UVA CS 6316/4501 – Fall 2016 Machine Learning

Lecture 9: Review of Regression

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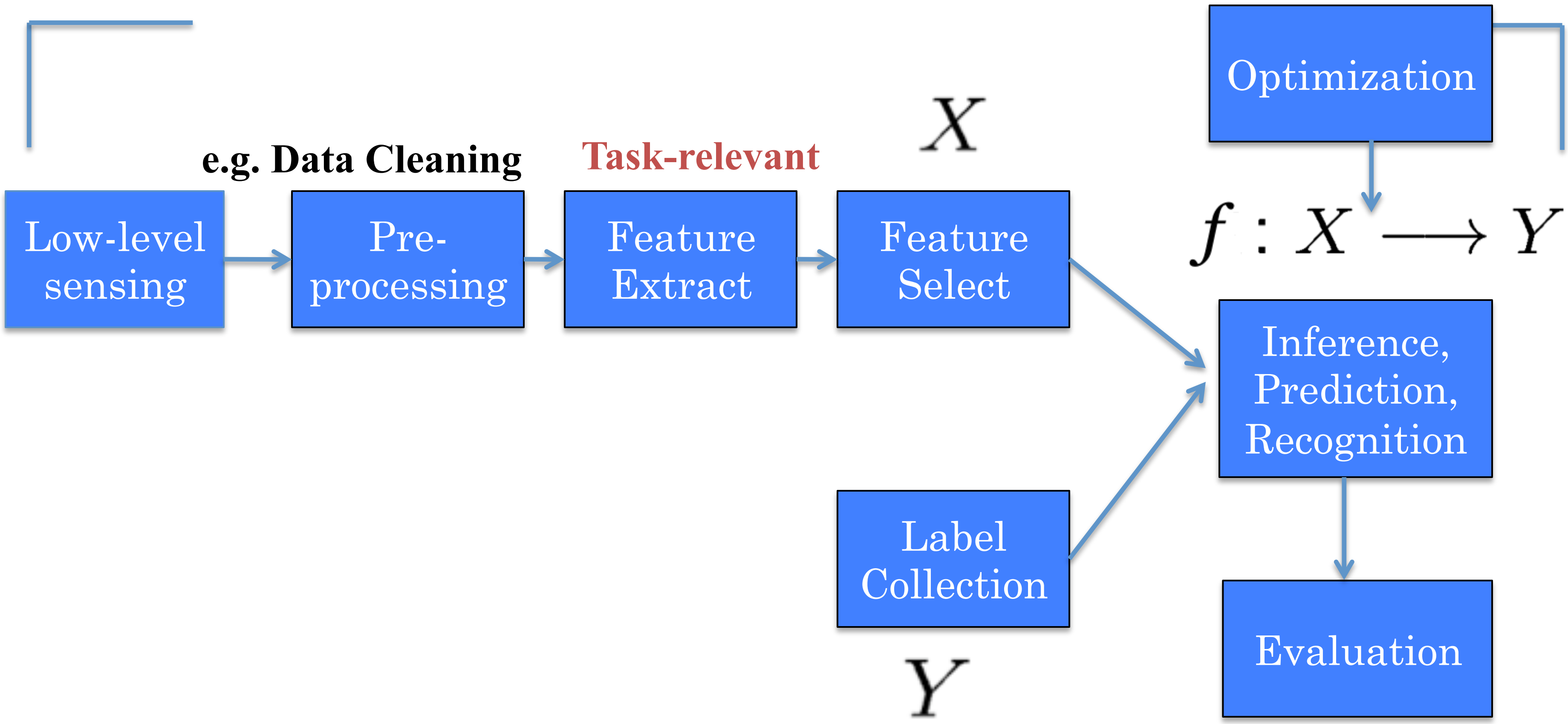
Where are we ? → Five major sections of this course

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

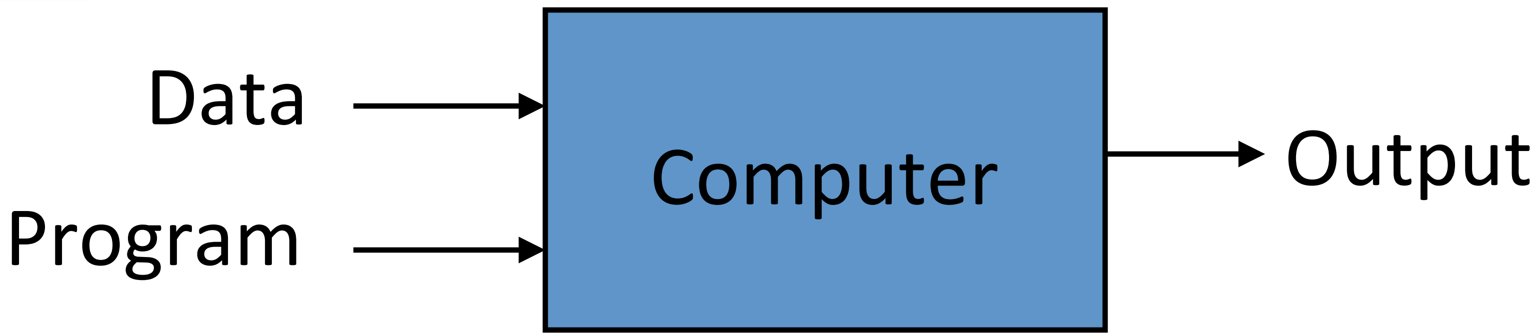
Today

- ❑ Review of basic pipeline
- ❑ Review of regression models
  - Linear regression (LR)
  - LR with non-linear basis functions
  - Locally weighted LR
  - LR with Regularizations
- ❑ Feature Selection
- ❑ Model Selection

