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KYOTO UNIVERSITY

Statistical Learning Theory
- Regression -

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Linear Regression

Regression: Supervised learning for predicting a real valued variable

- Regression learning is one of supervised learning problem settings with wide applications
- Goal: Obtain a function $f : \mathcal{X} \to \Re$ ($\Re$: real value)
  - Usually, input domain $\mathcal{X}$ is a D-dimensional vector space
    - E.g. $x \in \mathcal{X}$ is a house and $y \in \Re$ is its price (housing dataset in UCI Machine Learning Repository)
- Training dataset: N pairs of an input and an output $\{(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \ldots, (\mathbf{x}^{(N)}, y^{(N)})\}$
  - We use the training dataset to estimate f

Some applications of regression: From marketing prediction to chemo-informatics

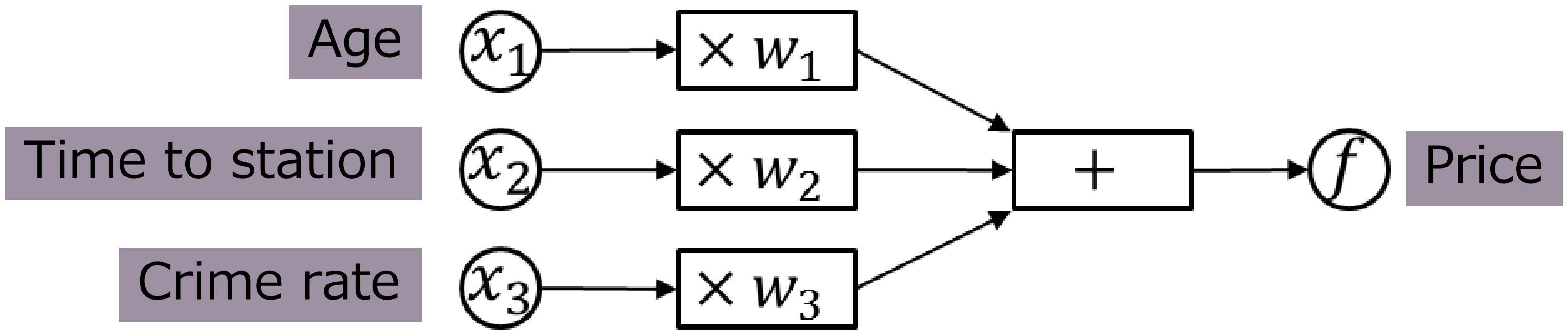
- Some applications:
  - Price prediction: Predict the price y of a product x
  - Demand prediction: Predict the demanded amount y of a product x
  - Sales prediction: Predict the sales amount y of a product x
  - Chemical activity: Predict the activity level y of a compound x
- Other applications:
  - Time series prediction: Predict the value y at the next time step given the past measurements x
  - Classification (has a discrete output domain)

Model:
Linear regression model

- Model: How does y depend on $\mathbf{x}$?
- We consider the simplest choices: Liner regression model

$$y = \mathbf{w}^\top \mathbf{x} = w_1 x_1 + w_2 x_2 + \cdots + w_D x_D$$

  - Prediction model of the price of a house:



Handling discrete features: Dummy variables

- We assume input $\mathbf{x}$ is a real vector
  - In the house price prediction example, features can be age, walk time to the nearest station, crime rate in the area, …
    - They are considered as real values
- How do we handle discrete features as real values?
  - Binary features: $\{\mathrm{Male}, \mathrm{Female}\}$ are encoded as $\{0,1\}$
  - One-hot encoding: $\{\mathrm{Kyoto}, \mathrm{Osaka}, \mathrm{Tokyo}\}$ are encoded with $(1,0,0)$, $(0,1,0)$, and $(0,0,1)$
  - Called dummy variables

Objective function of training: Squared loss

- Objective function (to minimize): Disagreement measure of the model to the training dataset
  - Loss function: $\ell\left(y^{(i)}, \mathbf{w}^\top \mathbf{x}^{(i)}\right)$ for the i-th instance
  - Objective function: $L(\mathbf{w}) = \sum_{i=1}^{N} \ell\left(y^{(i)}, \mathbf{w}^\top \mathbf{x}^{(i)}\right)$
- Squared loss function:

$$\ell\left(y^{(i)}, \mathbf{w}^\top \mathbf{x}^{(i)}\right) = \left(y^{(i)} - \mathbf{w}^\top \mathbf{x}^{(i)}\right)^2$$

