ECE 5984: Introduction to Machine Learning

Topics:

- Regression

Readings: Barber 17.1, 17.2

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Administrativia

- HW1
  - Due on Sun 02/15, 11:55pm
  - http://inclass.kaggle.com/c/VT-ECE-Machine-Learning-HW1

- Project Proposal
  - Due: Tue 02/24, 11:55 pm
  - <=2pages, NIPS format

- HW2
  - Out today
  - Due on Friday 03/06, 11:55pm
  - Please please please please please start early
  - Implement linear regression, Naïve Bayes, Logistic Regression

Recap of last time

Learning a Gaussian

- Collect a bunch of data
  - Hopefully, i.i.d. samples
  - e.g., exam scores
- Learn parameters
  - Mean
  - Variance

$$P(x \mid \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

MLE for Gaussian

- Prob. of i.i.d. samples $D=\{x_1,\ldots,x_N\}$:

$$P(\mathcal{D} \mid \mu, \sigma) = \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^N \prod_{i=1}^{N} e^{\frac{-(x_i-\mu)^2}{2\sigma^2}}$$

- Log-likelihood of data:

$$\begin{aligned} \ln P(\mathcal{D} \mid \mu, \sigma) &= \ln\left[\left(\frac{1}{\sigma\sqrt{2\pi}}\right)^N \prod_{i=1}^{N} e^{\frac{-(x_i-\mu)^2}{2\sigma^2}}\right] \\ &= -N \ln \sigma\sqrt{2\pi} - \sum_{i=1}^{N} \frac{(x_i-\mu)^2}{2\sigma^2} \end{aligned}$$

Your second learning algorithm: MLE for mean of a Gaussian

- What's MLE for mean?

$$\frac{d}{d\mu} \ln P(\mathcal{D} \mid \mu, \sigma) = \frac{d}{d\mu}\left[-N \ln \sigma\sqrt{2\pi} - \sum_{i=1}^{N} \frac{(x_i - \mu)^2}{2\sigma^2}\right]$$

Learning Gaussian parameters

- MLE:

$$\widehat{\mu}_{MLE} = \frac{1}{N}\sum_{i=1}^{N} x_i$$

$$\widehat{\sigma}^2_{MLE} = \frac{1}{N}\sum_{i=1}^{N} (x_i - \widehat{\mu})^2$$

Bayesian learning of Gaussian parameters

- Conjugate priors
  - Mean: Gaussian prior
  - Variance: Inverse Gamma or Wishart Distribution

- Prior for mean:

$$P(\mu \mid \eta, \lambda) = \frac{1}{\lambda\sqrt{2\pi}} e^{\frac{-(\mu-\eta)^2}{2\lambda^2}}$$

MAP for mean of Gaussian

$$P(\mu \mid \eta, \lambda) = \frac{1}{\lambda\sqrt{2\pi}} e^{\frac{-(\mu-\eta)^2}{2\lambda^2}} \qquad P(\mathcal{D} \mid \mu, \sigma) = \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^N \prod_{i=1}^{N} e^{\frac{-(x_i-\mu)^2}{2\sigma^2}}$$

$$\frac{d}{d\mu}\left[\ln P(\mathcal{D} \mid \mu) P(\mu)\right] = \frac{d}{d\mu}\left[\ln P(\mathcal{D} \mid \mu) + \ln P(\mu)\right]$$

