Overfitting

Machine Learning – CSE546
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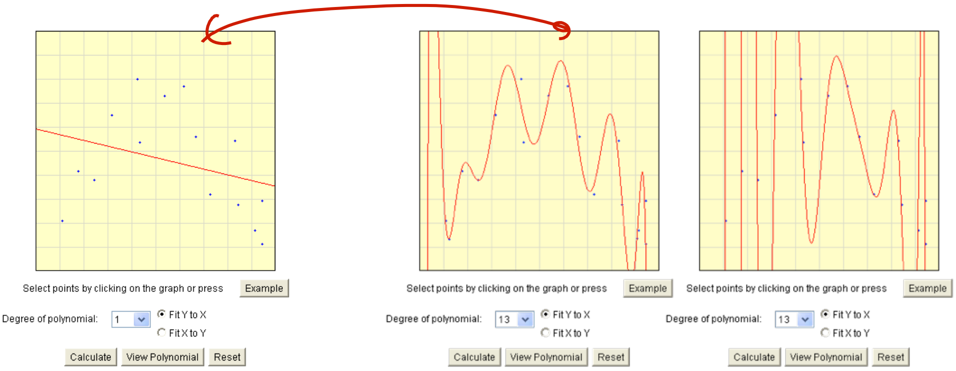
University of Washington

October 2, 2014

Bias-Variance Tradeoff

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



Select points by clicking on the graph or press

Degree of polynomial: 1

● Fit Y to X
○ Fit X to Y

Select points by clicking on the graph or press

Degree of polynomial: 13

● Fit Y to X
○ Fit X to Y

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Degree of polynomial: 13

● Fit Y to X
○ Fit X to Y

Training set error

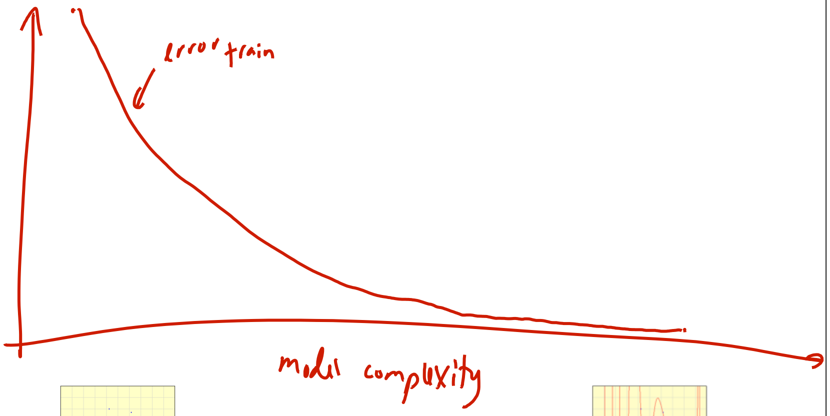
$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \sum_j \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

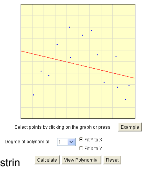
- Given a dataset (Training data)
- Choose a loss function
  - ☐ e.g., squared error (L_2) for regression
- **Training set error:** For a particular set of parameters, loss function on training data:

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

Training set error as a function of model complexity

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





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Degree of polynomial: 1

Select points by clicking on the graph or press

Degree of polynomial: 13

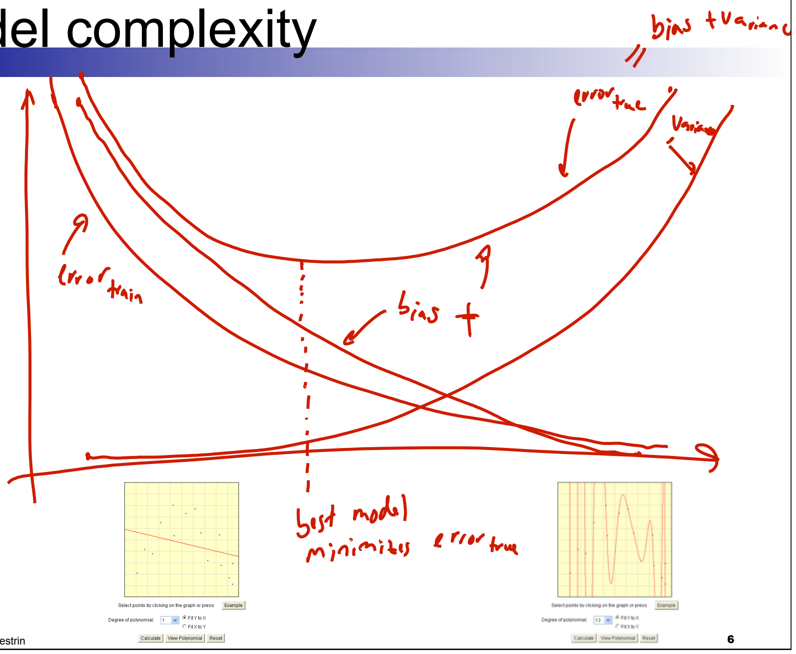
Prediction error

- 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:

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

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**

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

- 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

Sample avg of error

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

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Why training set error doesn't approximate prediction error?

- Sampling approximation of prediction error:

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

- Training error :

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

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

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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:

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

$\approx$

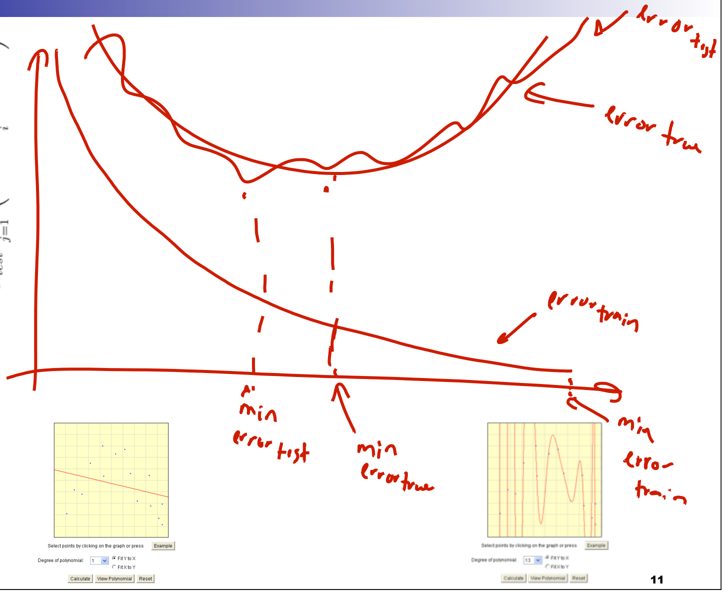
$error_{true}(\hat{w})$

Test set error as a function of model complexity

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

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

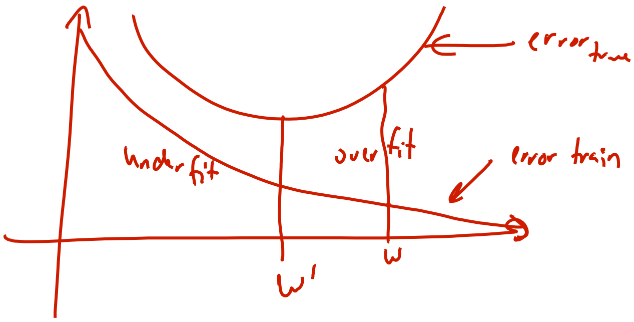
$$error_{test}(\mathbf{w}) = \frac{1}{N_{test}} \sum_{j=1}^{N_{test}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$



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:

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

- 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

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

← gold standard

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

← data for learning, optimistically biased

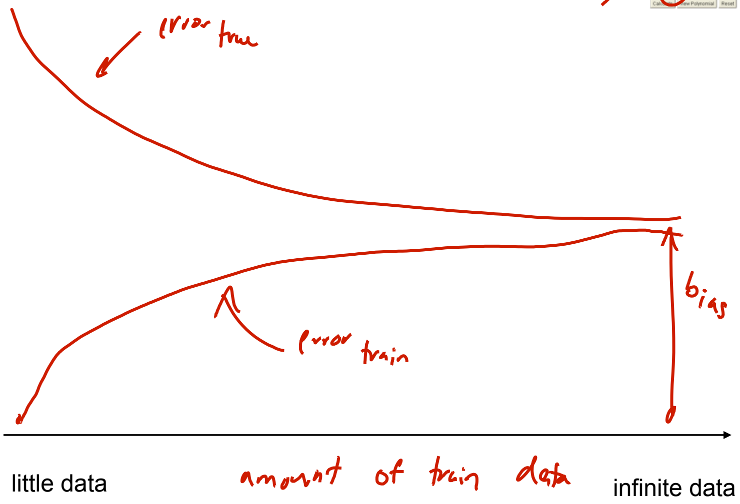
$$error_{test}(\mathbf{w}) \;=\; \frac{1}{N_{test}} \sum_{j=1}^{N_{test}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j)\right)^2$$

← Evaluate final model

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

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

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



Error 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)

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

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

Regularization

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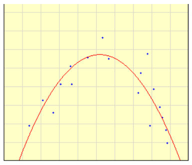
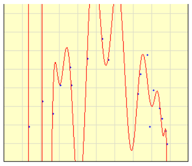
Regularization in Linear Regression

- Overfitting usually leads to very large parameter choices, e.g.:

$-2.2 + 3.1 X – 0.30 X^2$



$-1.1 + 4,700,910.7 X – 8,585,638.4 X^2 + …$



- ***Regularized*** or ***penalized*** regression aims to impose a "complexity" penalty by penalizing large weights
  - ☐ "Shrinkage" method

→ smaller curvatures or smoother fns

→ a kind of bias we can believe in

Ridge Regression

- Ameliorating issues with overfitting: penalizing large weights
- New objective:

$$\underbrace{\sum_{j=1}^{N} \left(t(x_j) - \overbrace{\left(w_0 + \sum_{i=1}^{k} w_i h_i(x_j) \right)}^{\hat{f}} \right)^2}_{\text{train error}} + \lambda \underbrace{\sum_{i=1}^{k} w_i^2}_{\|w_{1:k}\|_2^2}$$

regularization coeff $\lambda \geq 0$

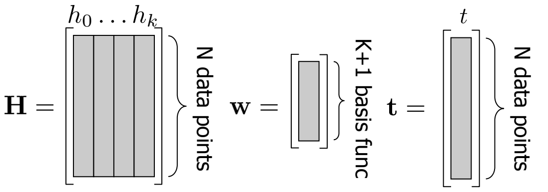
regularization penalty

practical note: don't regularize w_0

Ridge Regression in Matrix Notation

$$\hat{\mathbf{w}}_{ridge} = \arg\min_{w} \sum_{j=1}^{N} \left(t(x_j) - (w_0 + \sum_{i=1}^{k} w_i h_i(x_j)) \right)^2 + \lambda \sum_{i=1}^{k} w_i^2$$

$$= \arg\min_{\mathbf{w}} \underbrace{(\mathbf{Hw} - \mathbf{t})^T (\mathbf{Hw} - \mathbf{t})}_{\text{residual error}} + \lambda\ \mathbf{w}^T I_{0+k} \mathbf{w}$$



$$I_{0+k} = \begin{pmatrix} 0 & & & & 0 \\ & 1 & & & \\ & & 1 & & \\ 0 & & & 1 & \\ & & & & 1 \end{pmatrix}$$

Minimizing the Ridge Regression Objective

$$\hat{\mathbf{w}}_{ridge} = \arg\min_{w} \sum_{j=1}^{N} \left(t(x_j) - (w_0 + \sum_{i=1}^{k} w_i h_i(x_j)) \right)^2 + \lambda \sum_{i=1}^{k} w_i^2$$

$$F(w) = (H\mathbf{w} - \mathbf{t})^T (H\mathbf{w} - \mathbf{t}) + \lambda\ \mathbf{w}^T I_{0+k} \mathbf{w}$$

