Linear Regression

Machine Learning – CSE446
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Prediction of continuous variables

- Billionaire sayz: Wait, that's not what I meant!
- You sayz: Chill out, dude.
- He sayz: I want to predict a continuous variable for continuous inputs: I want to predict salaries from GPA.
- You sayz: **I can regress that…**

The regression problem

- **Instances:** <$\mathbf{x}_j$, t_j>
- **Learn:** Mapping from x to t(**x**)
- **Hypothesis space:**
  - Given, basis functions
  - Find coeffs **w**={w_1,…,w_k}

$$H = \{h_1, \ldots, h_K\}$$

$$\underbrace{t(\mathbf{x})}_{\text{data}} \approx \widehat{f}(\mathbf{x}) = \sum_i w_i h_i(\mathbf{x})$$

  - Why is this called linear regression???
    - model is linear in the parameters

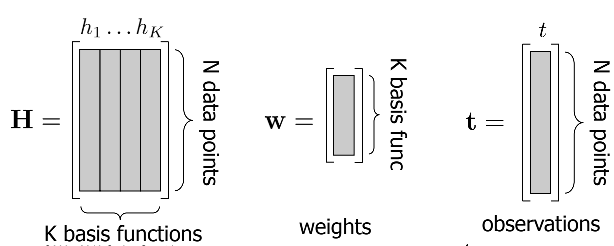
- Precisely, minimize the residual squared error:

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \sum_j \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

The regression problem in matrix notation

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \sum_j \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \underbrace{(\mathbf{H}\mathbf{w} - \mathbf{t})^T (\mathbf{H}\mathbf{w} - \mathbf{t})}_{\text{residual error}}$$



Minimizing the Residual

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \underbrace{(\mathbf{H}\mathbf{w}-\mathbf{t})^T(\mathbf{H}\mathbf{w}-\mathbf{t})}_{\text{residual error}}$$

Regression solution = simple matrix operations

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \underbrace{(\mathbf{H}\mathbf{w}-\mathbf{t})^T(\mathbf{H}\mathbf{w}-\mathbf{t})}_{\text{residual error}}$$

$$\text{solution: } \mathbf{w}^* = \underbrace{(\mathbf{H}^{\mathrm{T}}\mathbf{H})^{-1}}_{\mathbf{A}^{-1}} \underbrace{\mathbf{H}^{\mathrm{T}}\mathbf{t}}_{\mathbf{b}} = \mathbf{A}^{-1}\mathbf{b}$$

$$\text{where } \mathbf{A} = \mathbf{H}^{\mathrm{T}}\mathbf{H} = \underbrace{\begin{bmatrix} \square & \square & \square & \square \\ \square & \square & \square & \square \\ \square & \square & \square & \square \\ \square & \square & \square & \square \end{bmatrix}}_{\substack{\text{k×k matrix} \\ \text{for k basis functions}}} \qquad \mathbf{b} = \mathbf{H}^{\mathrm{T}}\mathbf{t} = \underbrace{\begin{bmatrix} \square \\ \square \\ \square \\ \square \end{bmatrix}}_{\text{k×1 vector}}$$

But, why?

- Billionaire (again) says: Why sum squared error???
- You say: Gaussians, Dr. Gateson, Gaussians…
- Model: prediction is linear function plus Gaussian noise
  - $t(\mathbf{x}) = \sum_i w_i h_i(\mathbf{x}) + \varepsilon_{\mathbf{x}}$
- Learn **w** using MLE

$$P(t \mid \mathbf{x}, \mathbf{w}, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-\left[t - \sum_i w_i h_i(\mathbf{x})\right]^2}{2\sigma^2}}$$

Maximizing log-likelihood

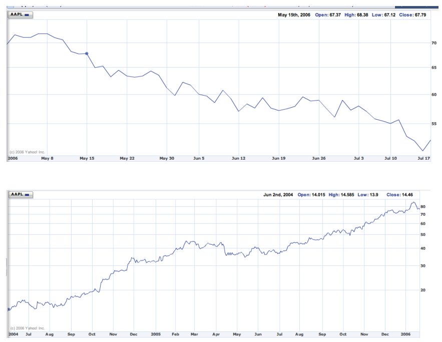
Maximize:

$$\ln P(\mathcal{D} \mid \mathbf{w}, \sigma) = \ln \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^N \prod_{j=1}^{N} e^{\frac{-\left[t_j - \sum_i w_i h_i(\mathbf{x}_j)\right]^2}{2\sigma^2}}$$

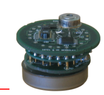
Least-squares Linear Regression is MLE for Gaussians!!!

