CSC2515 Tutorial 3

Jan 27 2015

Presented by Ali Punjani

Outline

- Multivariate Linear Regression, Demo
- Cross-Validation, Review
- *k*-NN Classification, Demo

Multivariate Linear Regression

- We want to predict output, such as the median house price, from multi-dimensional observations

- Each house is a data point *n*, with observations indexed by *j*:

$$\mathbf{x}^{(n)} = (x_1^{(n)}, \ldots, x_d^{(n)})$$

- Simple predictor is analogue of linear classifier, producing real-valued *y* for input **x** with parameters **w** (assuming $x_0 = 1$):

$$y = w_0 + \sum_{j=1}^{d} w_j x_j = \mathbf{w}^T \mathbf{x}$$

Multivariate Data

- Multiple measurements (sensors)
- d inputs/features/attributes
- N instances/observations/examples

$$\mathbf{X} = \begin{bmatrix} X_1^1 & X_2^1 & \cdots & X_d^1 \\ X_1^2 & X_2^2 & \cdots & X_d^2 \\ \vdots & & & \\ X_1^N & X_2^N & \cdots & X_d^N \end{bmatrix}$$

Multivariate Parameters

$$\text{Mean:} E[\mathbf{x}] = [\mu_1, ..., \mu_d]^T$$

$$\text{Covariance:} \sigma_{ij} \equiv \text{Cov}(X_i, X_j)$$

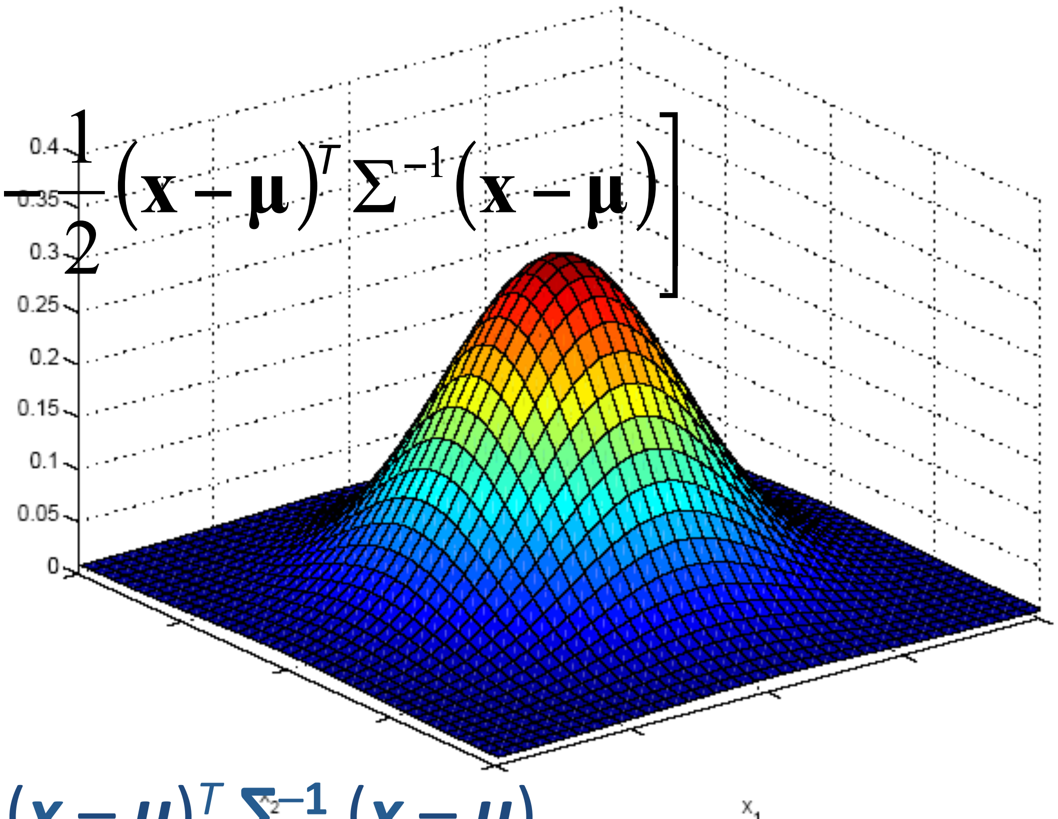
$$\text{Correlation: Corr}(X_i, X_j) \equiv \rho_{ij} = \frac{\sigma_{ij}}{\sigma_i \sigma_j}$$