  - Absolute loss, Huber loss: more robust choices
- Optimal parameter $\mathbf{w}^*$ is the one that minimizes $L(\mathbf{w})$:

$$\mathbf{w}^* = \operatorname{argmin}_{\mathbf{w}} L(\mathbf{w})$$

Solution of linear regression problem: One dimensional case

- Let us start with a case where inputs and outputs are both one-dimensional

- Objective function to minimize:

$$L(w) = \sum_{i=1}^{N} \left(y^{(i)} - wx^{(i)}\right)^2$$

- Solution: $w^* = \frac{\sum_{i=1}^{N} y^{(i)} x^{(i)}}{\sum_{i=1}^{N} {x^{(i)}}^2} = \frac{\mathrm{Cov}(x,y)}{\mathrm{Var}(x)}$

  – Solve $\frac{\partial L(w)}{\partial w} = 0$

Solution of linear regression problem: General multi-dimensional case

- Matrix and vector notations:
  - Design matrix $\boldsymbol{X} = \left[\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(N)}\right]^\top$
  - Target vector $\mathbf{y} = \left(y^{(1)}, y^{(2)}, \dots, y^{(N)}\right)^\top$
- Objective function:

$$L(\mathbf{w}) = \sum_{i=1}^{N}\left(y^{(i)} - \mathbf{w}^\top\mathbf{x}^{(i)}\right)^2 = \|\mathbf{y} - \boldsymbol{X}\mathbf{w}\|_2^2$$

$$= (\mathbf{y} - \boldsymbol{X}\mathbf{w})^\top(\mathbf{y} - \boldsymbol{X}\mathbf{w})$$

- Solution: $\mathbf{w}^* = \mathrm{argmin}_{\mathbf{w}}\, L(\mathbf{w}) = (\boldsymbol{X}^\top\boldsymbol{X})^{-1}\boldsymbol{X}^\top\mathbf{y}$

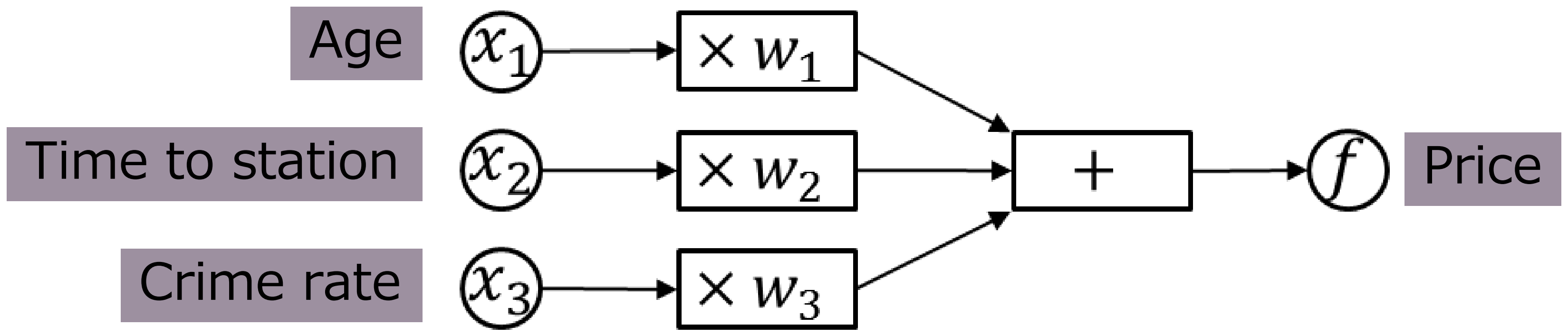
Example:
House price prediction

- Design matrix:

$$\boldsymbol{X} = \left[\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \mathbf{x}^{(3)}, \mathbf{x}^{(4)}\right]^\top = \left[\begin{pmatrix} 15 \\ 10 \\ 1.0 \end{pmatrix}, \begin{pmatrix} 3 \\ 1 \\ 0.1 \end{pmatrix}, \begin{pmatrix} 35 \\ 5 \\ 7.0 \end{pmatrix}, \begin{pmatrix} 40 \\ 70 \\ 1.0 \end{pmatrix}\right]^\top$$