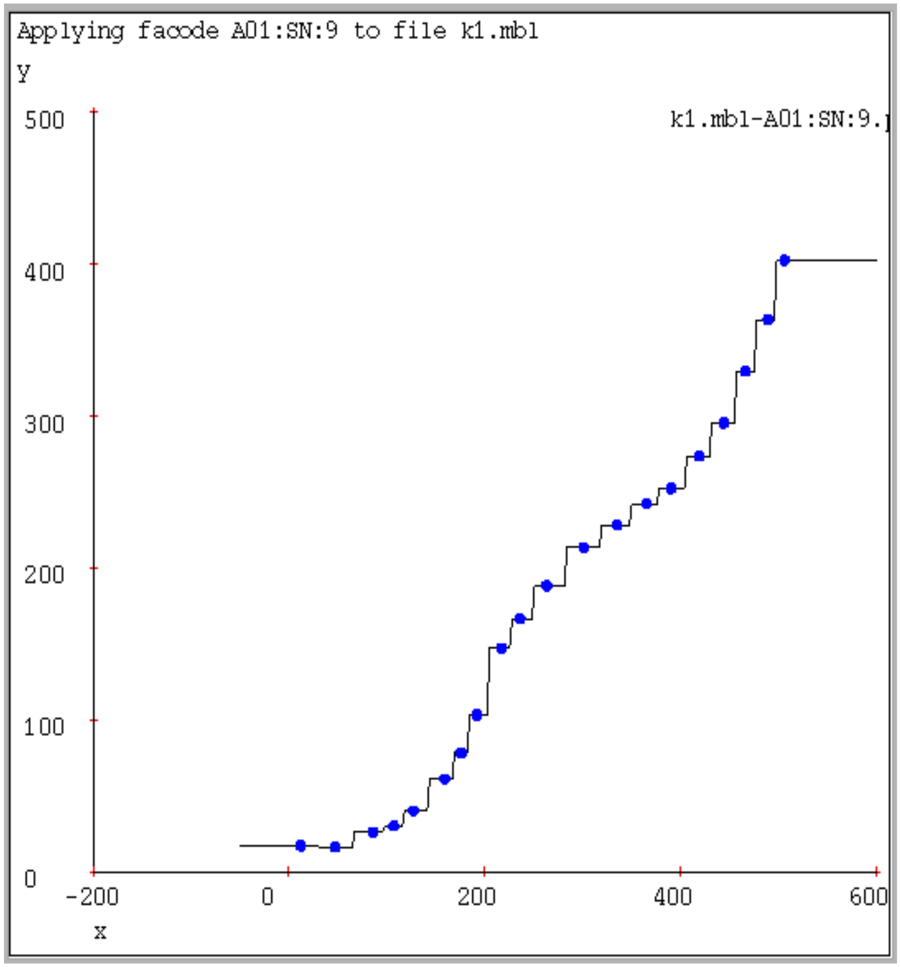
Plan for Today

- Regression
  - Linear Regression
  - Connections with Gaussians

New Topic: Regression

1-NN for Regression

- Often bumpy (overfits)



