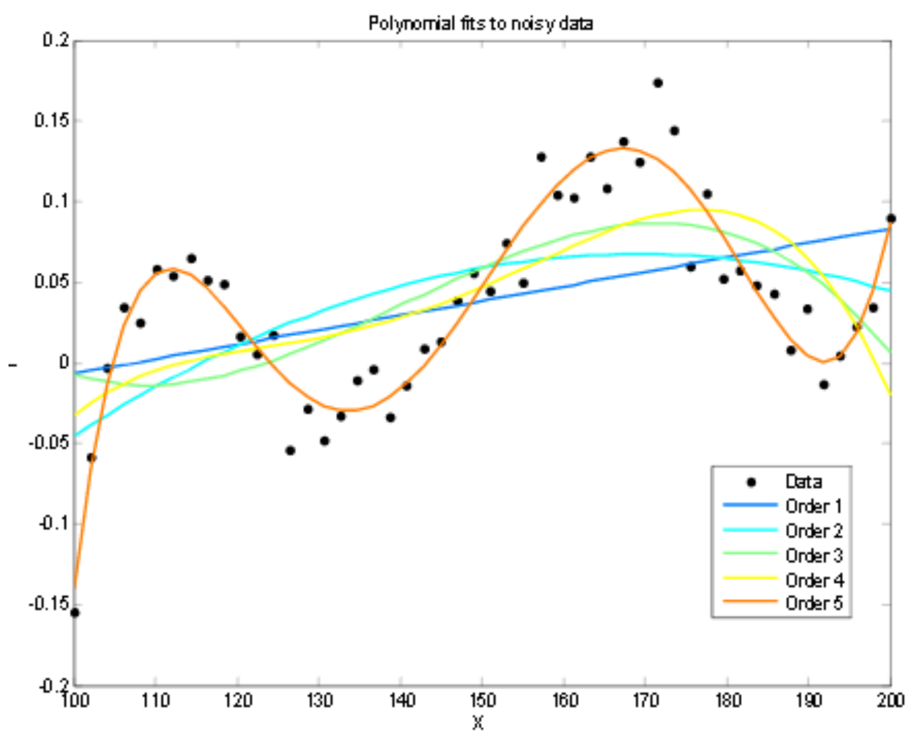
- case 1: complete problem
  $N = m$, i.e., # of data = # of parameters
  $\Rightarrow$ matrix X is square
  $\Rightarrow$ unique solution with zero prediction error

- case 2: over-complete problem
  $N > m$, i.e., # of data > # of parameters
  $\Rightarrow$ matrix X is short & fat
  $\Rightarrow$ unique solution with non-zero prediction error

- case 3: under-complete problem
  $N < m$, i.e., # of data < # of parameters
  $\Rightarrow$ matrix X is tall & thin
  $\Rightarrow$ non-unique solution with zero prediction error

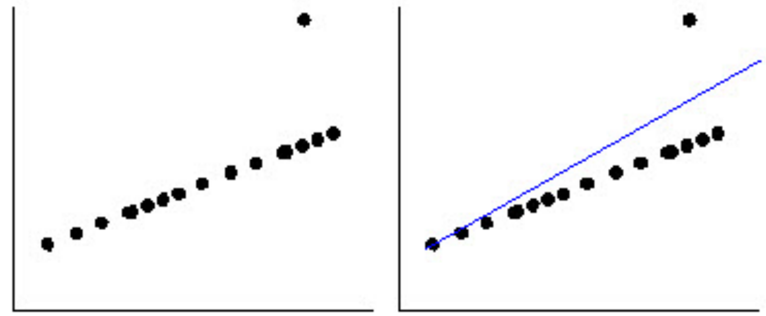
LLSE — general procedure

- Obtain training data X
- Decide number of base functions to use
- Choose a proper weight matrix W
- Form LSE objective function, and solve the normal equation for optimal solution



Issues

- Squared L2 loss is sensitive to outliers in training data
  - Using L1 loss is more robust to outliers in training data



- Data points may not come at the same time, we need to handle the data in an online manner
- Using a high degree of polynomial may overfit the data, how do we control that from occurring
- The number of base functions (degree of polynomials) is a hyper-parameter, how do we select it