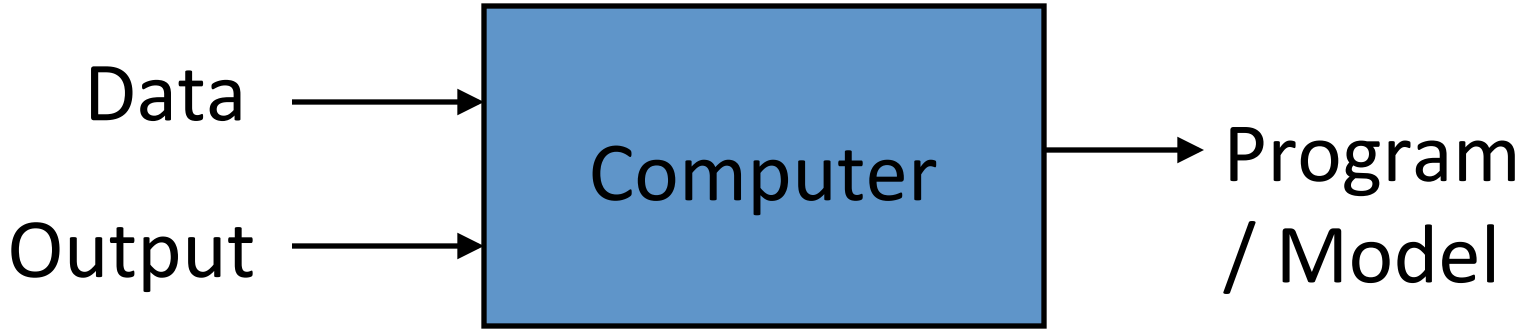
A Typical Machine Learning Pipeline



Traditional Programming



Machine Learning



e.g. SUPERVISED LEARNING

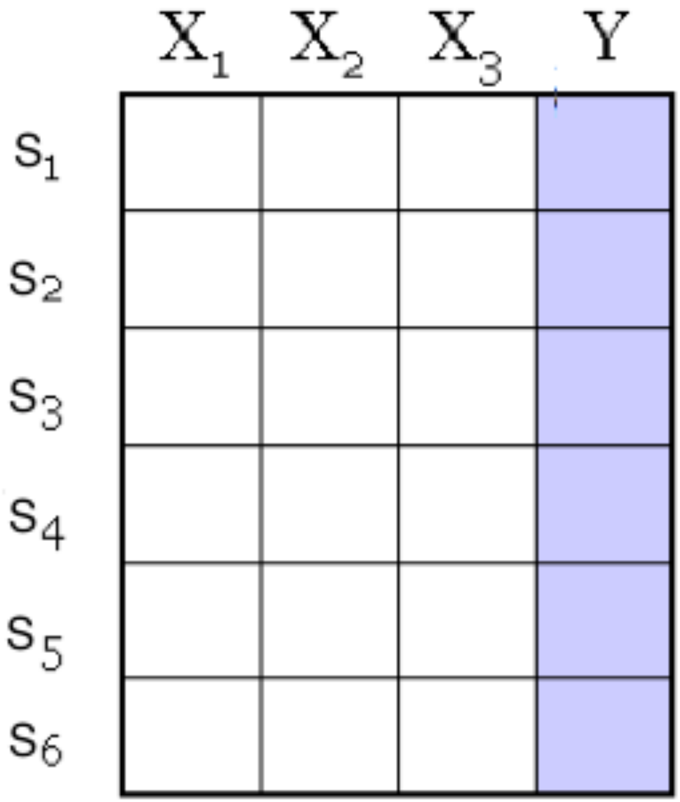
$$f : X \longrightarrow Y$$

- Find function to map input space X to output space Y

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

KEY

A Dataset

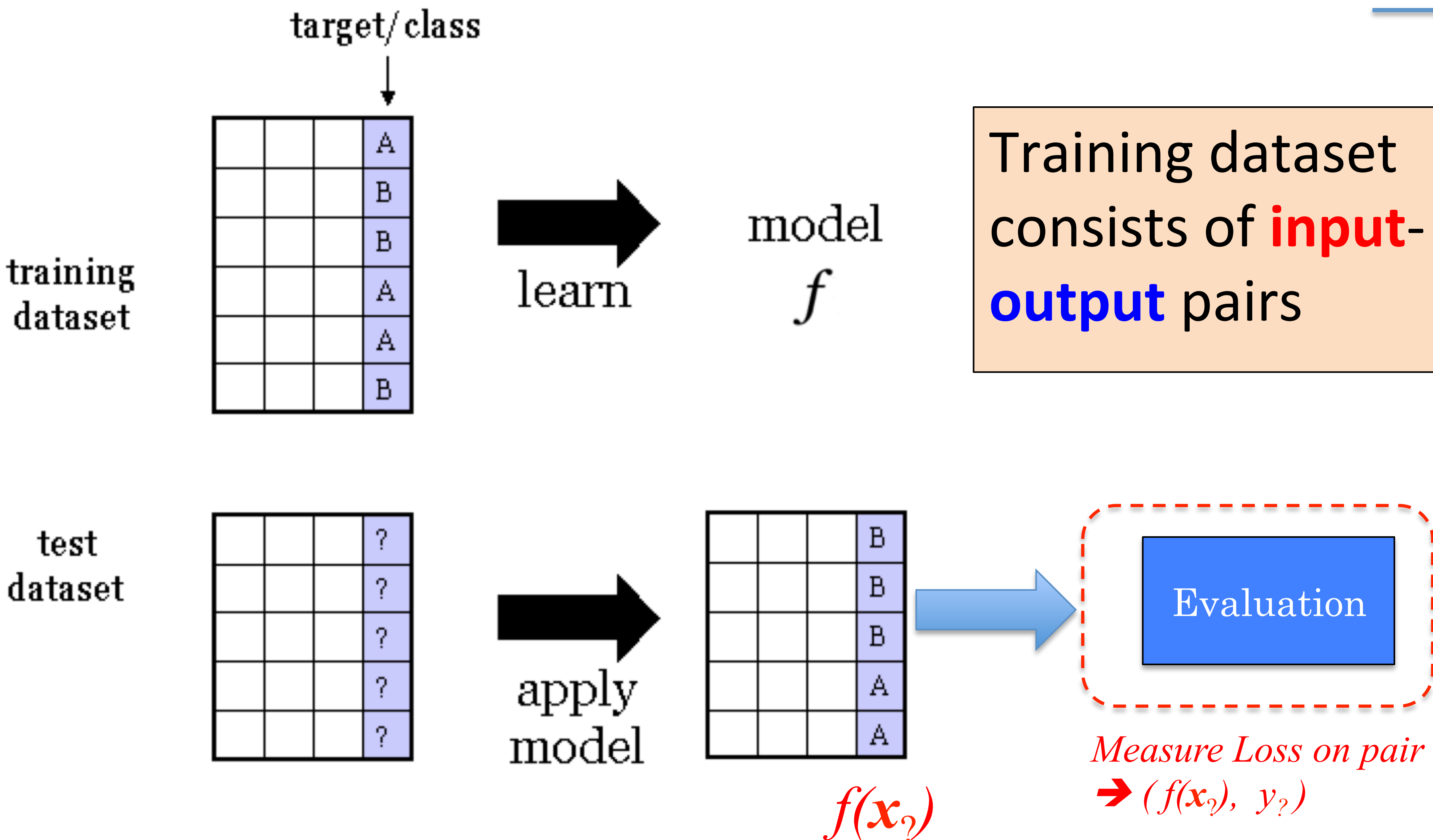


$$f : X \longrightarrow Y$$

- **Data**/*points/instances/examples/samples/records*: [rows]
- **Features**/*attributes/dimensions/independent variables/covariates/predictors/regressors*: [columns, except the last]
- **Target**/*outcome/response/label/dependent variable*: special column to be predicted [last column]

SUPERVISED LEARNING

Training dataset consists of **input-output** pairs



Evaluation Metric

e.g. for linear regression models

training dataset

$$\mathbf{X}_{train} = \begin{bmatrix} -- & \mathbf{x}_1^T & -- \\ -- & \mathbf{x}_2^T & -- \\ \vdots & \vdots & \vdots \\ -- & \mathbf{x}_n^T & -- \end{bmatrix} \qquad \vec{y}_{train} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

test dataset

$$\mathbf{X}_{test} = \begin{bmatrix} -- & \mathbf{x}_{n+1}^T & -- \\ -- & \mathbf{x}_{n+2}^T & -- \\ \vdots & \vdots & \vdots \\ -- & \mathbf{x}_{n+m}^T & -- \end{bmatrix} \qquad \vec{y}_{test} = \begin{bmatrix} y_{n+1} \\ y_{n+2} \\ \vdots \\ y_{n+m} \end{bmatrix}$$

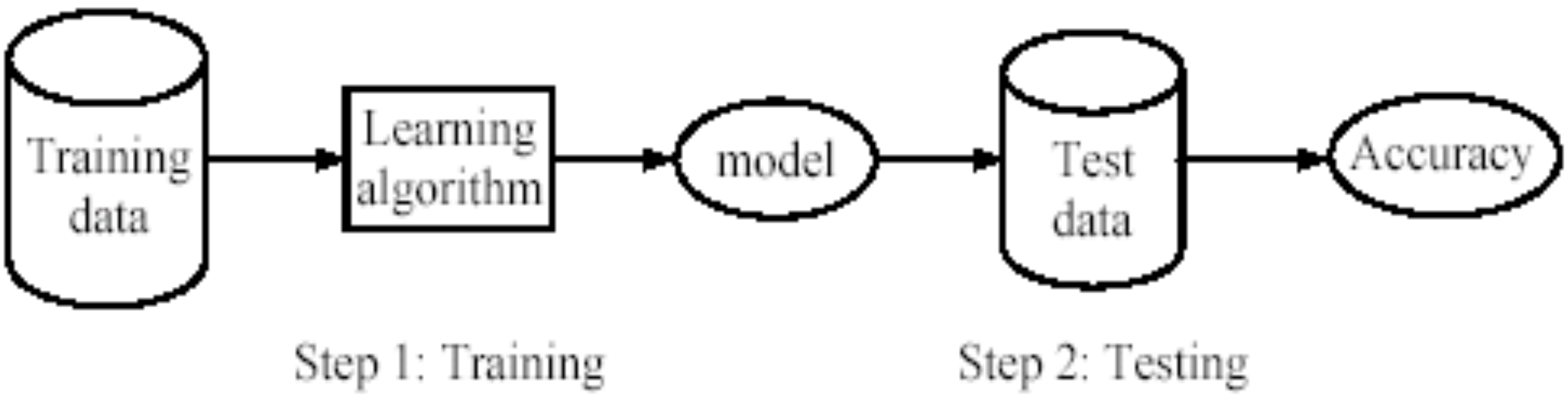
Evaluation Metric
e.g. for linear regression models

- Testing MSE (mean squared error) to report:

$$J_{test} = \frac{1}{m} \sum_{i=n+1}^{n+m} (\mathbf{x}_i^T \theta^* - y_i)^2$$

Evaluation Choice-I:

- ✓ Training (Learning): Learn a model using the training data
- ✓ Testing: Test the model using unseen test data to assess the model accuracy



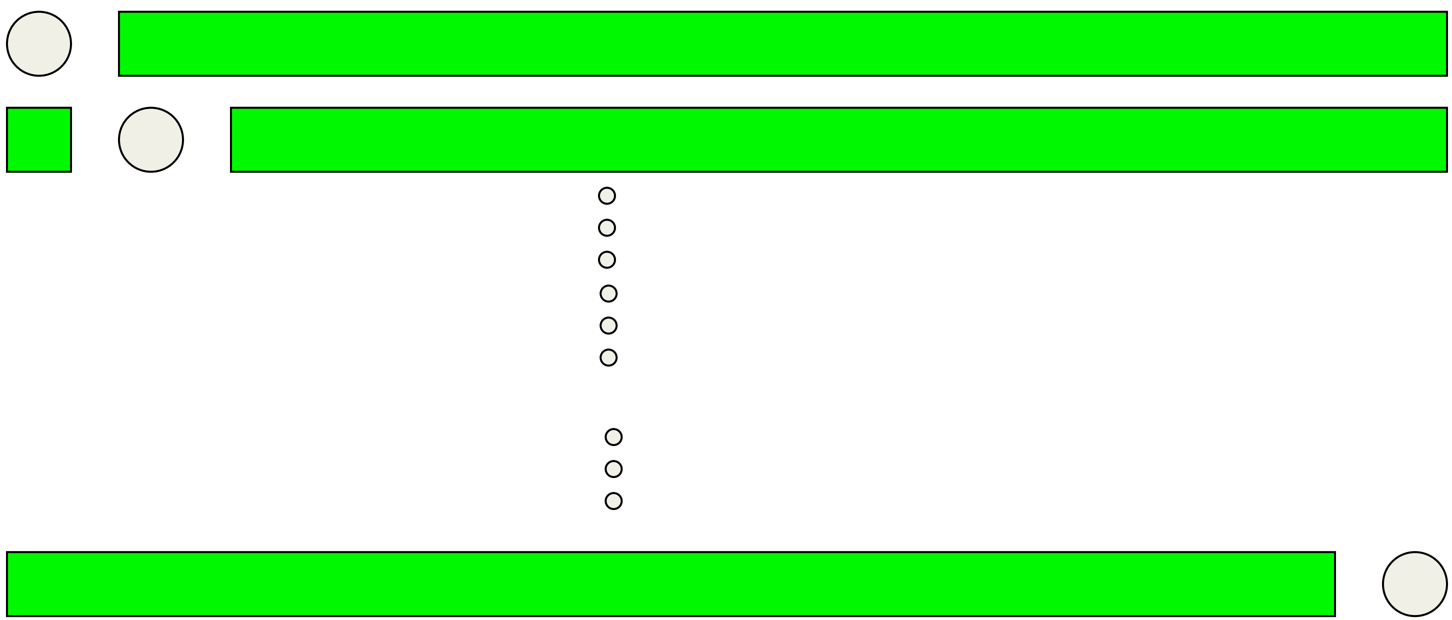
$$Accuracy = \frac{\text{Number of correct classifications}}{\text{Total number of test cases}},$$

Evaluation Choice-II:
e.g. 10 fold Cross Validation

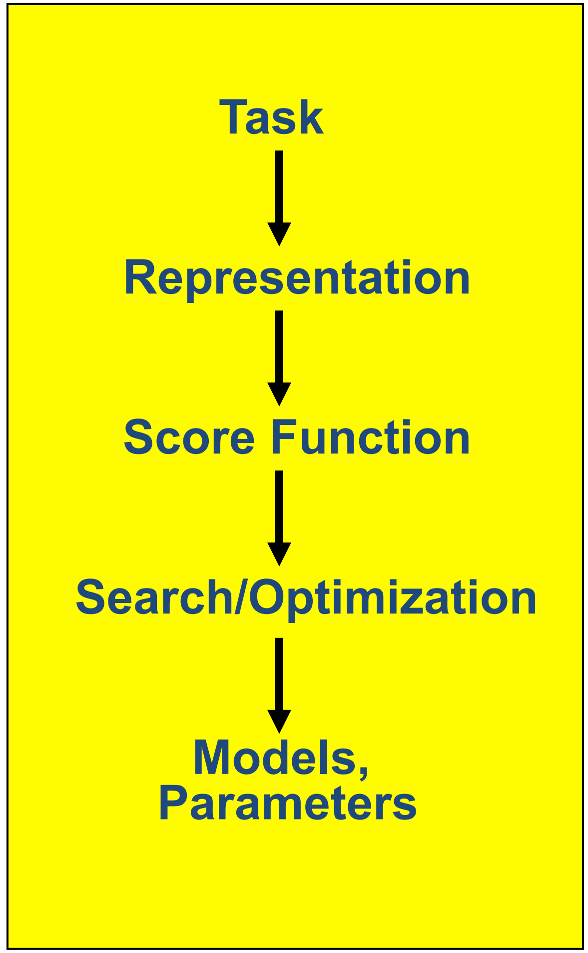
- Divide data into 10 equal pieces
- 9 pieces as training set, the rest 1 as test set
- Collect the scores from the diagonal

model	P1	P2	P3	P4	P5	P6	P7	P8	P9	P10
1	train	train	train	train	train	train	train	train	train	test
2	train	train	train	train	train	train	train	train	test	train
3	train	train	train	train	train	train	train	test	train	train
4	train	train	train	train	train	train	test	train	train	train
5	train	train	train	train	train	test	train	train	train	train
6	train	train	train	train	test	train	train	train	train	train
7	train	train	train	test	train	train	train	train	train	train
8	train	train	test	train	train	train	train	train	train	train
9	train	test	train	train	train	train	train	train	train	train
10	test	train	train	train	train	train	train	train	train	train