$$\nabla_w F(w) = 0$$

$$\nabla_w F(w) = 2H^T(Hw - t) + 2\lambda I_{0+k} w$$

$$\hat{w}_{ridge} = (H^T H + \lambda I_{0+k})^{-1} H^T t$$

MLE same but now adding

$\frac{d}{dw} \lambda w i w$

$= 2\lambda i w$

Regularization

$(H^T H)^{-1}$? $H^T H$ may not be invertible

λI_{0+k} adds a little to diagonal & makes $H^T H$ more invertible

Shrinkage Properties

$\hat{w}_{MLE} = (H^T H)^{-1} H^T t$

$= \begin{pmatrix} 1 & & 0 \\ & 1 & \\ 0 & & 1 \end{pmatrix} H^T t$

$$\hat{\mathbf{w}}_{ridge} = (H^T H + \lambda\ I_{0+k})^{-1} H^T \mathbf{t}$$

- If orthonormal features/basis: $\underline{H^T H = I}$

$\hat{w}_{ridge} = (I + \lambda I_{0+k})^{-1} H^T t$

$= \begin{pmatrix} 1 & & 0 \\ & \frac{1}{1+\lambda} & \\ 0 & & \frac{1}{1+\lambda} & \\ & & & \ddots \end{pmatrix} H^T t$

For i > 0

$$\{\hat{w}_{ridge}\}_i = \frac{\{\hat{w}_{MLE}\}_i}{1+\lambda}$$

For degree 1 polynomial

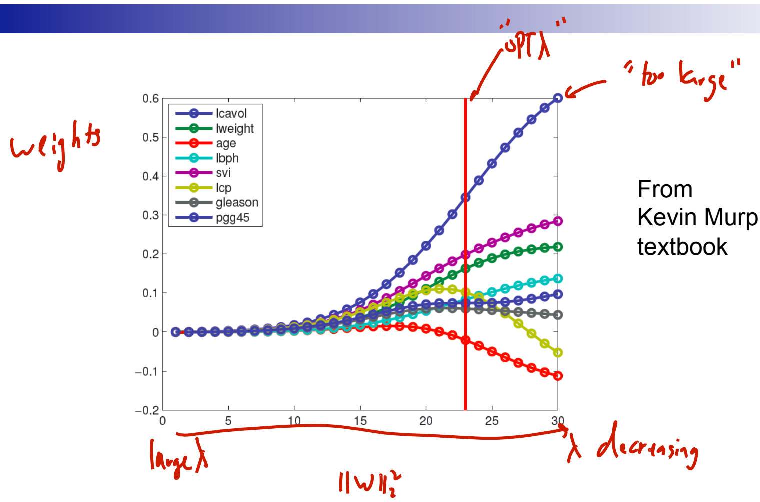
Ridge Regression: Effect of Regularization

$$\hat{\mathbf{w}}_{ridge} = \arg\min_w \sum_{j=1}^{N} \Big(t(x_j) - \underbrace{(w_0 + \sum_{\underset{\uparrow}{i=1}}^{k} w_i h_i(x_j))}_{\hat{f}} \Big)^2 + \lambda \sum_{\underset{\uparrow}{i=1}}^{k} w_i^2$$

- Solution is indexed by the regularization parameter λ
- Larger λ   higher regularization
- Smaller λ   lower regularization
- As λ → 0 $\hat{w}_{ridge} \to \hat{w}_{MLE}$
- As λ →∞ $\hat{w}_{ridge} \to w_0$ ← converges to avg of $t(x_j)$ in train data

  flat line

Ridge Coefficient Path



From
Kevin Murphy
textbook

- Typical approach: select λ using cross validation, more on this later in the quarter

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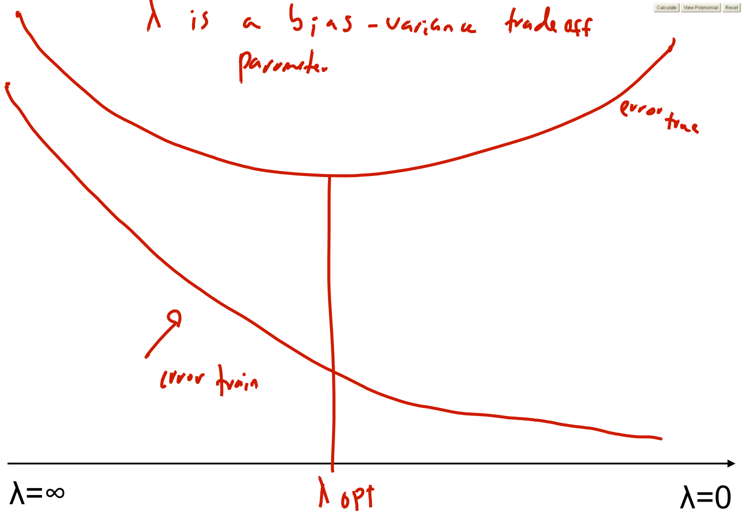
Error as a function of regularization parameter for a fixed model complexity