- Target vector:

$$\mathbf{y} = \left(y^{(1)}, y^{(2)}, y^{(3)}, y^{(4)}\right)^\top = (140, 85, 220, 115)^\top$$



Regularization

Ridge regression: Include penalty on the norm of $\mathbf{w}$ to avoid instability

- Existence of the solution $\mathbf{w}^* = (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}\mathbf{y}$ requires that $\boldsymbol{X}^\top \boldsymbol{X}$ is non-singular, i.e. full-rank
  - This is often secured when the number of data instances N is much larger than the number of dimensions D
- Regularization: Adding some constant $\lambda > 0$ to the diagonals of $\boldsymbol{X}^\top \boldsymbol{X}$ for numerical stability
  - Modified solution: $\mathbf{w}^* = (\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I})^{-1} \boldsymbol{X}^\top \mathbf{y}$
- Back to its objective function, the new solution corresponds to

$$L(\mathbf{w}) = ||\mathbf{y} - \boldsymbol{X}\mathbf{w}||_2^2 + \lambda ||\mathbf{w}||_2^2$$

  - $\lambda ||\mathbf{w}||_2^2$ is called a (L2-)regularization term

Overfitting:
Degradation of predictive performance for future data

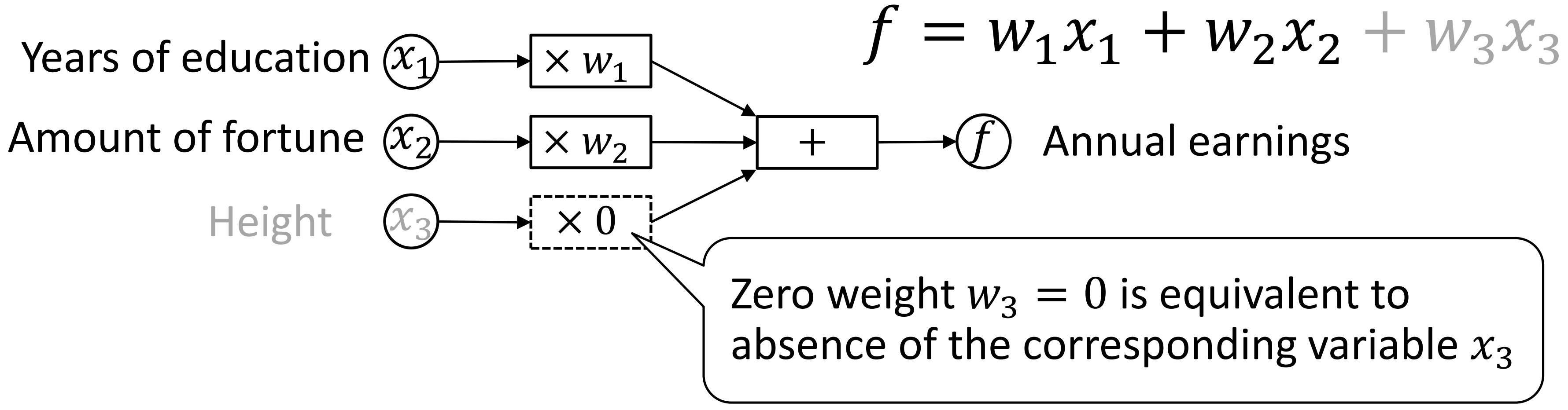
- Previously, we introduced the regularization term to avoid numerical stability
- Another interpretation: To avoid *overfitting* to the training data
  - Our goal is to make correct predictions for future data, not for the training data
  - Overfitting: Too much adaptation to the training data degrades predictive performance on future data
- When the number of data instances N is less than the number of dimensions D, the solution is not unique
  - Infinite number of solutions exist

Occam's razor: Adopt the simplest model

- We have infinite number of models that equally fit to the training data (=minimize the loss function)
  - Some perform well, some perform badly
- Which is the "best" model among them?
- Occam's razor principle: "Take the simplest model"
  - We will discuss why the simple model is good later in the "statistical learning theory"
- What is the measure of simplicity?
  For example, number of features = the number of non-zero elements in $\mathbf{w}$