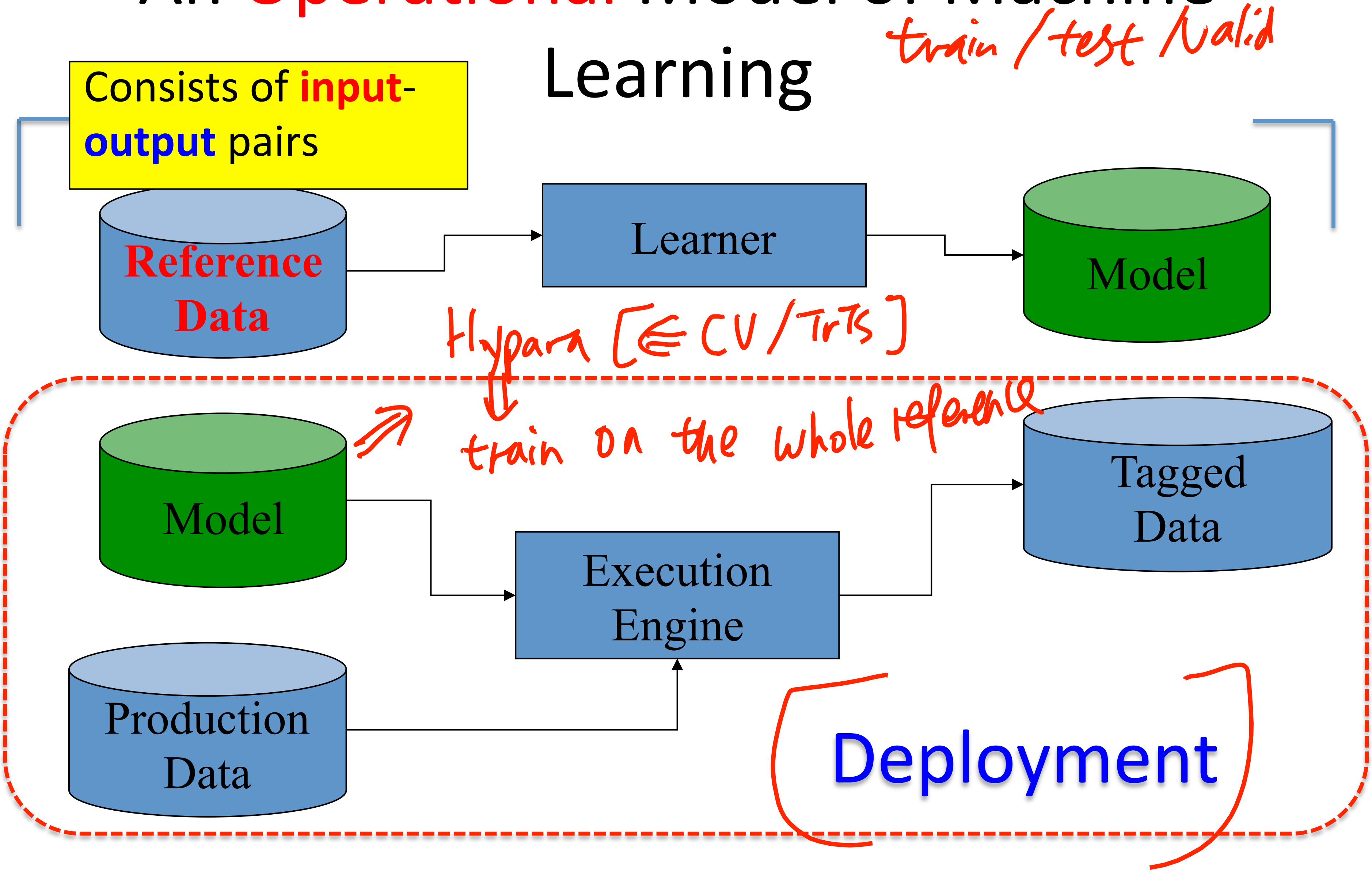
e.g. Leave-one-out (n-fold cross validation)



Machine Learning in a Nutshell



An Operational Model of Machine Learning



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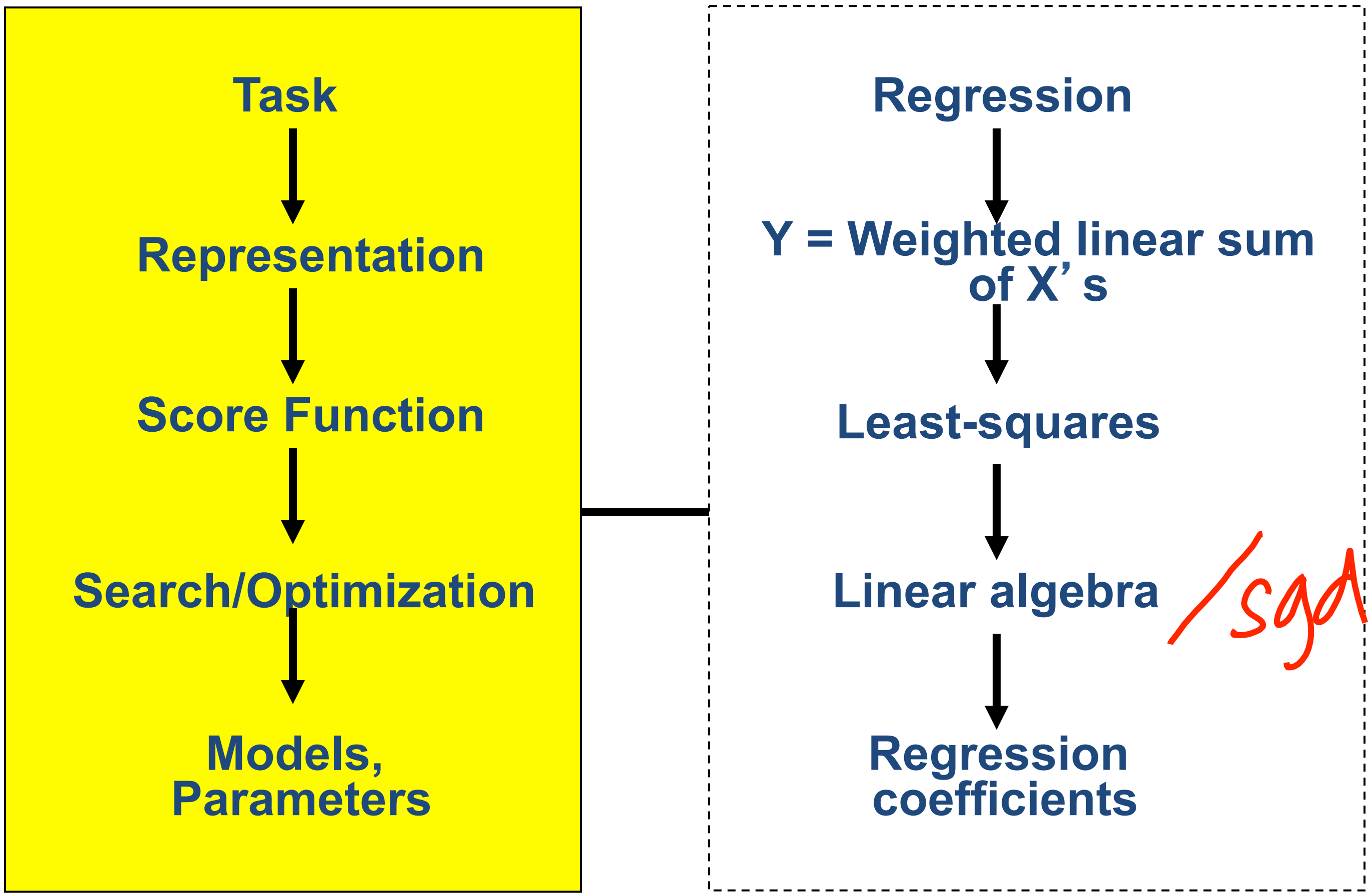
(1) Multivariate Linear Regression



$$\hat{y} = f(x) = \theta_0 + \theta_1 x^1 + \theta_2 x^2$$

(1) Linear Regression (LR)