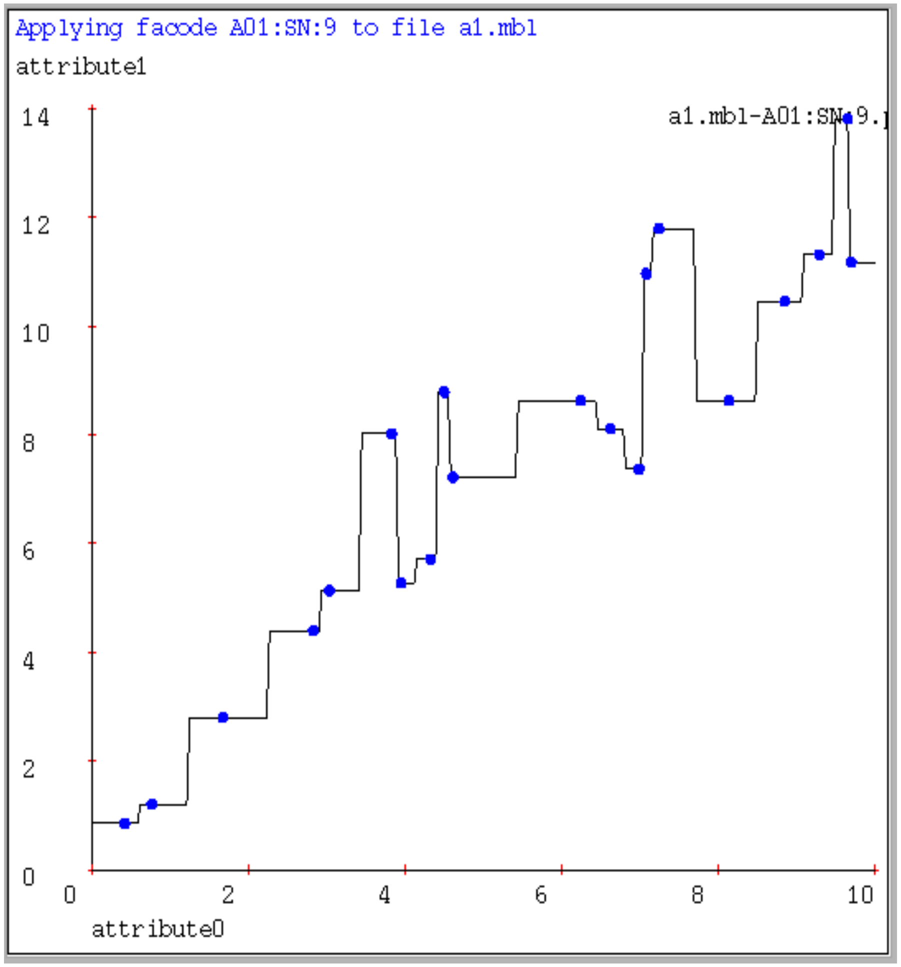
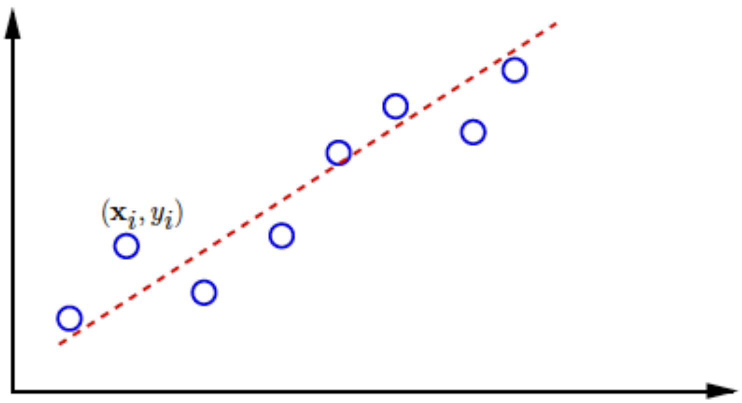


Figure Credit: Andrew Moore

Linear fitting to data

- We want to fit a linear function to an observed set of points $X = [\mathbf{x}_1, \ldots, \mathbf{x}_N]$ with associated labels $Y = [y_1, \ldots, y_N]$.
  - Once we fit the function, we want to use it to *predict* the y for new $\mathbf{x}$.



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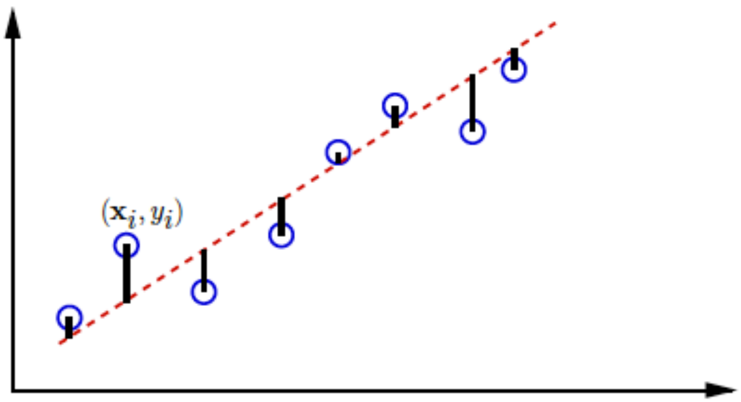
- Least squares (LSQ) fitting criterion: find the function that minimizes sum (or average) of square distances between actual ys in the training set and predicted ones.