$$\Sigma \equiv \text{Cov}(\mathbf{X}) = E\left[(\mathbf{X} - \mu)(\mathbf{X} - \mu)^T\right] = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1d} \\ \sigma_{21} & \sigma_2^2 & \cdots & \sigma_{2d} \\ \vdots & & & \\ \sigma_{d1} & \sigma_{d2} & \cdots & \sigma_d^2 \end{bmatrix}$$

Multivariate Normal Distribution

$$\mathbf{x} \sim \mathcal{N}_d(\boldsymbol{\mu}, \Sigma)$$

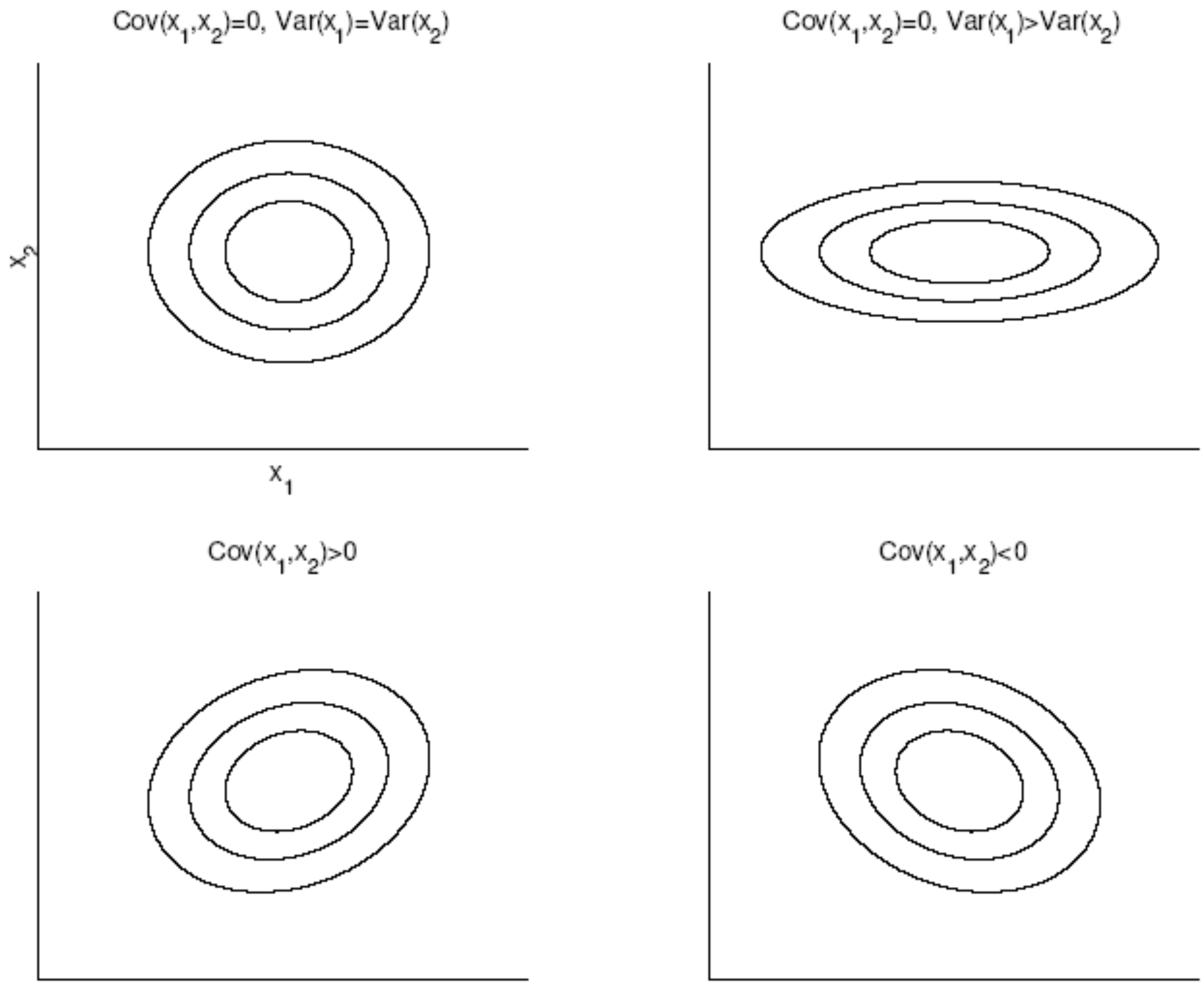
$$p(\mathbf{x}) = \frac{1}{(2\pi)^{d/2} |\Sigma|^{1/2}} \exp\left[-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right]$$