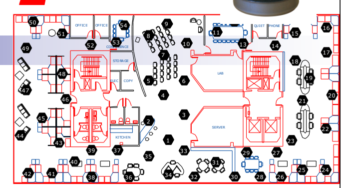
Applications Corner 1

- Predict stock value over time from
  - past values
  - other relevant vars
    - e.g., weather, demands, etc.

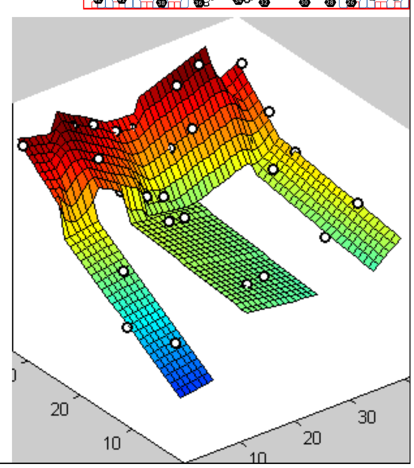


Applications Corner 2





- Measure temperatures at some locations
- Predict temperatures throughout the environment



[Guestrin et al. '04]

Applications Corner 3

- Predict when a sensor will fail
  - based several variables
    - age, chemical exposure, number of hours used,…

Bias-Variance Tradeoff

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Bias-Variance tradeoff – Intuition

- Model too "simple" ➔ does not fit the data well
  - A biased solution
- Model too complex ➔ small changes to the data, solution changes a lot
  - A high-variance solution

(Squared) Bias of learner

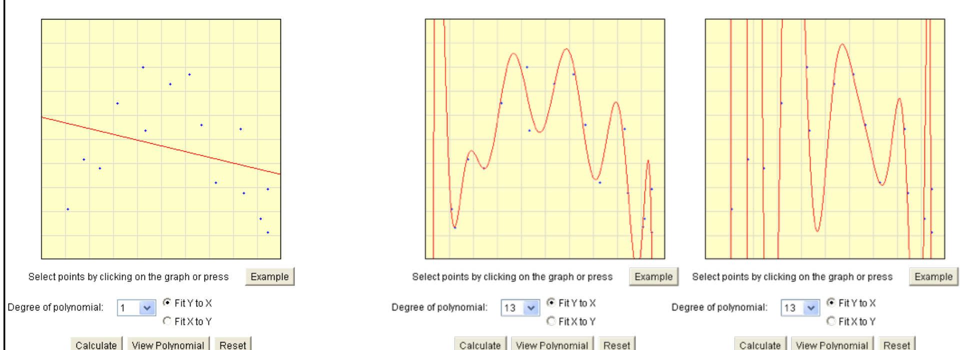
- Given dataset *D* with *N* samples, learn function $h_D(x)$
- If you sample a different dataset *D'* with *N* samples, you will learn different $h_D'(x)$
- **Expected hypothesis**: $E_D[h_D(x)]$
- **Bias:** difference between what you expect to learn and truth
  - Measures how well you expect to represent true solution
  - Decreases with more complex model
  - Bias^2 at one point *x*:
  - Average Bias^2:

Variance of learner

- Given dataset D with N samples, learn function $h_D(x)$
- If you sample a different dataset D' with N samples, you will learn different $h_D'(x)$
- **Variance:** difference between what you expect to learn and what you learn from a particular dataset
  - Measures how sensitive learner is to specific dataset
  - Decreases with simpler model
  - Variance at one point x:
  - Average pariance:

Bias-Variance Tradeoff

- Choice of hypothesis class introduces learning bias
  - More complex class → less bias
  - More complex class → more variance



Bias-Variance Decomposition of Error

$\bar{h}_N(x) = E_D[h_D(x)]$

- Expected mean squared error: $\mathrm{MSE} = E_D\left[E_x\left[(t(x) - h_D(x))^2\right]\right]$
- To simplify derivation, drop x:
- Expanding the square:

Moral of the Story: Bias-Variance Tradeoff Key in ML

- Error can be decomposed:

$$\mathrm{MSE} = E_D\left[E_x\left[(t(x) - h_D(x))^2\right]\right]$$
$$= E_x\left[\left(t(x) - \bar{h}_N(x)\right)^2\right] + E_D\left[E_x\left[\left(\bar{h}(x) - h_D(x)\right)^2\right]\right]$$