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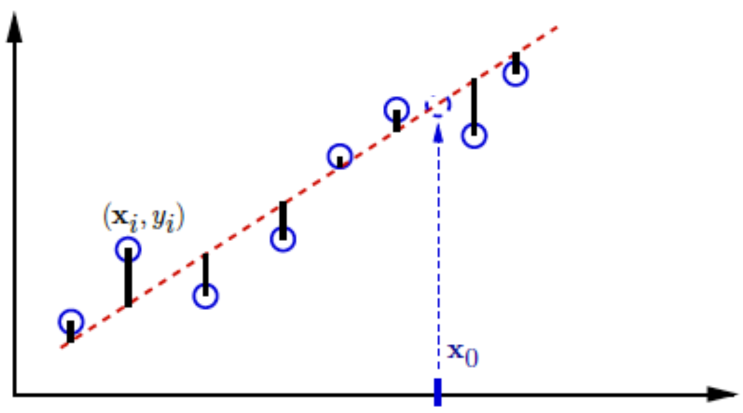


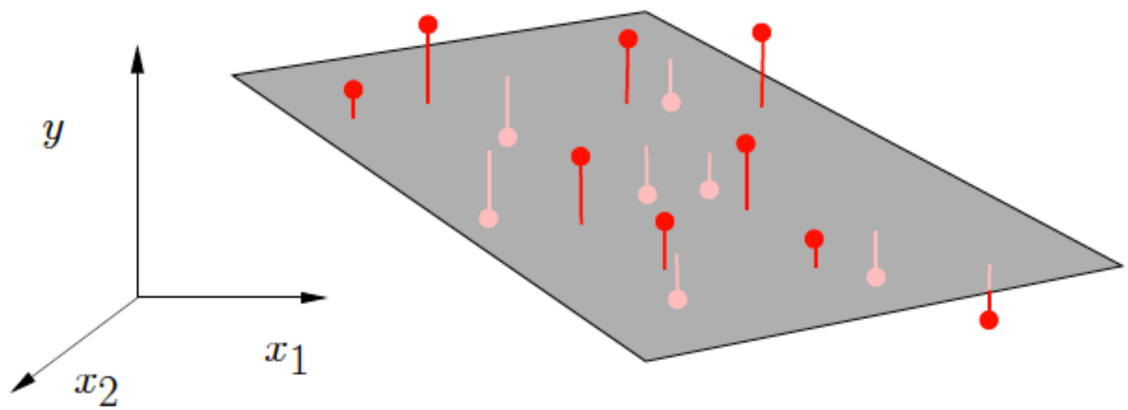
The fitted line is used as a predictor

Linear Regression

- Demo
  - http://hspm.sph.sc.edu/courses/J716/demos/LeastSquares/LeastSquaresDemo.html

Linear functions

- General form: $f(\mathbf{x}; \mathbf{w}) = w_0 + w_1 x_1 + \ldots + w_d x_d$
- 1D case ($\mathcal{X} = \mathbb{R}$): a line
- $\mathcal{X} = \mathbb{R}^2$: a plane



- *Hyperplane* in general, d-D case.

Least squares: estimation

- We need to minimize w.r.t. $\mathbf{w}$

$$L(\mathbf{w}, \mathbf{X}) = L(\mathbf{w}) = \frac{1}{N}\sum_{i=1}^{N}\left(y_i - \mathbf{w}^T\mathbf{x}_i\right)^2$$
$$= \frac{1}{N}\sum_{i=1}^{N}\left(y_i - w_0 - w_1 x_{i1} - \ldots - w_d x_{id}\right)^2$$

- Necessary condition to minimize L: derivatives w.r.t. w_0, w_1,...,w_d must be zero.

Least squares in matrix form

$$\mathbf{X} = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1d} \\ \vdots & & \vdots & \\ 1 & x_{N1} & \cdots & x_{Nd} \end{bmatrix}, \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}, \qquad \mathbf{w} = \begin{bmatrix} w_0 \\ \vdots \\ w_d \end{bmatrix}.$$

- Predictions: $\hat{\mathbf{y}} = \mathbf{X}\mathbf{w}$, errors: $\mathbf{y} - \mathbf{X}\mathbf{w}$, empirical loss:

$$L(\mathbf{w}, \mathbf{X}) = \frac{1}{N}(\mathbf{y} - \mathbf{X}\mathbf{w})^T(\mathbf{y} - \mathbf{X}\mathbf{w})$$