$$f : X \longrightarrow Y$$

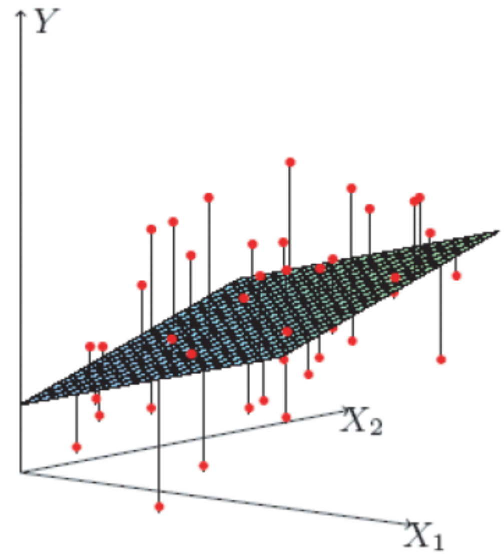
➔ e.g. Linear Regression Models

$$\hat{y} = f(x) = \theta_0 + \theta_1 x^1 + \theta_2 x^2$$

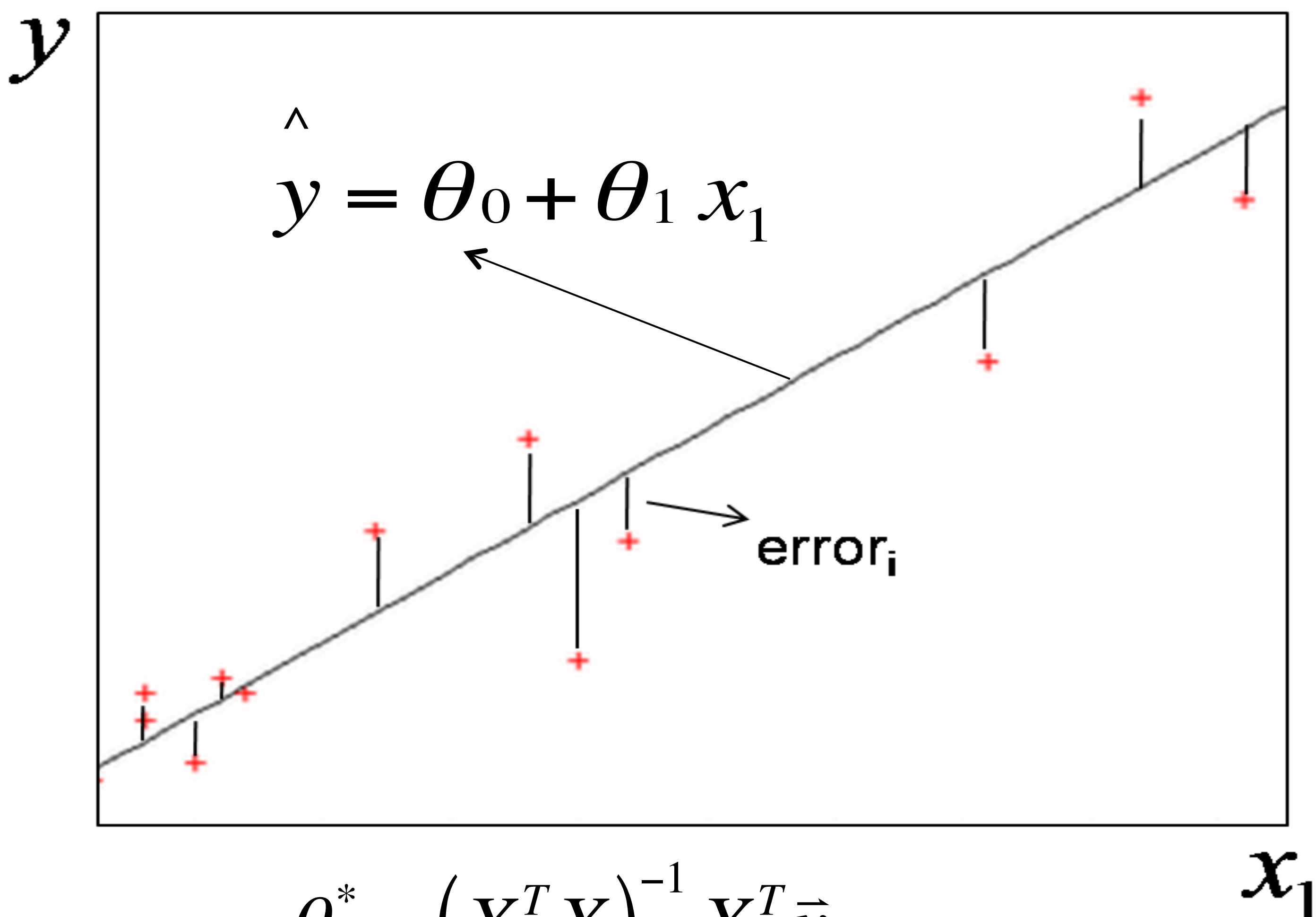
➔ To minimize the " least square " cost function:

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

➔ θ



Linear regression (1D example)



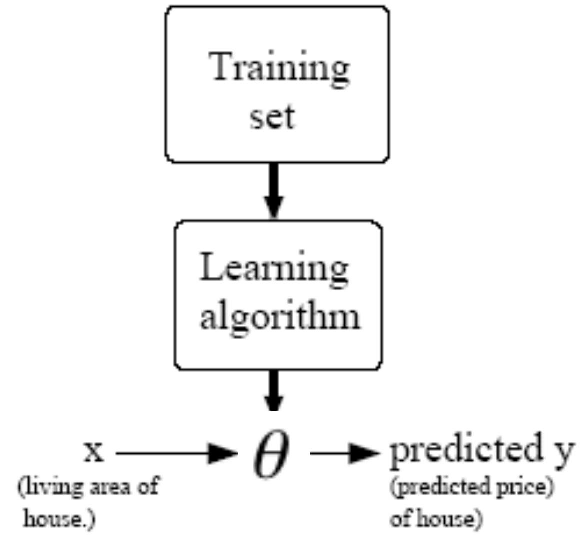
$$\hat{y} = \theta_0 + \theta_1 x_1$$

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

Our goal:

- We can represent the whole Training set:

$$\mathbf{X} = \begin{bmatrix} -- & \mathbf{x}_1^T & -- \\ -- & \mathbf{x}_2^T & -- \\ \vdots & \vdots & \vdots \\ -- & \mathbf{x}_n^T & -- \end{bmatrix} = \begin{bmatrix} x_1^0 & x_1^1 & \ldots & x_1^{p-1} \\ x_2^0 & x_2^1 & \ldots & x_2^{p-1} \\ \vdots & \vdots & \vdots & \vdots \\ x_n^0 & x_n^1 & \ldots & x_n^{p-1} \end{bmatrix}$$



$$\mathbf{Y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

- Predicted output for each training sample:

$$\begin{bmatrix} f(\mathbf{x}_1^T) \\ f(\mathbf{x}_2^T) \\ \vdots \\ f(\mathbf{x}_n^T) \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1^T\theta \\ \mathbf{x}_2^T\theta \\ \vdots \\ \mathbf{x}_n^T\theta \end{bmatrix} = X\theta$$

Method I: normal equations

- Write the cost function in matrix form:

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{n}(\mathbf{x}_i^T\theta - y_i)^2$$
$$= \frac{1}{2}\left(X\theta - \vec{y}\right)^T\left(X\theta - \vec{y}\right)$$
$$= \frac{1}{2}\left(\theta^T X^T X\theta - \theta^T X^T \vec{y} - \vec{y}^T X\theta + \vec{y}^T\vec{y}\right)$$

$$\mathbf{X} = \begin{bmatrix} -- & \mathbf{x}_1^T & -- \\ -- & \mathbf{x}_2^T & -- \\ \vdots & \vdots & \vdots \\ -- & \mathbf{x}_n^T & -- \end{bmatrix} \qquad \vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

To minimize $J(\theta)$, take derivative and set to zero:

$$\Rightarrow \quad X^T X\theta = X^T\vec{y}$$

The normal equations

$$\Downarrow$$

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

Method II: LR with batch Steepest descent / Gradient descent

For the t-th epoch

$$\theta_t = \theta_{t-1} - \alpha \nabla J(\theta_{t-1})$$

$$\nabla_\theta J = \left[\frac{\partial}{\partial \theta_1} J, \ldots, \frac{\partial}{\partial \theta_k} J \right]^T = -\sum_{i=1}^{n} (y_i - \vec{\mathbf{x}}_i^T \theta) \mathbf{x}_i$$

$$\theta_j^{t+1} = \theta_j^t + \alpha \sum_{i=1}^{n} (y_i - \vec{\mathbf{x}}_i^T \theta^t) x_i^j$$

– This is as a **batch** gradient descent algorithm

Method III: LR with Stochastic GD →

- From the batch steepest descent rule:

$$\theta_j^{t+1} = \theta_j^{t} + \alpha \sum_{i=1}^{n} (y_i - \vec{\mathbf{x}}_i^T \theta^t) x_i^j$$

- For a single training point, we have:

$$\theta^{t+1} = \theta^{t} + \alpha (y_i - \vec{\mathbf{x}}_i^T \theta^t) \vec{\mathbf{x}}_i$$

  – a "**stochastic**", "**coordinate**" descent algorithm
  – This can be used as an **on-line** algorithm

Method IV: Newton's method for optimization

- The most basic second-order optimization algorithm

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \mathbf{H}_K^{-1} \mathbf{g}_k$$

- Updating parameter with

$$\Rightarrow \theta^{t+1} = \theta^{t} - H^{-1} \nabla f(\theta)$$

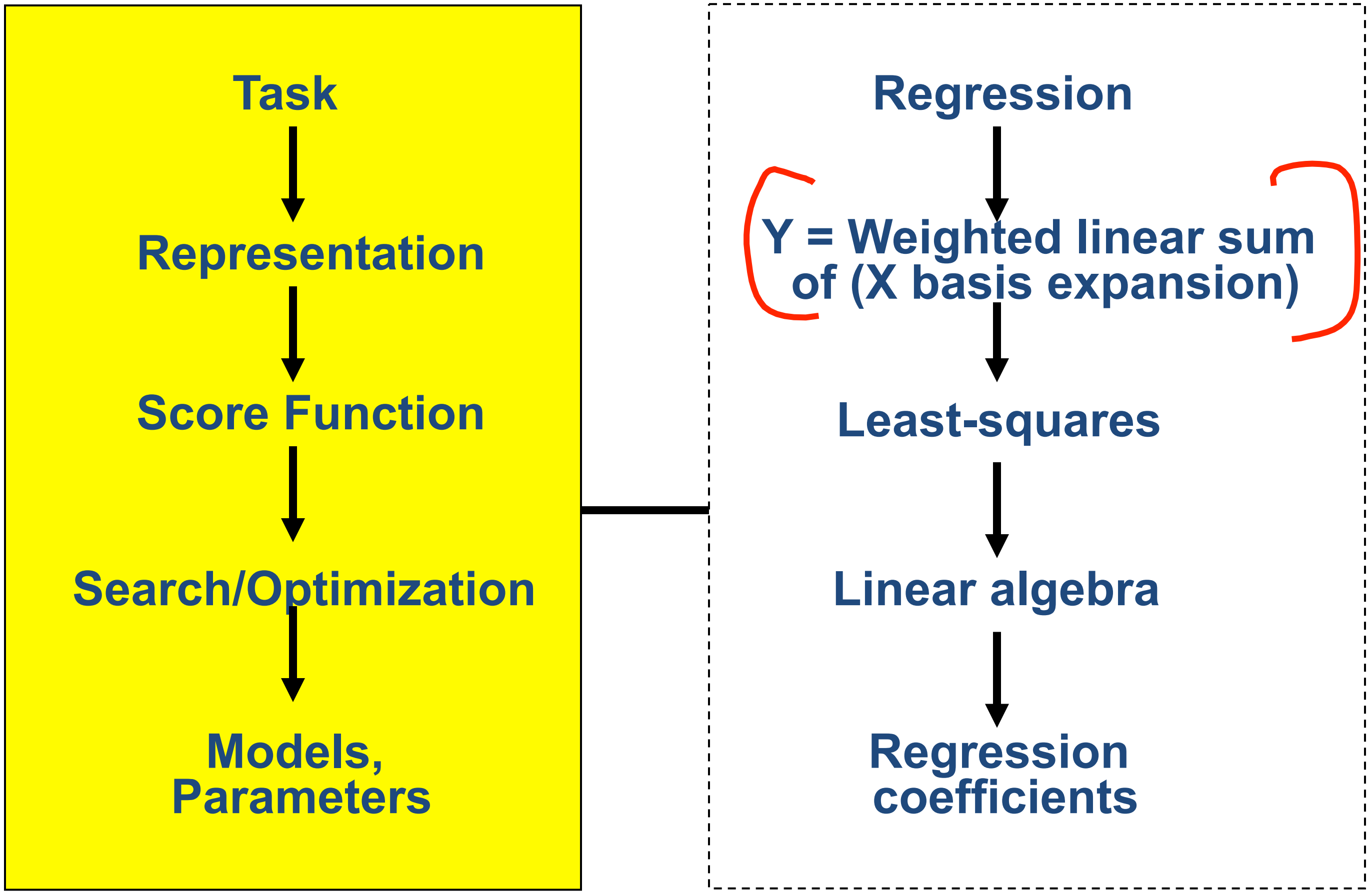
$$= \theta^{t} - (X^T X)^{-1} [X^T X \theta^{t} - X^T \vec{y}]$$

$$= (X^T X)^{-1} X^T y$$

WHY ???
Normal Eq?