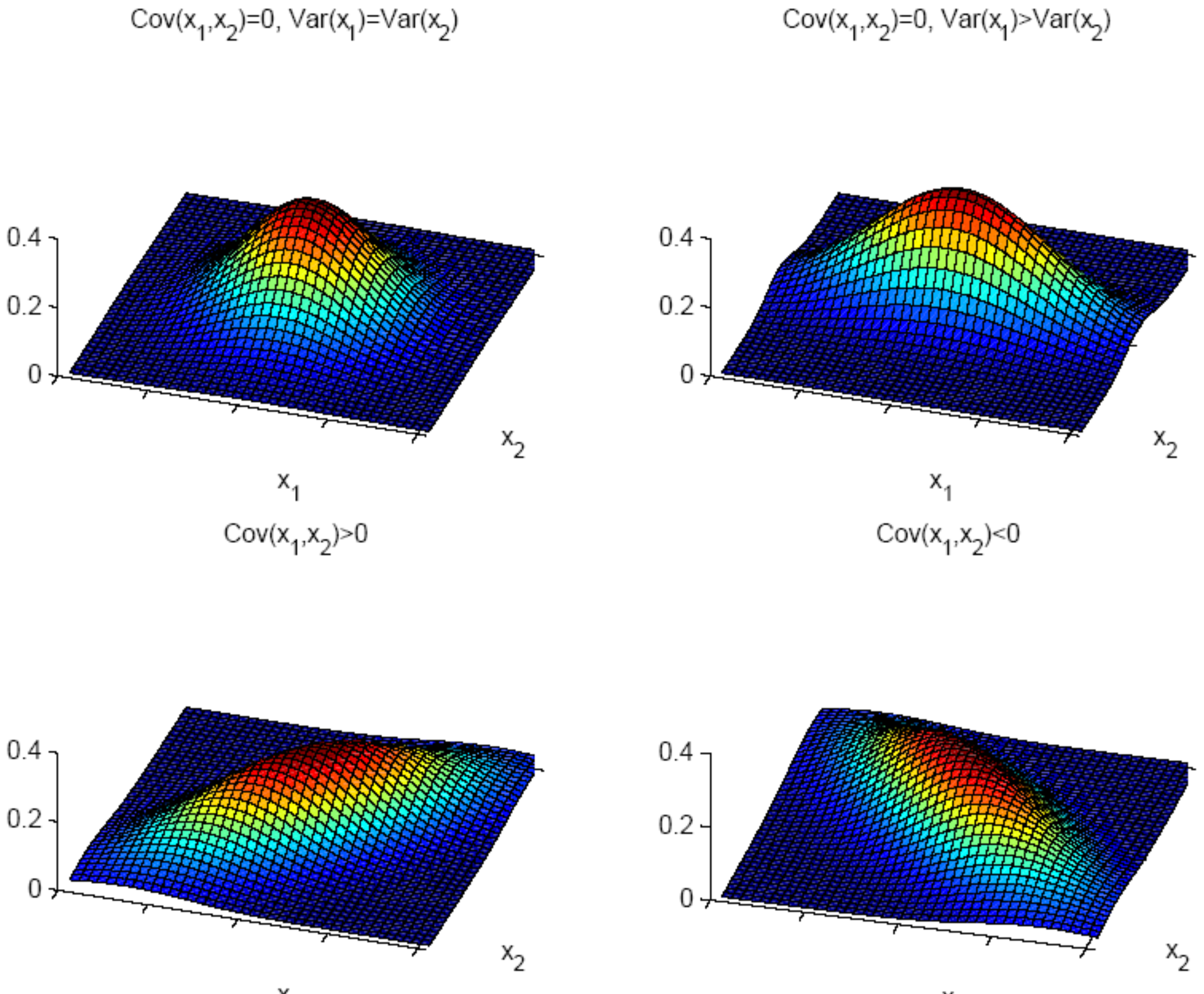


- Mahalanobis distance: $(\boldsymbol{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{x} - \boldsymbol{\mu})$

  measures the distance from $\boldsymbol{x}$ to $\boldsymbol{\mu}$ in terms of Σ (normalizes for difference in variances and correlations)

Bivariate Normal




Cov(x1,x2)=0, Var(x1)=Var(x2)
Cov(x1,x2)=0, Var(x1)>Var(x2)
Cov(x1,x2)>0
Cov(x1,x2)<0
0.4
0.2
0
x1
x2

Independent Inputs: Naive Bayes

- If x_i are independent, offdiagonals of ∑ are 0, Mahalanobis distance reduces to weighted (by $1/\sigma_i$) Euclidean distance:

$$p(\mathbf{x}) = \prod_{i=1}^{d} p_i(x_i) = \frac{1}{(2\pi)^{d/2} \prod_{i=1}^{d} \sigma_i} \exp\left[-\frac{1}{2} \sum_{i=1}^{d} \left(\frac{x_i - \mu_i}{\sigma_i} \right)^2 \right]$$

- If variances are also equal, reduces to Euclidean distance

Parametric Classification

- If $p\,(\boldsymbol{x} \mid C_i) \sim N\,(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$

$$p(\mathbf{x} \mid C_i) = \frac{1}{(2\pi)^{d/2} |\Sigma_i|^{1/2}} \exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_i)^T \Sigma_i^{-1} (\mathbf{x}-\boldsymbol{\mu}_i)\right]$$

- Discriminant functions

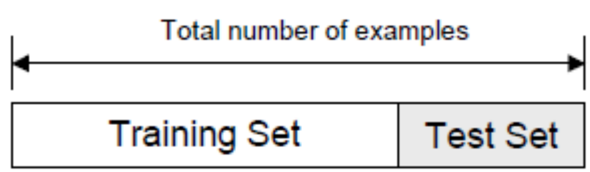
$$\begin{aligned} g_i(\mathbf{x}) &= \log p(\mathbf{x} \mid C_i) + \log P(C_i) \\ &= -\frac{d}{2}\log 2\pi - \frac{1}{2}\log|\Sigma_i| - \frac{1}{2}(\mathbf{x}-\mu_i)^T \Sigma_i^{-1} (\mathbf{x}-\mu_i) + \log P(C_i) \end{aligned}$$