Derivative of loss

$$L(\mathbf{w}) = \frac{1}{N}\left(\mathbf{y}^T - \mathbf{w}^T\mathbf{X}^T\right)(\mathbf{y} - \mathbf{X}\mathbf{w}).$$

$$\frac{\partial \mathbf{a}^T\mathbf{b}}{\partial \mathbf{a}} = \frac{\partial \mathbf{b}^T\mathbf{a}}{\partial \mathbf{a}} = \mathbf{b}, \quad \frac{\partial \mathbf{a}^T\mathbf{B}\mathbf{a}}{\partial \mathbf{a}} = 2\mathbf{B}\mathbf{a}$$

Derivative of loss

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$$\begin{aligned}\frac{\partial L(\mathbf{w})}{\partial \mathbf{w}} &= \frac{1}{N}\frac{\partial}{\partial \mathbf{w}}\left[\mathbf{y}^T\mathbf{y} - \mathbf{w}^T\mathbf{X}^T\mathbf{y} - \mathbf{y}^T\mathbf{X}\mathbf{w} + \mathbf{w}^T\mathbf{X}^T\mathbf{X}\mathbf{w}\right] \\ &= \frac{1}{N}\left[\mathbf{0} - \mathbf{X}^T\mathbf{y} - (\mathbf{y}^T\mathbf{X})^T + 2\mathbf{X}^T\mathbf{X}\mathbf{w}\right] \\ &= -\frac{2}{N}\left(\mathbf{X}^T\mathbf{y} - \mathbf{X}^T\mathbf{X}\mathbf{w}\right)\end{aligned}$$

Least squares solution

$$\frac{\partial}{\partial \mathbf{w}} L(\mathbf{w}) = -\frac{2}{N} \left(\mathbf{X}^T \mathbf{y} - \mathbf{X}^T \mathbf{X} \mathbf{w} \right) = 0$$

Least squares solution

$$\frac{\partial}{\partial \mathbf{w}} L(\mathbf{w}) = -\frac{2}{N}\left(\mathbf{X}^T\mathbf{y} - \mathbf{X}^T\mathbf{X}\mathbf{w}\right) = 0$$

$$\mathbf{X}^T\mathbf{y} = \mathbf{X}^T\mathbf{X}\mathbf{w} \Rightarrow \mathbf{w}^* = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y}$$

- $\mathbf{X}^\dagger \triangleq \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T$ is called the *Moore-Penrose pseudoinverse* of $\mathbf{X}$.
- Linear regression in Matlab:

```
% X(i,:) is i-th example, y(i) is i-th label
wLSQ = pinv([ones(size(X,1),1) X])*y;
```

- Prediction:

$$\hat{y} = \mathbf{w}^{*T}\begin{bmatrix}1\\ \mathbf{x}_0\end{bmatrix} = \mathbf{y}^T\mathbf{X}^{\dagger T}\begin{bmatrix}1\\ \mathbf{x}_0\end{bmatrix}$$

But, why?

- Why sum squared error???
- Gaussians, Watson, Gaussians…

Gaussian noise model

$$y = f(\mathbf{x}; \mathbf{w}) + \nu, \quad \nu \sim \mathcal{N}\left(\nu; 0, \sigma^2\right)$$

- Given the input $\mathbf{x}$, the label y is a random variable

$$p(y|\mathbf{x}; \mathbf{w}, \sigma) \; = \; \mathcal{N}\left(y; \; f(\mathbf{x}; \mathbf{w}), \sigma^2\right)$$

  that is,

$$p(y|\mathbf{x}; \mathbf{w}, \sigma) \; = \; \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(y - f(\mathbf{x}; \mathbf{w}))^2}{2\sigma^2}\right)$$

- This is an explicit model of y that allows us, for instance, to *sample* y for a given $\mathbf{x}$.

MLE Under Gaussian Model

- On board

Is OLS Robust?

- Demo
  - http://www.calpoly.edu/~srein/StatDemo/All.html

- Bad things happen when the data does not come from your model!

- How do we fix this?

Robust Linear Regression

- y ~ Lap(w'x, b)
- On board