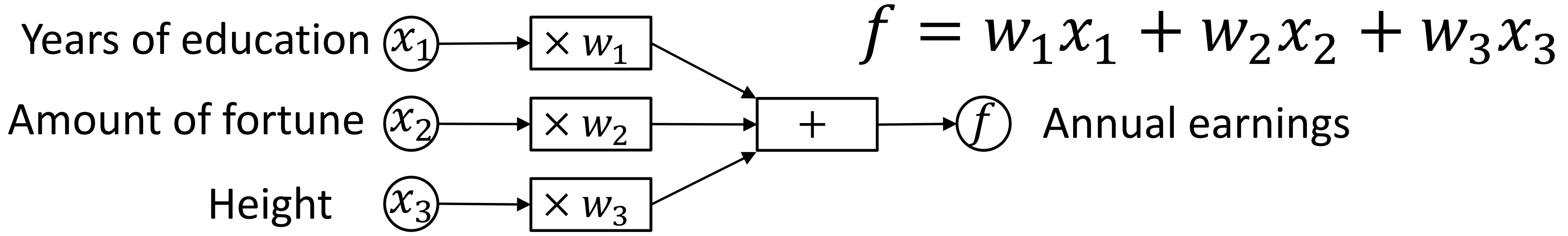
Occam's razor:
Prefers models with smaller number of variables

- Occam's razor principle prefers



Zero weight $w_3 = 0$ is equivalent to absence of the corresponding variable x_3

to



0-norm regularization: Reduces the number of non-zero elements in $\mathbf{w}$

- Number of non-zero elements in $\mathbf{w}$ = "0-norm of $\mathbf{w}$"

Number of features used in the model

- Use 0-norm constraint:

$$\text{minimize}_{\mathbf{w}} \; \|\mathbf{y} - \boldsymbol{X}\mathbf{w}\|_2^2 \;\; \text{s.t.} \;\; \|\mathbf{w}\|_0 \leq \eta$$

or 0-norm penalty:

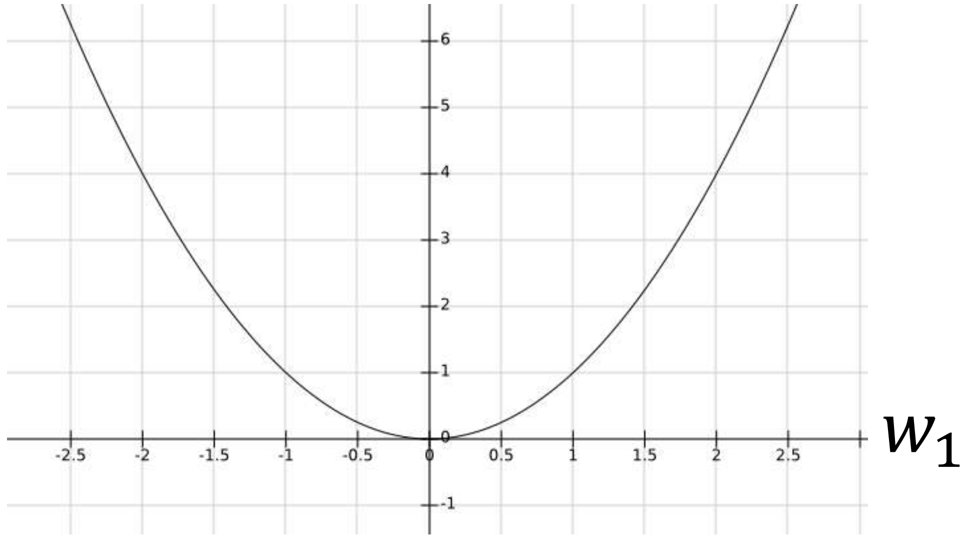
$$\text{minimize}_{\mathbf{w}} \; \|\mathbf{y} - \boldsymbol{X}\mathbf{w}\|_2^2 + \lambda\|\mathbf{w}\|_0$$

  – There is some one-to-one correspondence between η and λ

- However, they are non-convex optimization problems …
  – Hard to find the optimal solution