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

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

λ is a bias-variance tradeoff parameter



What you need to know…

- Regularization
  - Penalizes for complex models
- Ridge regression
  - L_2 penalized least-squares regression
  - Regularization parameter trades off model complexity with training error

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Cross-Validation

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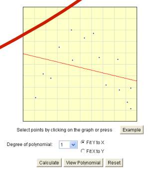
Test set error as a function of model complexity

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

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

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



Select points by clicking on the graph or press Example

Degree of polynomial: 1 ● Fit Y to X ○ Fit X to Y

Calculate View Polynomial Reset

Select points by clicking on the graph or press Example

Degree of polynomial: 13 ● Fit Y to X ○ Fit X to Y

Calculate View Polynomial Reset

How… How… How???????

- How do we pick the regularization constant λ…
  - ☐ And all other constants in ML, 'cause one thing ML doesn't lack is constants to tune… ☹

- We could use the test data, but…

1. don't learn on test data
2. don't learn on test data
3. may not be enough data for a good train test split

(LOO) Leave-one-out cross validation

- Consider a **validation set with 1 example**: ← choose λ using 1 train example
  - ☐ *D* – training data ← N data points
  - ☐ *D*\j – training data with *j* th data point moved to validation set
- **Learn ~~classifier~~ regression $h_{D\backslash j}$ with *D*\j dataset** ← using N-1 data points, for each λ
- **Estimate true error** as squared error on predicting t($\mathbf{x}_j$):
  - ☐ Unbiased estimate of $\text{error}_{\text{true}}(h_{D\backslash j})$!

    $E[(t(x_j) - h_{D/j}(x_j))^2] = \text{error}_{\text{true}}(h_{D/j})$
  - ☐ Seems really bad estimator, but wait!

- **LOO cross validation**: Average over all data points *j*:
  - ☐ **For each data point you leave out, learn a new classifier $h_{D\backslash j}$**
  - ☐ **Estimate error** as:

$$error_{LOO} = \frac{1}{N}\sum_{j=1}^{N}\left(t(\mathbf{x}_j) - h_{\mathcal{D}\backslash j}(\mathbf{x}_j)\right)^2$$

LOO cross validation is (almost) unbiased estimate of true error of h_D!

- When computing **LOOCV error, we only use *N-1* data points**
  - ☐ So it's not estimate of true error of learning with *N* data points!
  - ☐ Usually pessimistic, though – learning with less data typically gives worse answer
- **LOO is almost unbiased**!

  $\text{error}_{\text{true}}(h_D^{\lambda}) \approx \text{error}_{\text{LOO}}$

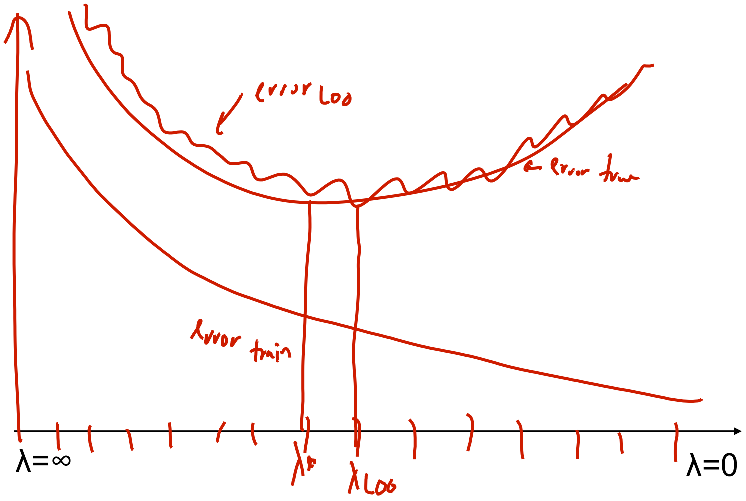
- **Great news!**
  - ☐ **Use LOO error for model selection!!!**
  - ☐ **E.g., picking λ**