Newton's method for Linear Regression

(2) Multivariate Linear Regression with basis Expansion



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

(2) LR with polynomial basis functions

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

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

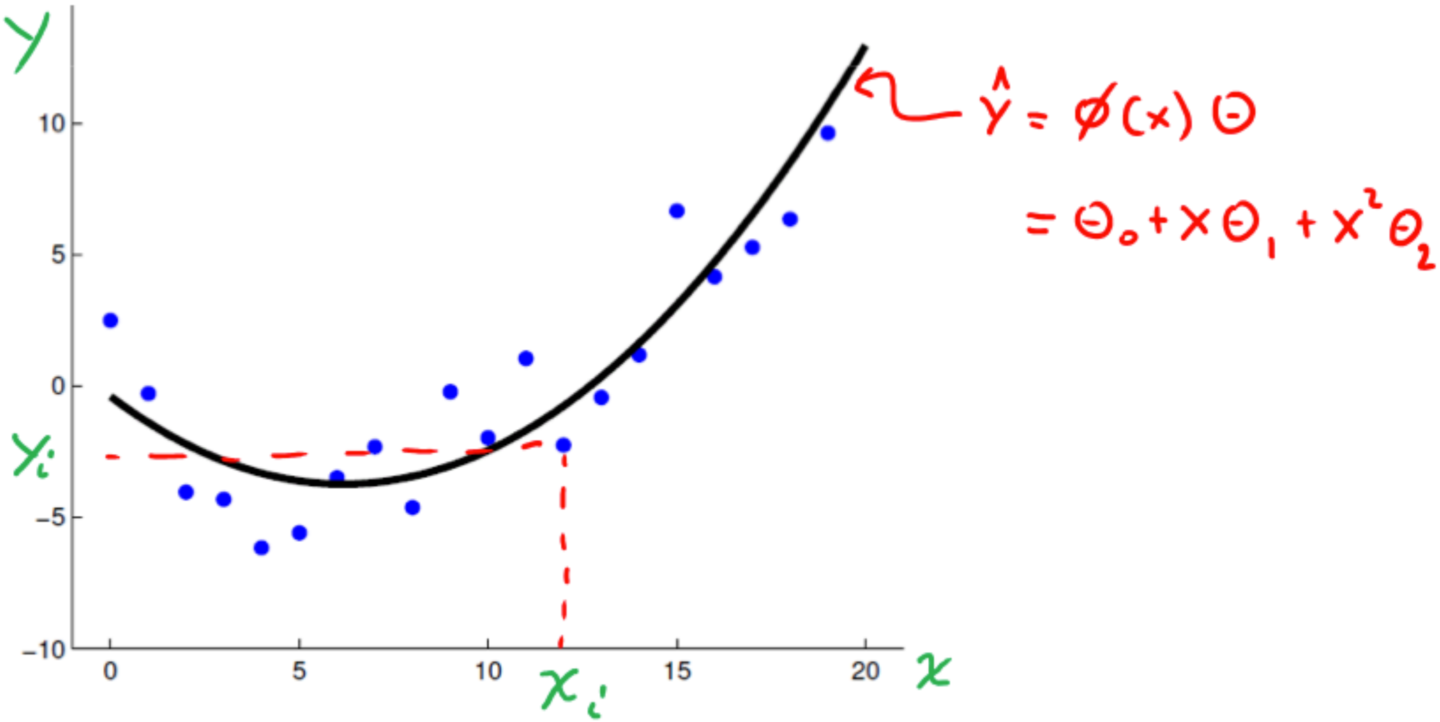
- E.g.: polynomial regression:

$$\varphi(x) := \left[1, x, x^2, x^3\right]$$

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

e.g. **polynomial regression**

For example, $\phi(x) = [1, x, x^2]$



Dr. Nando de Freitas's tutorial slide

LR with radial-basis functions

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

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

- E.g.: LR with RBF regression: $K_\lambda(\underline{x}, r) = \exp\left(-\frac{(\underline{x} - r)^2}{2\lambda^2}\right)$

$$\varphi(x) := \left[1, K_{\lambda=1}(x,1), K_{\lambda=1}(x,2), K_{\lambda=1}(x,4)\right]$$

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

(3) Locally Weighted / Kernel Regression

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

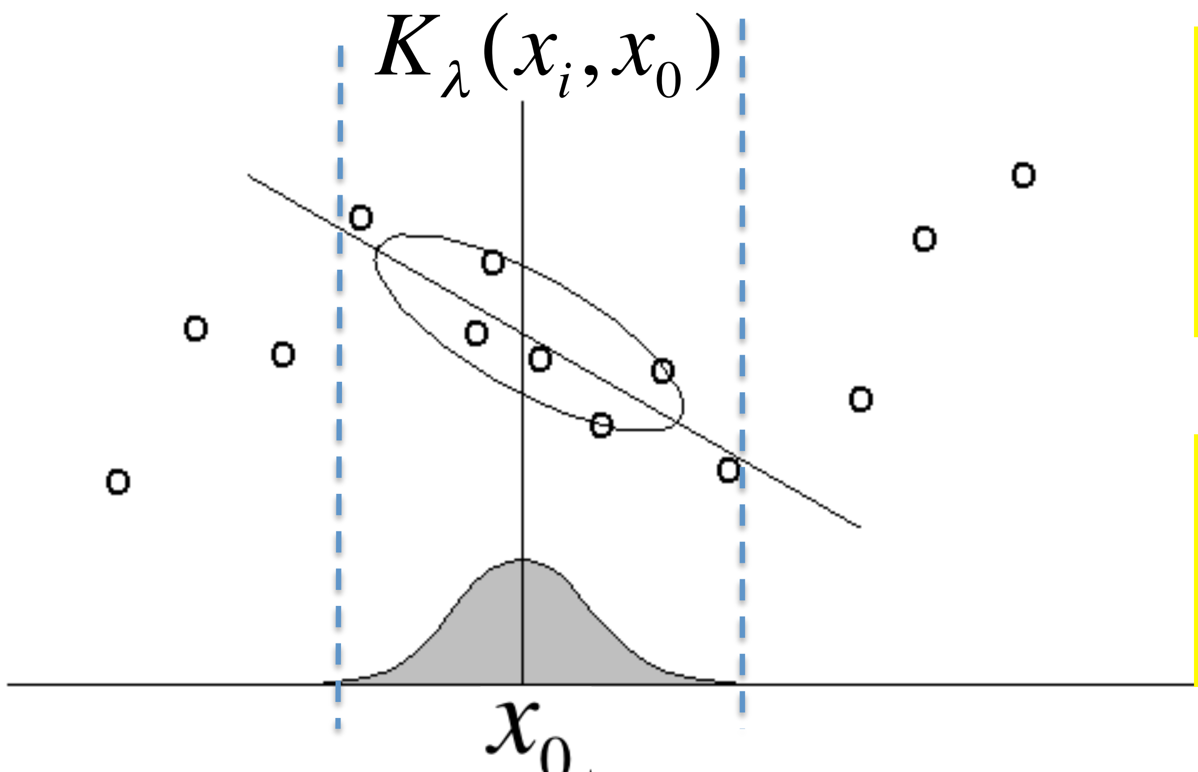
Regression → Y = Weighted linear sum of X' s → Weighted Least-squares → Linear algebra → Local Regression coefficients (conditioned on each test point)

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

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

(3) Locally weighted regression

- *aka* locally weighted regression, locally linear regression, LOESS, …



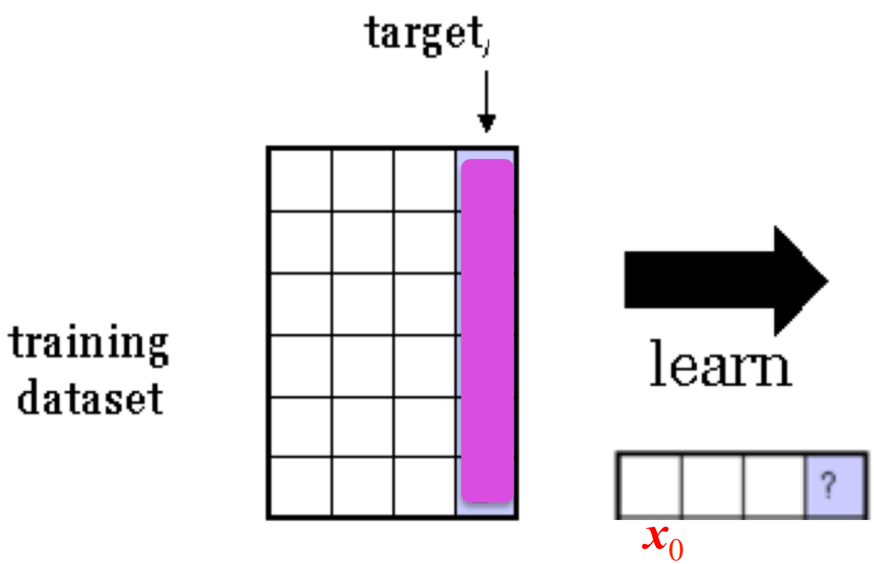
linear_func(x)->y
➔
could represent only the neighbor region of x_0

Use RBF function to pick out/emphasize the neighbor region of x_0 ➔

$K_\lambda(x_i, x_0)$

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.