Ridge regression :
2-norm regularization as a convex surrogate for 0-norm

- Instead of the zero-norm $||\mathbf{w}||_0$, we use 2-norm $||\mathbf{w}||_2^2$



- Ridge regression: $L(\mathbf{w}) = ||\mathbf{y} - \boldsymbol{X}\mathbf{w}||_2^2 + \lambda||\mathbf{w}||_2^2$

Convex ☺

  – Can be seen as a relaxed(?) version of

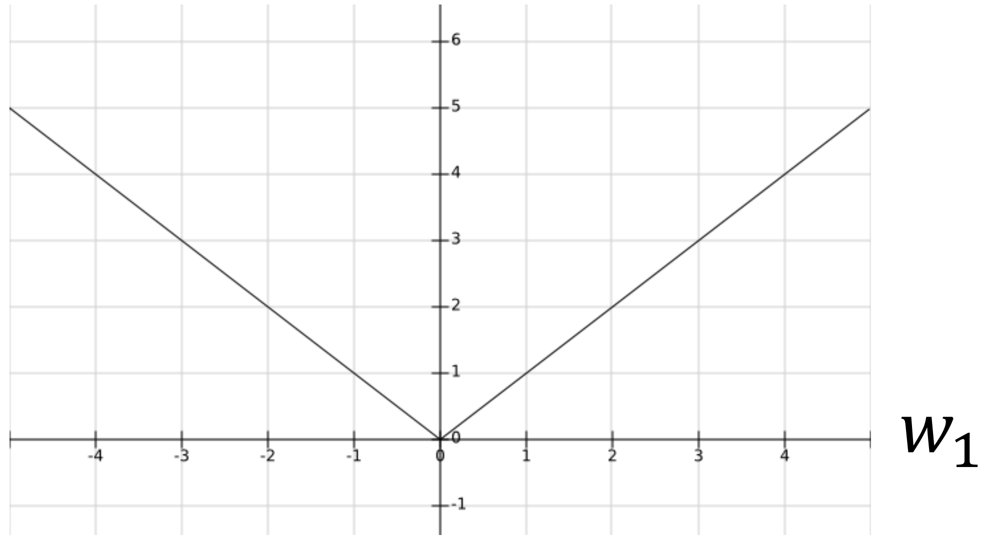
$$L(\mathbf{w}) = ||\mathbf{y} - \boldsymbol{X}\mathbf{w}||_2^2 + \lambda||\mathbf{w}||_0$$

Non-convex ☹

  – The closed form solution: $\mathbf{w}^* = (\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I})^{-1}\boldsymbol{X}^\top \mathbf{y}$

Lasso :
1-norm regularization further induces sparsity

- Instead, we can use 1-norm $\|\mathbf{w}\|_1 = |w_1| + |w_2| + \cdots + |w_D|$



- Lasso: $L(\mathbf{w}) = \|\mathbf{y} - \boldsymbol{X}\mathbf{w}\|_2^2 + \lambda\|\mathbf{w}\|_1$
  – Convex optimization, but no closed form solution
- Sparsity inducing norm: 1-norm induces sparse $\mathbf{w}^*$

Statistical Interpretation

Interpretation as statistical inference : Regression as maximum likelihood estimation

- So far we have formulated the regression problem in *loss minimization framework*
  - Function (prediction model) $f: \mathcal{X} \to \Re$ is deterministic
  - Least squares: Minimization of the sum of squared losses
- We have not considered any statistical inference
- Actually, we can interpret the previous formulation in a statistical inference framework, namely, *maximum likelihood estimation*

Maximum likelihood estimation (MLE): Find the parameter that best reproduces training data

- We consider f as a conditional distribution $f_{\mathbf{w}}(y|\mathbf{x})$

Conditional probability

- Maximum likelihood estimation (MLE):
  - Find $\mathbf{w}$ that maximizes the likelihood function: $L(\mathbf{w}) = \prod_{i=1}^{N} f_{\mathbf{w}}(y^{(i)}|\mathbf{x}^{(i)})$
    - Likelihood function: Probability that the training data is reproduced by the model
    - We assume i.i.d. (which will be explained next)
  - It is often convenient to use *log* likelihood instead:

$$L(\mathbf{w}) = \sum_{i=1}^{N} \log f_{\mathbf{w}}(y^{(i)}|\mathbf{x}^{(i)})$$

Important assumption on data: Identically and independently distributed

- We assume data are *identically and independently distributed*:
  - Data instances are generated from the same data generation mechanism (i.e. probability distribution)
    - Furthermore, past data (training data) and future data (test data) have the same property
  - Data instances are independent of each other