MATLAB Demo

- Multivariate Linear Regression

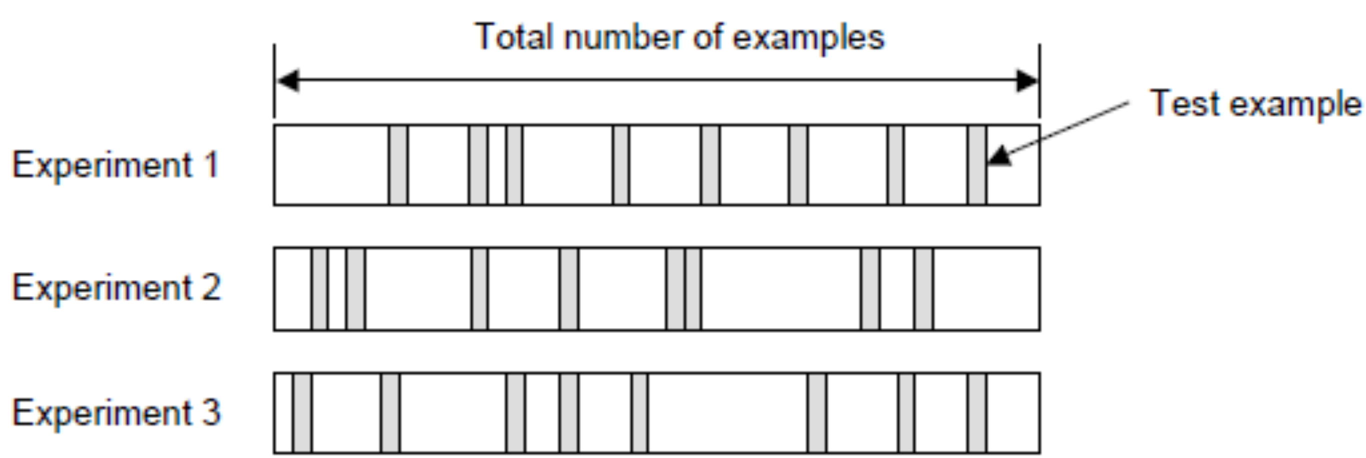
Cross-Validation

- why validation?
  - performance estimation
  - model selection (e.g. hyper parameters)
- hold-out validation
  - **split dataset into training set and test set**
  - drawbacks: waste of dataset, estimation of error rate maybe misleading
- cross-validation



Cross-Validation

- **random subsampling**
- k-fold cross-validation
- leave-1-out cross-validation (k=N)



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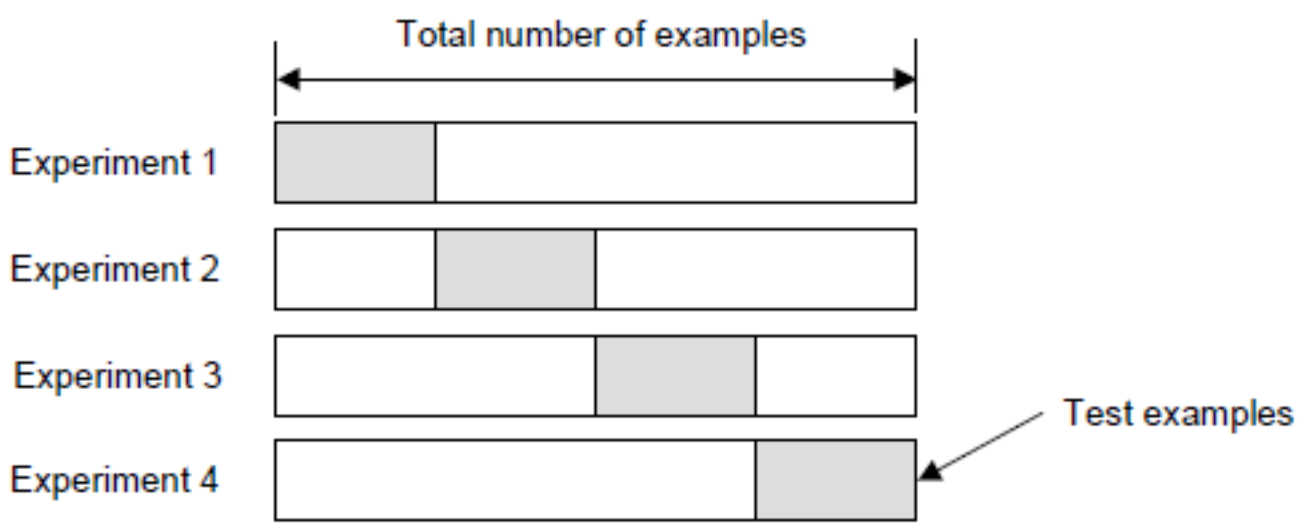