LEARNING of Locally weighted linear regression

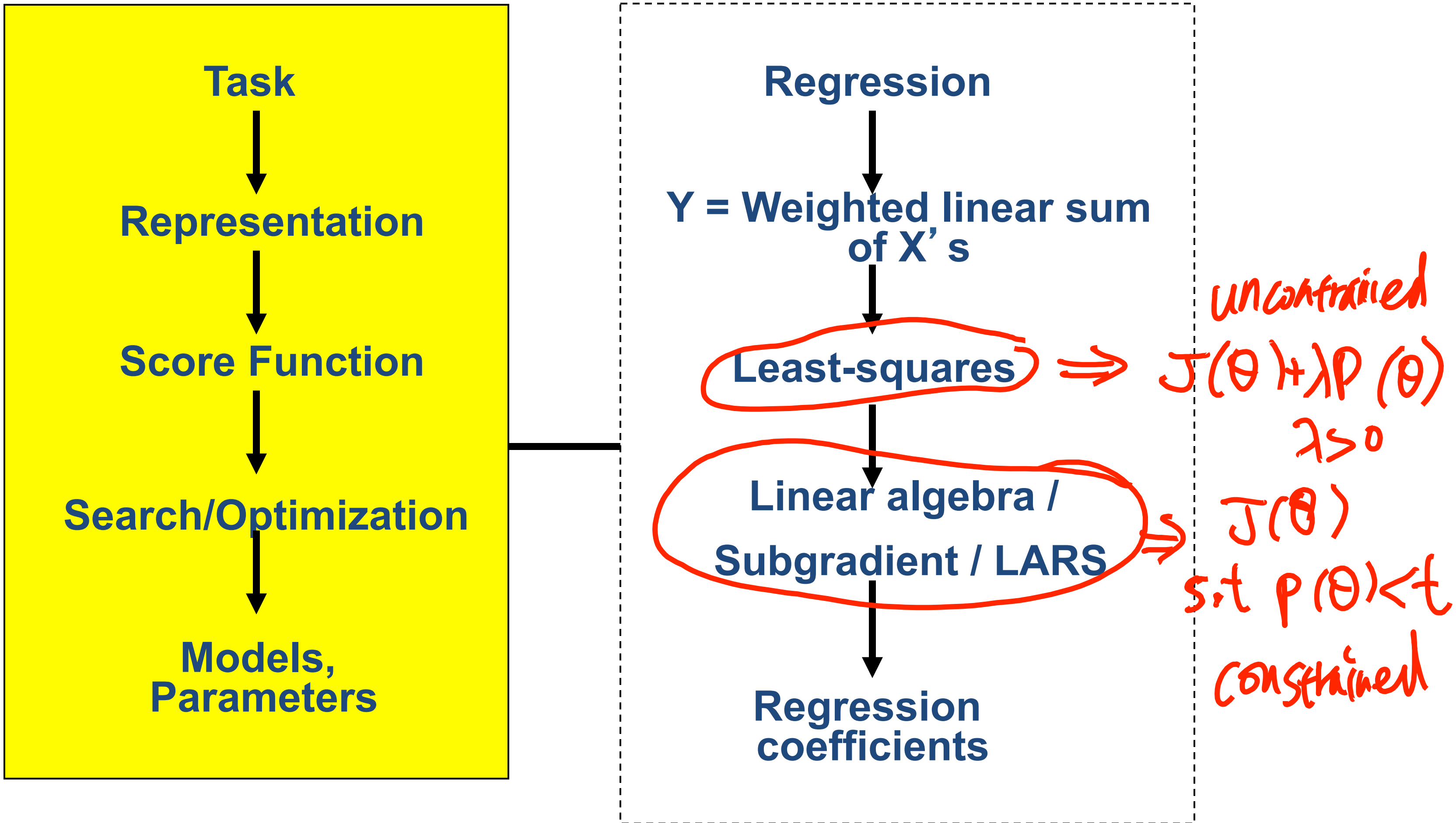


$$\hat{f}(x_0) = \hat{\alpha}(x_0) + \hat{\beta}(x_0) x_0$$

➔ Separate weighted least squares **at each target point x_0**

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

(4) Regularized multivariate linear regression



$$\min J(\beta) = \sum_{i=1}^{n}\left(Y - \hat{Y}\right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2$$

(4) LR with Regularizations / Regularized multivariate linear regression

- Basic model $$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \cdots + \hat{\beta}_p x_p$$
- LR estimation: $$\min J(\beta) = \sum \left(Y - \hat{Y}\right)^2$$
- LASSO estimation: $$\min J(\beta) = \sum_{i=1}^{n} \left(Y - \hat{Y}\right)^2 + \lambda \sum_{j=1}^{p} \left|\beta_j\right|$$
- Ridge regression estimation: $$\min J(\beta) = \sum_{i=1}^{n} \left(Y - \hat{Y}\right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2$$

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Error on data + Regularization

LR with Regularizations / Ridge Estimator

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \cdots + \hat{\beta}_p x_p$$

$$\beta^* = \left(X^T X + \lambda I\right)^{-1} X^T \vec{y}$$

- The ridge estimator is solution from RSS (regularized sum of square errors)

$$\hat{\beta}^{ridge} = \arg\min J(\beta) = \arg\min (y - X\beta)^T (y - X\beta) + \lambda \beta^T \beta$$

to minimize, take derivative and set to zero

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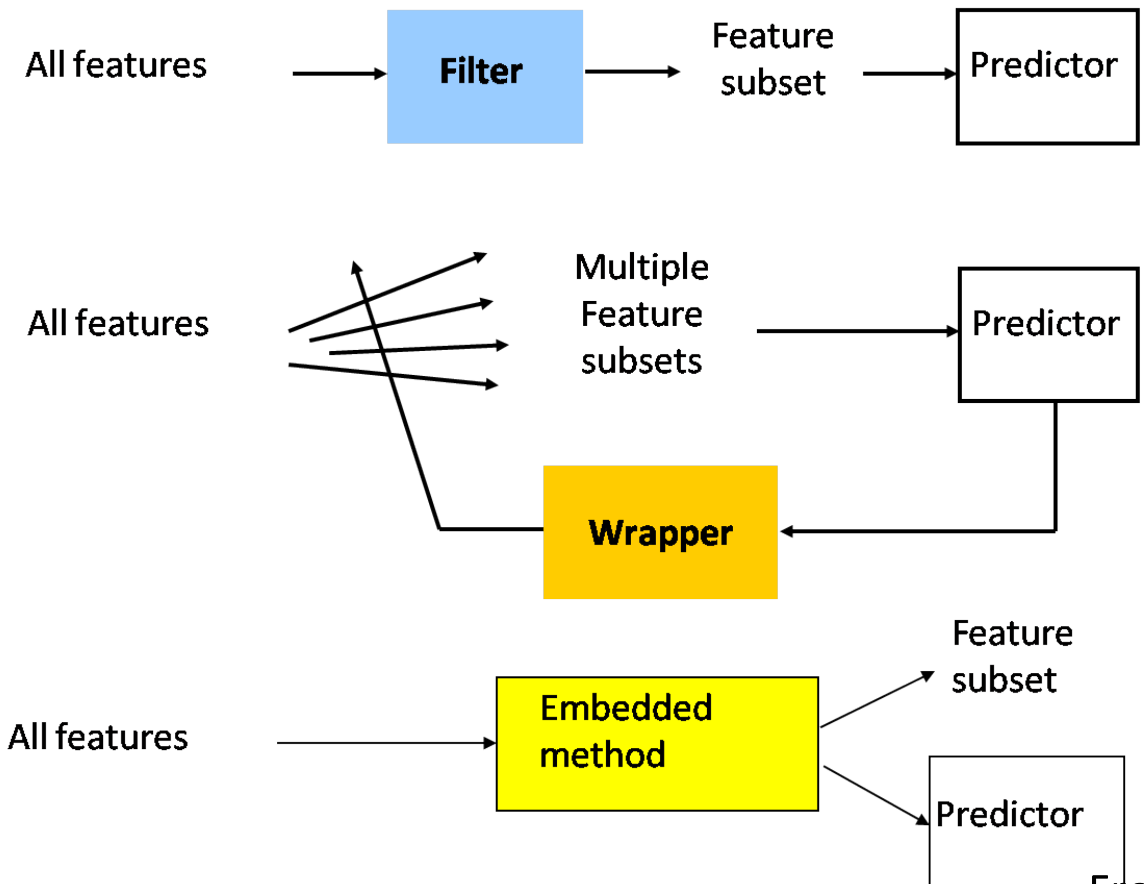
Summary: filters vs. wrappers vs. embedding

- **Main goal**: rank subsets of useful features



From Dr. **Isabelle Guyon**

$$(X^T X + \lambda I)^{-1} X y$$

$\Rightarrow \underset{p \times n}{X^T} \underset{n \times p}{X}$: $O(np^2)$

$\Rightarrow \underbrace{(X^T X + \lambda I)}_{p \times p}^{-1}$: $O(p^3)$

$\Rightarrow X y$: $O(np)$

$\Rightarrow$ Computationally, choose to make $p \downarrow$ if we can ☆

The principle of Occam's razor

image at: [ww.butterflyeffe ct.ca/.../ OccamsRazor.ht mlRemove frame](ww.butterflyeffect.ca/.../OccamsRazor.html)

Occam's razor:
states that the explanation of any phenomenon should make as few assumptions as possible, eliminating those that make no difference to any observable predictions of the theory

Occam's razor: law of parsimony

Basically it says that explanations must not include elements that have nothing to do with the phenomenon under analysis.

...not as often stated:
"The simplest explanation is the correct one"

As it is not about simplicity or complexity

William of Occam 1288 - 1348

parsimony: extreme unwillingness to spend money or use resources.