Probabilistic version of the linear regression model: Gaussian linear model

- Probabilistic version of the linear regression model $y = \mathbf{w}^\top \mathbf{x}$
- $y \sim \mathcal{N}\left(\mathbf{w}^\top \mathbf{x}, \sigma^2\right)$: Gaussian distribution with mean $\mathbf{w}^\top \mathbf{x}$ and variance σ^2

$$f_{\mathbf{w}}(y|\mathbf{x}) = \mathcal{N}\left(\mathbf{w}^\top \mathbf{x}, \sigma^2\right) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y - \underbrace{\mathbf{w}^\top \mathbf{x}}_{\text{Linear regression model}})^2}{2\sigma^2}\right)$$

  – In other words, $y = \mathbf{w}^\top \mathbf{x} + \epsilon$, where $\epsilon \sim \mathcal{N}\left(0, \sigma^2\right)$

Relation between least squares and MLE: Maximum likelihood is equivalent to least squares

- Log-likelihood function:

$$L(\mathbf{w}) = \sum_{i=1}^{N} \log f_{\mathbf{w}}(y^{(i)}|\mathbf{x}^{(i)})$$

$$= \sum_{i=1}^{N} \log \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\left(y^{(i)} - \mathbf{w}^\top \mathbf{x}^{(i)}\right)^2}{2\sigma^2}\right)$$

$$= -\frac{1}{2\sigma^2}\sum_{i=1}^{N}\left(y^{(i)} - \mathbf{w}^\top \mathbf{x}^{(i)}\right)^2 + \mathrm{const.}$$

- Maximization of $L(\mathbf{w})$ is equivalent to minimization of the squared loss $\sum_{i=1}^{N}\left(y^{(i)} - \mathbf{w}^\top \mathbf{x}^{(i)}\right)^2$

Some More Applications

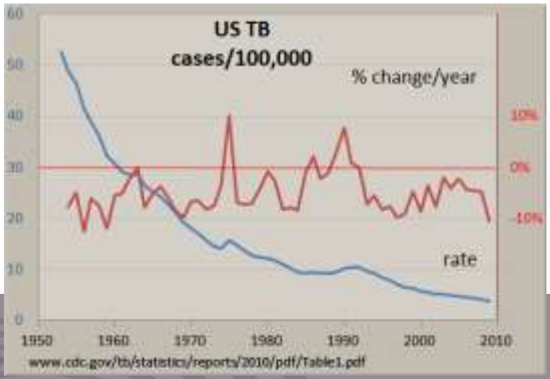
Time series prediction: Auto regressive (AR) model

- Time series data: A sequence of real valued data $x_1, x_2, \ldots, x_t, \ldots \in \Re$ associated with time stamps $t = 1,2,\ldots$
- Time series prediction: Given $x_1, x_2, \ldots, x_{t-1}$, predict x_t
- Auto regressive (AR) model:

$$x_t = w_1 x_{t-1} + w_2 x_{t-2} + \cdots + w_D x_{t-D}$$

  – x_t is determined by the recent length-D history

- AR model as a linear regression model $y = \mathbf{w}^\top \mathbf{x}$:
  – $\mathbf{w} = (w_1, w_2, \ldots, w_D)^\top$
  – $\mathbf{x} = (x_{t-1}, x_{t-2}, \ldots, x_{t-D})^\top$



Classification as regression: Regression is also applicable to classification

- Binary classification: $y \in \{+1, -1\}$
- Apply regression to predict $y \in \{+1, -1\}$
- Rigorously, such application is not valid
  - Since an output is either $+1$ or -1, the Gaussian noise assumption does not hold
  - However, since solution of regression is often easier than that of classification, this application can be compromise
- Fisher discriminant: Instead of $\{+1, -1\}$, use $\left\{+\frac{1}{N^+}, -\frac{1}{N^-}\right\}$
  - $N^+ (N^-)$ is the number of positive (negative) data

Nonlinear Regression

Nonlinear regression: Introducing nonlinearity in linear models

- So far we have considered only linear models
- How to introduce non-linearity in the models?