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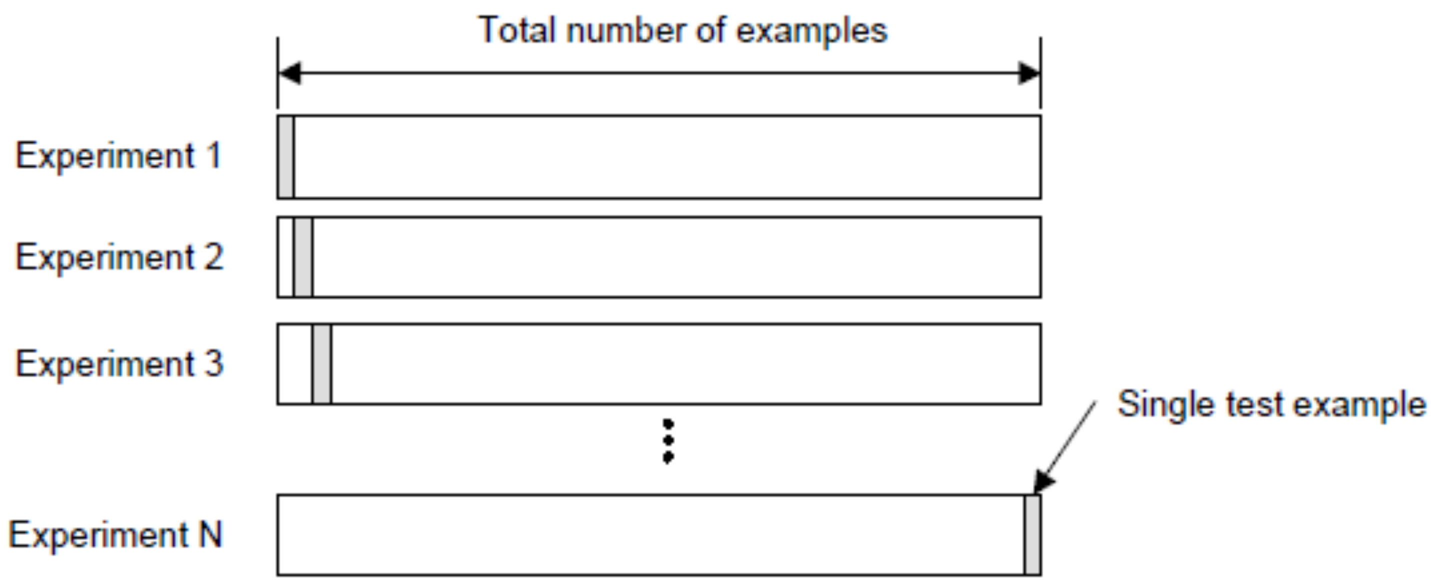

Cross-Validation

- how many folds do we need ?
- with larger k
  - error estimation tends to be more accurate
  - but computational time will be larger
- in practice, larger dataset, smaller k
- a common choice for k-fold cross-validation is k = 10

Some Issues with Cross-Validation

- intensive use of cross-validation can overfit if you explore too many models, by tuning hyper parameters to predict the whole training set well
    - hold out an additional test set before doing any model selection. Check the best model performs well even on the additional test set
- time consuming (always if done naively)
    - there are efficient tricks that can save work over brute force

k-Nearest Neighbors

- *k*-NN is a simple algorithm which stores all available training examples and predict value/class of an unseen instance based on a similarity measure
    - *k* = 1
        - predict the same value/class as the nearest instance in the training set
    - *k* > 1
        - find the k closet training examples
        - predict class: majority vote
        - predict value: average weighted by inverse distance
- memory based, no explicit training or model

k-NN Classification

- similarity measure: Euclidean distance, etc.
  - assumption behind Euclidean distance: uncorrelated inputs with equal variances
- predict class: majority vote
- *k* preferably odd to avoid ties for binary classification
- choice of *k*
  - smaller *k*: higher variance (less stable)
  - larger *k*: higher bias (less precise)
  - cross-validation can help
- MATLAB demo