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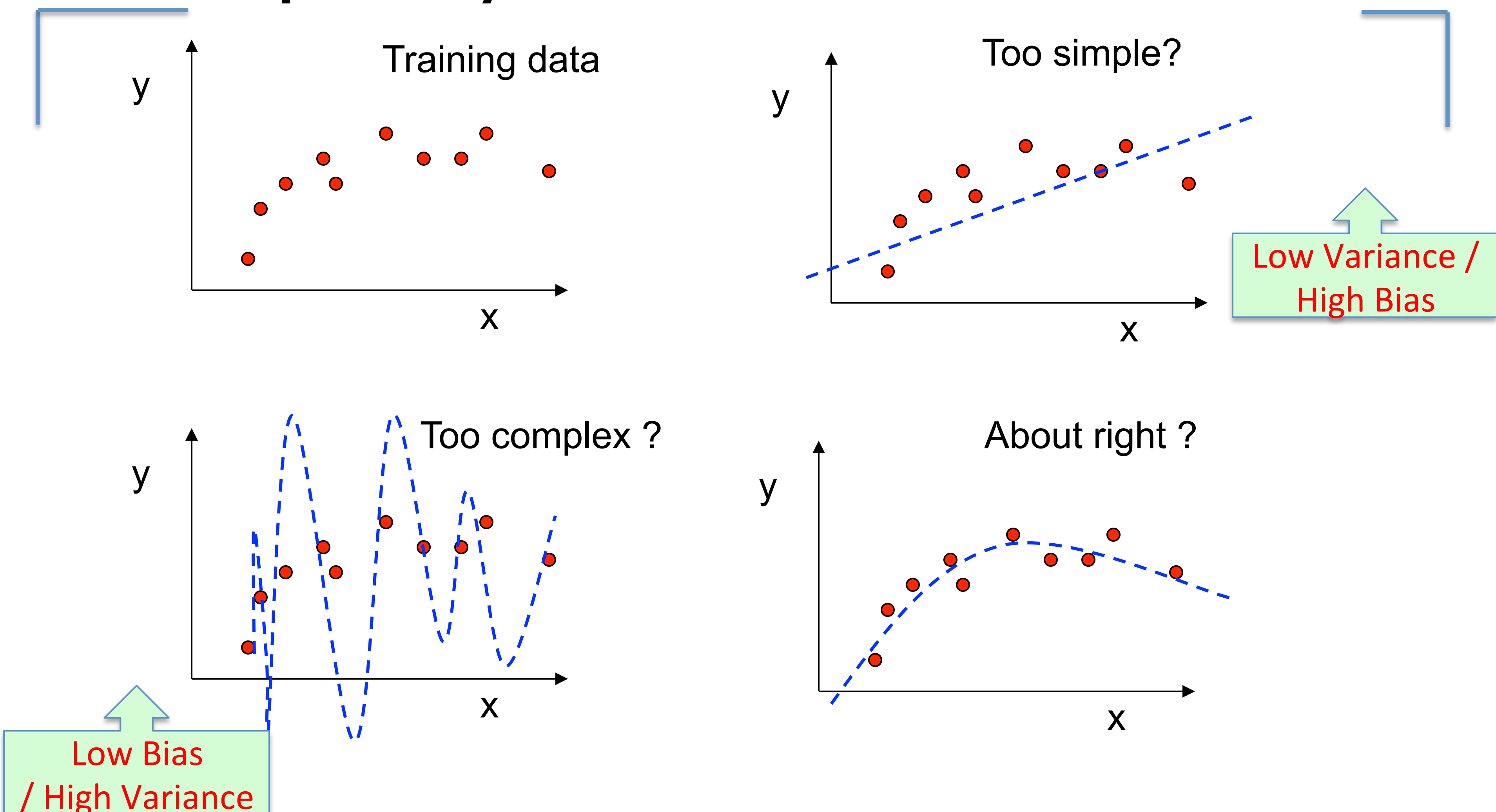
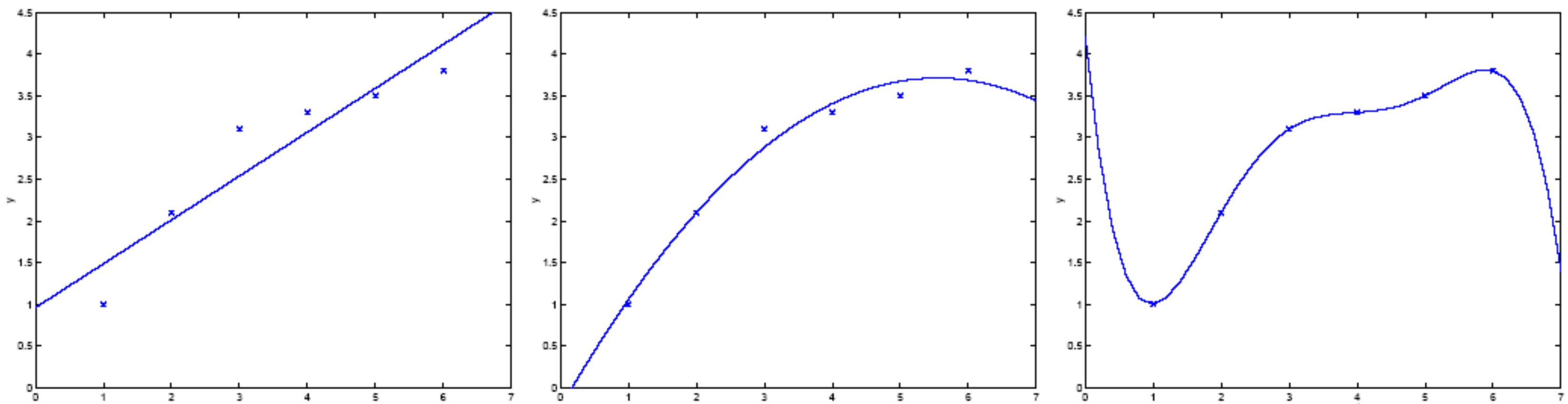
Regression: Complexity versus Goodness of Fit



What ultimately matters: ***GENERALIZATION***

Which function *f* *to choose*? Many possible choices , e.g. LR with polynomial basis functions

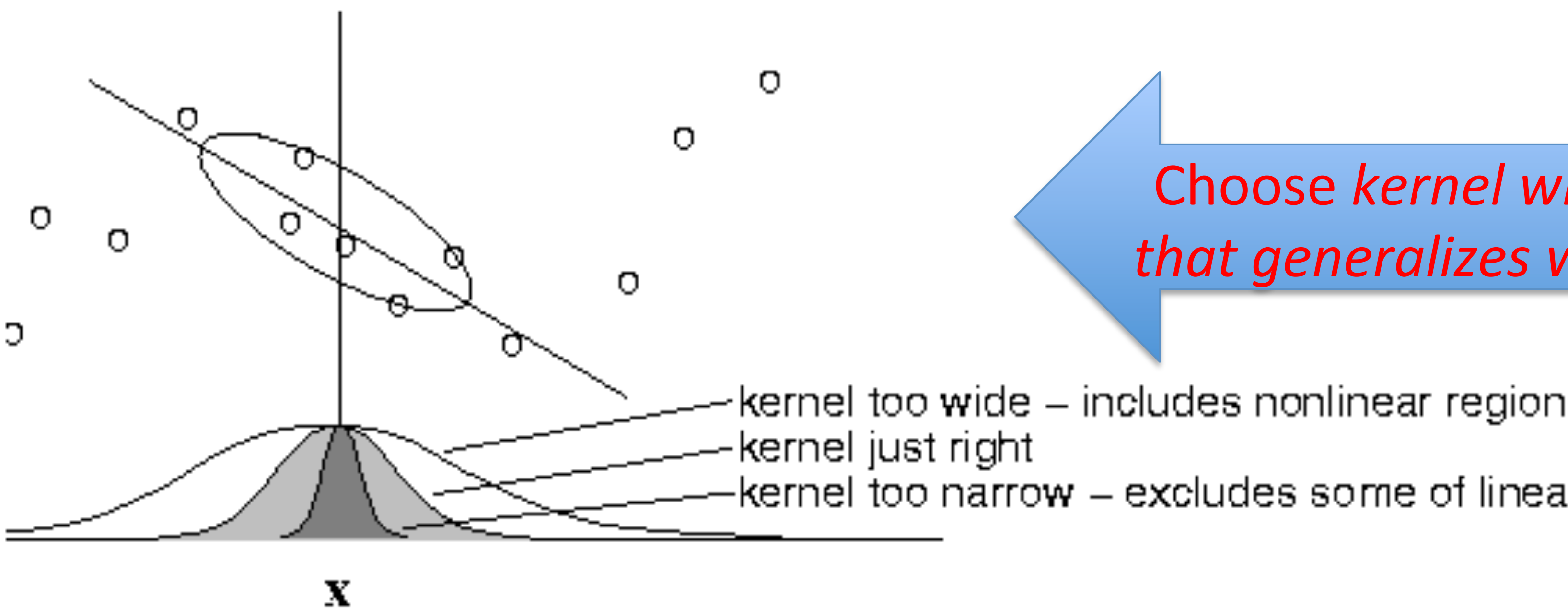


$y = \theta_0 + \theta_1 x$ $\qquad$ $y = \theta_0 + \theta_1 x + \theta_2 x^2$ $\qquad$ $y = \sum_{j=0}^{5} \theta_j x^j$

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

Choose f that generalizes well !

Which kernel width to choose ? e.g. locally weighted LR

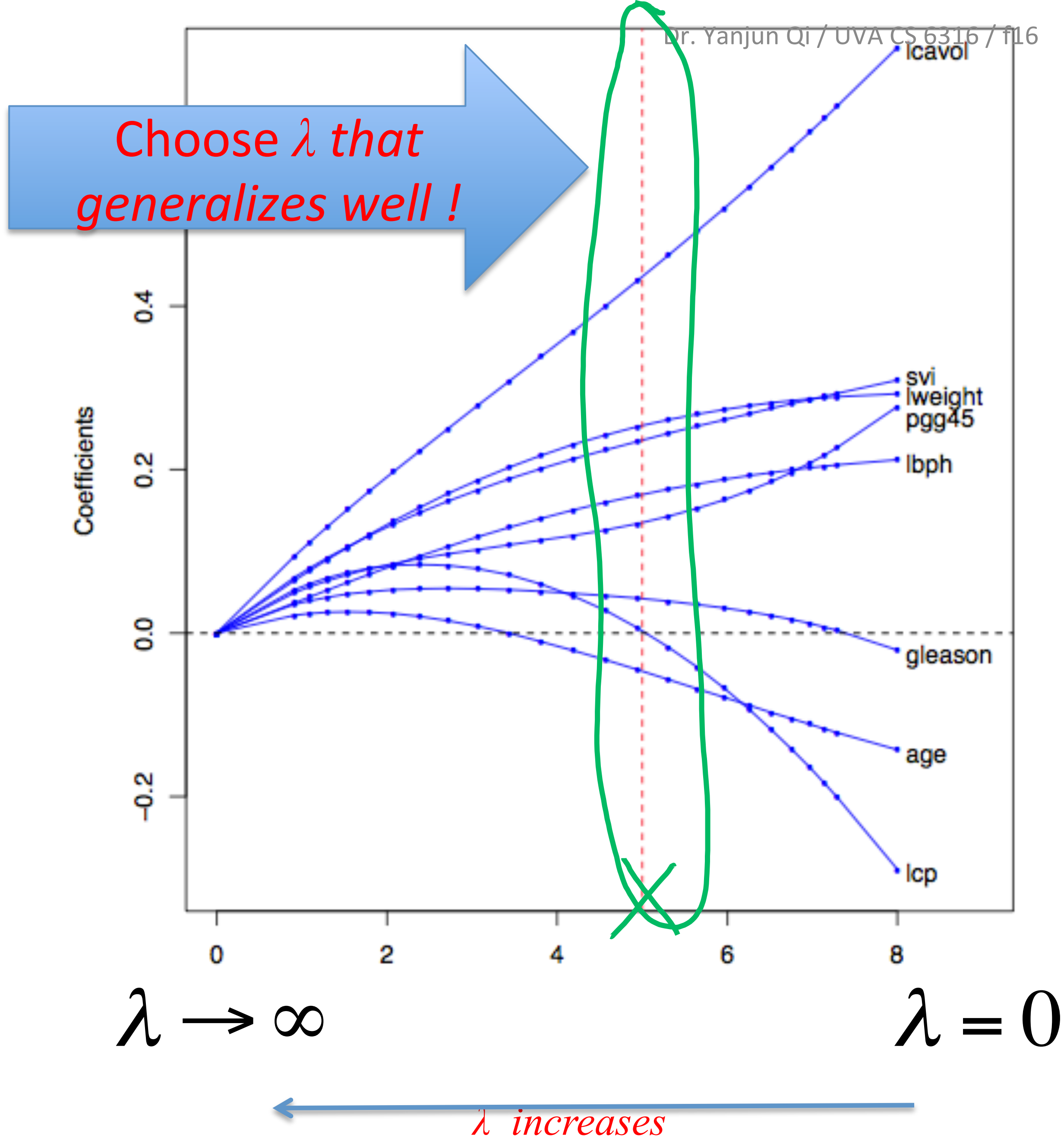


Choose *kernel width that generalizes well !*

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.

an example (ESL Fig3.8), Ridge Regression

when varying λ, how θ_j varies.