1. Introduce nonlinear basis functions:
   - Transformed features: e.g. $x \to \log x$
   - Cross terms: e.g. $x_1, x_2 \to x_1 x_2$
   - Kernels: $\mathbf{x} \to \boldsymbol{\phi}(\mathbf{x})$ (some nonlinear mapping to a high-dimensional space)
2. Intrinsically nonlinear models:
   - Regressoin tree / random forest
   - Neural network

Nonlinear transformation of features: Simplest way to introduce nonlinearity in linear models

- Nonlinear basis function: $x \rightarrow \log x, e^x, x^2, \frac{1}{x}, \dots$
  - Sometimes used for converting the range
    - E.g. $\log: \mathfrak{R}^+ \rightarrow \mathfrak{R}$, $\exp: \mathfrak{R} \rightarrow \mathfrak{R}^+$
- Interpretations of log transformation:

	y	$\log y$
x	$y = \beta x + \alpha$ Increase of x by 1 will increase y by β	$\log y = \beta x + \alpha$ Increase of x by 1 will multiply y by $1 + \beta$
$\log x$	$y = \beta \log x + \alpha$ Doubling x will increase y by β	$\log y = \beta \log x + \alpha$ Doubling x will multiply y by $1 + \beta$

Cross terms:
Can include synergetic effects among different features

- Not only the original features $x_1, x_2, \dots, x_D$, use their cross terms products $\{x_d x_{d'}\}_{d,d'}$

- Model has a matrix parameter $\boldsymbol{W}$:

$$y = \mathrm{Trace}\left(\begin{bmatrix} w_{1,1} & \cdots & w_{1,D} \\ \vdots & \ddots & \vdots \\ w_{D,1} & \cdots & w_{D,D} \end{bmatrix}^\top \begin{bmatrix} x_1^2 & x_1 x_2 & \cdots & x_1 x_D \\ x_2 x_1 & x_2^2 & & x_2 x_D \\ \vdots & & \ddots & \vdots \\ x_D x_1 & x_D x_2 & \cdots & x_D^2 \end{bmatrix} \right)$$

$$= \mathbf{x}^\top \boldsymbol{W}^\top \mathbf{x}$$

- $L(\boldsymbol{W}) = \sum_{i=1}^{N} \left(y^{(i)} - \mathbf{x}^{(i)\top} \boldsymbol{W}^\top \mathbf{x}^{(i)} \right)^2 + \lambda \|\boldsymbol{W}\|_{\mathrm{F}}^2$

(e.g. factorization machines)

Kernels: Linear model in a high-dimensional feature space

- High dimensional non-linear mapping: $\mathbf{x} \to \boldsymbol{\phi}(\mathbf{x})$
  - $\boldsymbol{\phi}: \Re^D \to \Re^{\bar{D}}$ is some nonlinear mapping from D-dimensional space to a $\bar{D}$-dimensional space ($D \ll \bar{D}$)
- Linear model $y = \bar{\mathbf{w}}^\top \boldsymbol{\phi}(\mathbf{x})$
- Kernel regression model: $y = \sum_{i=1}^{N} \alpha^{(i)} k\left(\mathbf{x}^{(i)}, \mathbf{x}\right)$
  - Kernel function $k\left(\mathbf{x}^{(i)}, \mathbf{x}\right) = \langle \boldsymbol{\phi}\left(\mathbf{x}^{(i)}\right), \boldsymbol{\phi}(\mathbf{x}) \rangle$: inner product
  - Kernel trick: Instead of working in the $\bar{D}$-dimensional space, we use an equivalent form in an N -dimensional space
    - Foundation of kernel machines, e.g. SVM, Gaussian process, ...