- Choice of hypothesis class introduces learning bias
  - More complex class → less bias
  - More complex class → more variance

What you need to know

- Regression
  - Basis function = features
  - Optimizing sum squared error
  - Relationship between regression and Gaussians
- Bias-variance trade-off
- Play with Applet

Overfitting

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Bias-Variance Tradeoff

- Choice of hypothesis class introduces learning bias
  - More complex class → less bias
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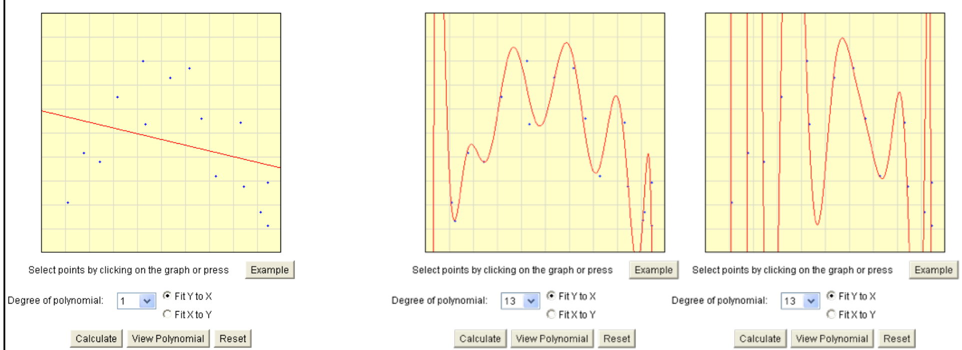


Training set error

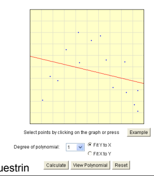
$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \sum_j \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

- Given a dataset (Training data)
- Choose a loss function
  - e.g., squared error (L_2) for regression
- **Training set error:** For a particular set of parameters, loss function on training data:

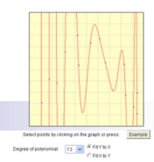
$$error_{train}(\mathbf{w}) = \frac{1}{N_{train}} \sum_{j=1}^{N_{train}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

Training set error as a function of model complexity

$$error_{train}(\mathbf{w}) = \frac{1}{N_{train}} \sum_{j=1}^{N_{train}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$



Prediction error



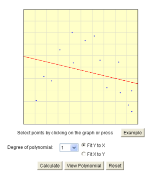
- Training set error can be poor measure of "quality" of solution
- **Prediction error:** We really care about error over all possible input points, not just training data:

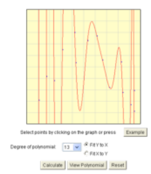
$$\begin{aligned} error_{true}(\mathbf{w}) &= E_{\mathbf{x}}\left[\left(t(\mathbf{x}) - \sum_i w_i h_i(\mathbf{x})\right)^2\right] \\ &= \int_{\mathbf{x}} \left(t(\mathbf{x}) - \sum_i w_i h_i(\mathbf{x})\right)^2 p(\mathbf{x}) d\mathbf{x} \end{aligned}$$

Prediction error as a function of model complexity

$$error_{train}(\mathbf{w}) = \frac{1}{N_{train}} \sum_{j=1}^{N_{train}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

$$error_{true}(\mathbf{w}) = \int_{\mathbf{x}} \left(t(\mathbf{x}) - \sum_i w_i h_i(\mathbf{x}) \right)^2 p(\mathbf{x}) d\mathbf{x}$$





Computing prediction error

- Computing prediction
  - Hard integral
  - May not know t(**x**) for every **x**

$$error_{true}(\mathbf{w}) = \int_{\mathbf{x}} \left(t(\mathbf{x}) - \sum_i w_i h_i(\mathbf{x}) \right)^2 p(\mathbf{x}) d\mathbf{x}$$

- Monte Carlo integration (sampling approximation)
  - Sample a set of i.i.d. points {$\mathbf{x}_1,\ldots,\mathbf{x}_M$} from p(**x**)
  - Approximate integral with sample average

$$error_{true}(\mathbf{w}) \approx \frac{1}{M} \sum_{j=1}^{M} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

Why training set error doesn't approximate prediction error?