Using LOO to Pick λ

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

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

$$error_{LOO} = \frac{1}{N} \sum_{j=1}^{N} \left(t(\mathbf{x}_j) - h_{\mathcal{D}\backslash j}(\mathbf{x}_j) \right)^2$$



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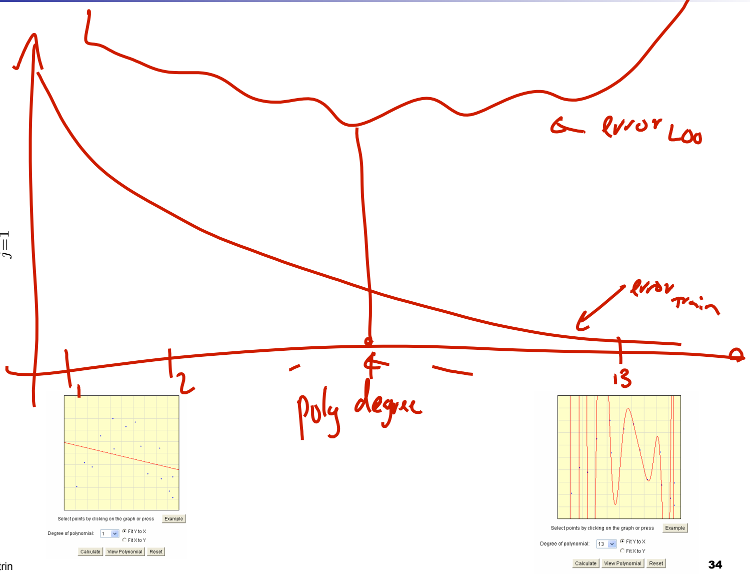
Using LOO error for model selection

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

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

$$error_{LOO} = \frac{1}{N} \sum_{j=1}^{N} \left(t(\mathbf{x}_j) - h_{\mathcal{D}\backslash j}(\mathbf{x}_j) \right)^2$$



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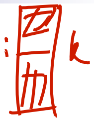
Computational cost of LOO

- Suppose you have 100,000 data points
- You implemented a great version of your learning algorithm
  - ☐ Learns in only 1 second
- Computing LOO will take about 1 day!!! or λ
  - ☐ If you have to do for each choice of basis functions, it will take fooooooreeeve'!!!
- Solution 1: Preferred, but not usually possible
  - ☐ Find a cool trick to compute LOO (e.g., see homework)

Solution 2 to complexity of computing LOO: (More typical) **Use *k*-fold cross validation**

LOO ≡ N-fold



- Randomly **divide training data into *k* equal parts**
  - ☐ $D_1,\ldots,D_k$
- For each *i*
  - ☐ **Learn classifier $h_{D\backslash D_i}$ using data point not in D_i**
  - ☐ **Estimate error of $h_{D\backslash D_i}$ on validation set D_i**:

$$error_{\mathcal{D}_i} = \frac{k}{N} \sum_{\mathbf{x}_j \in \mathcal{D}_i} \left(t(\mathbf{x}_j) - h_{\mathcal{D}\backslash\mathcal{D}_i}(\mathbf{x}_j)\right)^2$$

- ***k*-fold cross validation error is average** over data splits:

$$error_{k-fold} = \frac{1}{k}\sum_{i=1}^{k} error_{\mathcal{D}_i}$$

- *k*-fold cross validation properties:
  - ☐ **Much faster to compute** than LOO
  - ☐ **More (pessimistically) biased** – using much less data, only N *m(k-1)/k*
  - ☐ Usually, **k = 10** ☺

What you need to know…

- Never ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever train on the test data
- Use cross-validation to choose magic parameters such as λ
- Leave-one-out is the best you can do, but sometimes too slow
  - In that case, use k-fold cross-validation