Bayesian Statistical Interpretation

Bayesian interpretation of regression: Ridge regression as MAP estimation

- We consider another statistical interpretation of linear regression in terms of Bayesian statistics
  - Which justifies ridge regression
- Ridge regression as MAP estimation
  - Posterior distribution of parameters
  - Maximum A Posteriori (MAP) estimation

Least square regression $\Longleftrightarrow$ Maximum likelihood estimation

Ridge regression $\Longleftrightarrow$ MAP estimation

Bayesian modeling: Posterior distribution instead of likelihood

- In maximum likelihood estimation (MLE), we obtain $\mathbf{w}$ that maximizes data *likelihood*:

$$P(\mathbf{y} \mid \boldsymbol{X}, \mathbf{w}) = \prod_{i=1}^{N} f_{\mathbf{w}}(y^{(i)}|\mathbf{x}^{(i)})$$

or $\log P(\mathbf{y} \mid \boldsymbol{X}, \mathbf{w}) = \sum_{i=1}^{N} \log f_{\mathbf{w}}(y^{(i)}|\mathbf{x}^{(i)})$

  – The probability of the data reproduced with the parameter: $P(\text{Data} \mid \text{Parameters})$

- In Bayesian modeling, we consider the *posterior distribution* $P(\text{ Parameters} \mid \text{Data })$

  – Posterior distribution is the distribution over model parameters given data

Posterior distribution:
Log posterior = log likelihood + log prior

- Posterior distribution:

$$P(\text{Parameters} \mid \text{Data}) = \frac{P(\text{Data} \mid \text{Parameters})P(\text{Parameters})}{P(\text{Data})}$$

(Bayes' formula)

- Log posterior:

$$\log P(\text{Parameters} \mid \text{Data}) = \underbrace{\log P(\text{Data} \mid \text{Parameters})}_{\text{Likelihood}} + \underbrace{\log P(\text{Parameters})}_{\text{Prior}} - \log P(\text{Data})$$

  - $P(\text{Data})$ is a constant term and often neglected because it does not depend on the parameters

Maximum a posteriori (MAP) estimation: Find parameter that maximizes the posterior

- Maximum a posteriori (MAP) estimation finds the parameter that maximizes the (log) posterior:
  $\text{Parameters}^* = \text{argmax}_{\text{Parameters}} \log P(\text{ Parameters} \mid \text{Data })$

- Maximization of the log posterior:
  $\log P(\text{ Parameters} \mid \text{Data })$
  $= \log P(\text{ Data} \mid \text{Parameters }) + \log P(\text{Parameters}) + \text{const.}$

  - MLE considers only $\log P(\text{ Data} \mid \text{Parameters })$
  - MAP has an additional term (log prior) : $\log P(\text{Parameters})$

Ridge regression as MAP estimation: MAP with Gaussian linear model + Gaussian prior

- Log posterior: $\log P(\text{ Parameters } | \text{ Data })=$
  $$\underbrace{\log P(\text{ Data } | \text{ Parameters })}_{\text{Log likelihood}} + \underbrace{\log P(\text{Parameters})}_{\text{Log prior}} + \text{const.}$$
  - Log-likelihood: $\sum_{i=1}^{N} \log \frac{1}{\sqrt{2\pi}\sigma'} \exp\left(-\frac{\left(y^{(i)}-\mathbf{w}^\top\mathbf{x}^{(i)}\right)^2}{2\sigma'^2}\right)$
  - Prior $P(\mathbf{w}) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\mathbf{w}^\top\mathbf{w}}{2\sigma^2}\right)$ (Gaussian prior)
- Ridge regression is equivalent to MAP estimation:

$$\mathbf{w}^* = \operatorname{argmin}_{\mathbf{w}} \frac{1}{2\sigma^2}\sum_{i=1}^{N}\left(y^{(i)} - \mathbf{w}^\top\mathbf{x}^{(i)}\right)^2 + \frac{1}{2\sigma'^2}\|\mathbf{w}\|_2^2$$

Regression: Supervised learning for predicting a real valued variable

- A supervised learning problem to make real-valued predictions
- Regression problem is often formulated as a least-square minimization problem
  - Closed form solution is given
- Regularization framework to avoid overfitting
  - Reduce the number of features: 0-norm, 2-norm (ridge regression), 1-norm (lasso)
- Nonlinear regression
- Statistical interpretations: maximum likelihood estimation, maximum a posteriori (MAP) estimation