- Sampling approximation of prediction error:

$$error_{true}(\mathbf{w}) \approx \frac{1}{M}\sum_{j=1}^{M}\left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j)\right)^2$$

- Training error :

$$error_{train}(\mathbf{w}) = \frac{1}{N_{train}}\sum_{j=1}^{N_{train}}\left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j)\right)^2$$

- Very similar equations!!!
  - Why is training set a bad measure of prediction error???

Why training set error doesn't approximate prediction error?

Because you cheated!!!

Training error good estimate for a single **w,**
But you optimized **w** with respect to the training error, and found **w** that is good for this set of samples

Training error is a (optimistically) biased estimate of prediction error

- Very similar equations!!!
  - Why is training set a bad measure of prediction error???

Test set error

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \sum_j \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

- Given a dataset, **randomly** split it into two parts:
  - Training data – $\{\mathbf{x}_1,\ldots, \mathbf{x}_{Ntrain}\}$
  - Test data – $\{\mathbf{x}_1,\ldots, \mathbf{x}_{Ntest}\}$
- Use training data to optimize parameters **w**
- **Test set error:** For the ***final output*** $\hat{\mathbf{w}}$, evaluate the error using:

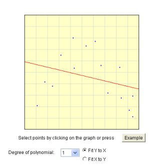
$$error_{test}(\mathbf{w}) = \frac{1}{N_{test}} \sum_{j=1}^{N_{test}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

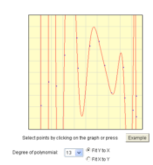
Test set error as a function of model complexity

$$error_{train}(\mathbf{w}) = \frac{1}{N_{train}} \sum_{j=1}^{N_{train}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

$$error_{true}(\mathbf{w}) = \int_{\mathbf{x}} \left(t(\mathbf{x}) - \sum_i w_i h_i(\mathbf{x}) \right)^2 p(\mathbf{x}) d\mathbf{x}$$

$$error_{test}(\mathbf{w}) = \frac{1}{N_{test}} \sum_{j=1}^{N_{test}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$





Overfitting

- **Overfitting:** a learning algorithm overfits the training data if it outputs a solution **w** when there exists another solution **w'** such that:

$$[error_{train}(\mathbf{w}) < error_{train}(\mathbf{w}')] \wedge [error_{true}(\mathbf{w}') < error_{true}(\mathbf{w})]$$

How many points to I use for training/testing?

- Very hard question to answer!
  - Too few training points, learned **w** is bad
  - Too few test points, you never know if you reached a good solution
- Bounds, such as Hoeffding's inequality can help:

$$P(|\ \widehat{\theta} - \theta^* \ | \geq \epsilon) \quad \leq \quad 2e^{-2N\epsilon^2}$$

- More on this later this quarter, but still hard to answer
- Typically:
  - If you have a reasonable amount of data, pick test set "large enough" for a "reasonable" estimate of error, and use the rest for learning
  - If you have little data, then you need to pull out the big guns…
    - e.g., bootstrapping

Error estimators

$$error_{true}(\mathbf{w}) = \int_{\mathbf{x}} \left(t(\mathbf{x}) - \sum_i w_i h_i(\mathbf{x}) \right)^2 p(\mathbf{x}) d\mathbf{x}$$

$$error_{train}(\mathbf{w}) = \frac{1}{N_{train}} \sum_{j=1}^{N_{train}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

$$error_{test}(\mathbf{w}) = \frac{1}{N_{test}} \sum_{j=1}^{N_{test}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

Error as a function of number of training examples for a fixed model complexity

$$error_{train}(\mathbf{w}) = \frac{1}{N_{train}} \sum_{j=1}^{N_{train}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

$$error_{test}(\mathbf{w}) = \frac{1}{N_{test}} \sum_{j=1}^{N_{test}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

little data

infinite data

Error estimators

err

err

Be careful!!!

Test set only unbiased if you never never ever ever do any any any any learning on the test data

For example, if you use the test set to select the degree of the polynomial… no longer unbiased!!!
(We will address this problem later in the quarter)

$$error_{test}(\mathbf{w}) = \frac{1}{N_{test}} \sum_{j=1}^{N_{test}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

What you need to know

- True error, training error, test error
  - Never learn on the test data
  - Never learn on the test data
  - Never learn on the test data
  - Never learn on the test data
  - Never learn on the test data
- Overfitting