Choose λ *that generalizes well !*

Regularization path of a Lasso Estimator

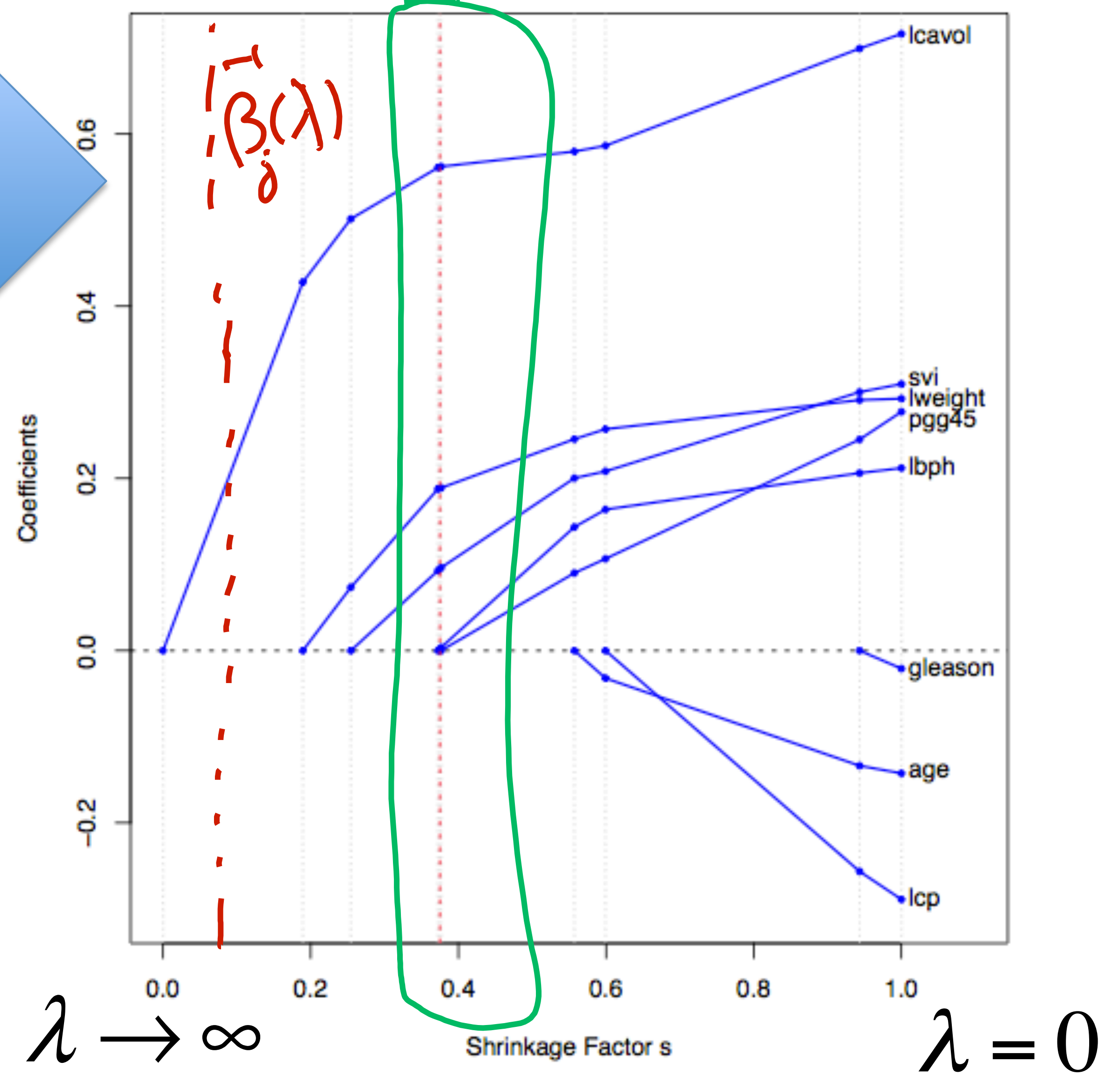
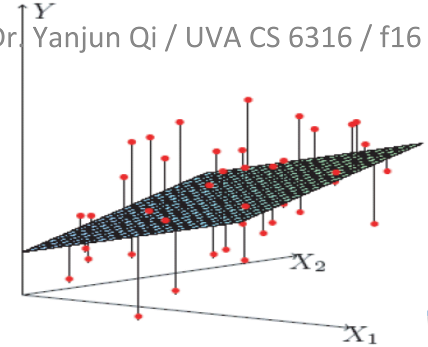


FIGURE 3.10. *Profiles of lasso coefficients, as the tuning parameter t is varied. Coefficients are plotted versus $s = t / \sum_1^p |\hat{\beta}_j|$. A vertical line is drawn at $s = 0.36$, the value chosen by cross-validation. Compare Figure 3.8 on page 65; the lasso profiles hit zero, while those for ridge do not. The profiles are piece-wise linear, and so are computed only at the points displayed; see Section 3.4.4 for details.*

Probabilistic Interpretation of Linear Regression (LATER)



- Let us assume that the target variable and the inputs are related by the equation:

$$y_i = \theta^T \mathbf{x}_i + \varepsilon_i$$

error data on each point

where ε is an error term of unmodeled effects or random noise

- Now assume that ε follows a Gaussian $N(0,\sigma)$, then we have:

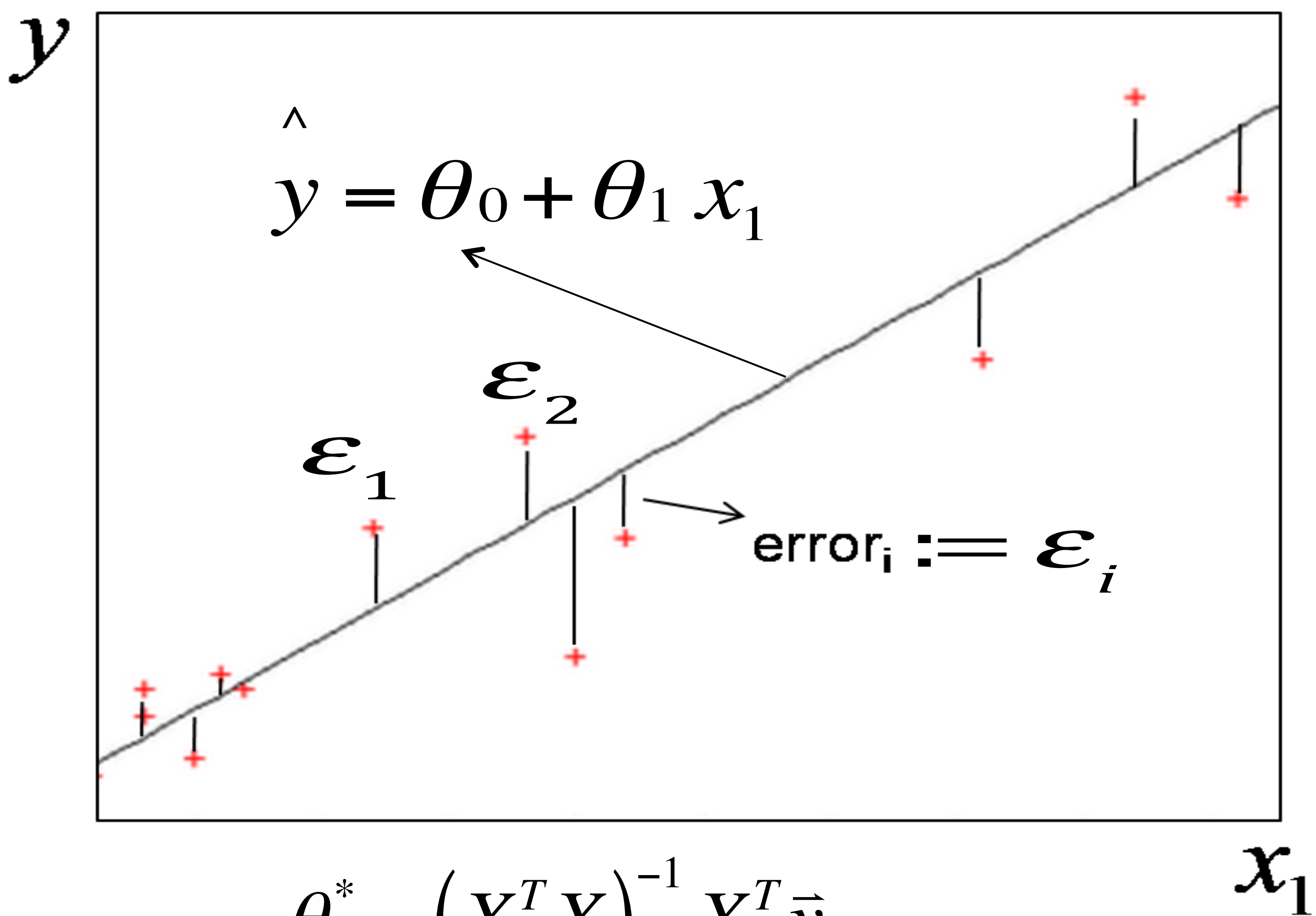
$$p(y_i \mid x_i;\theta) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{(y_i - \theta^T \mathbf{x}_i)^2}{2\sigma^2}\right)$$

Many more variations of LR from this perspective, e.g. binomial / poisson (LATER)

- By iid (among samples) assumption:

$$L(\theta) = \prod_{i=1}^{n} p(y_i \mid x_i;\theta) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^n \exp\left(-\frac{\sum_{i=1}^{n}(y_i - \theta^T \mathbf{x}_i)^2}{2\sigma^2}\right)$$

Linear regression (1D example)



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

References

- Big thanks to Prof. Eric Xing @ CMU for allowing me to reuse some of his slides
- Prof. Alexander Gray's slides