CSE446: Linear Regression

Spring 2017

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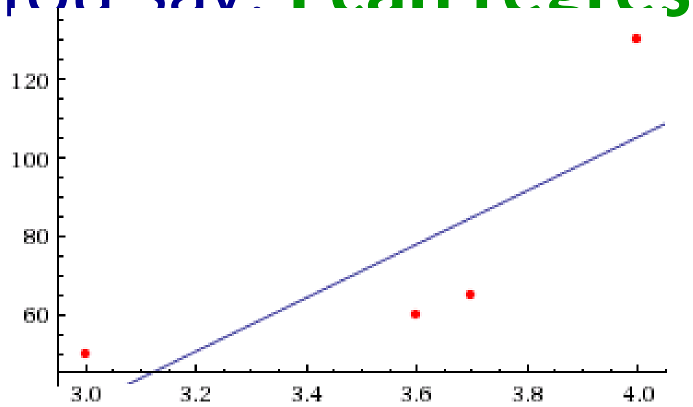
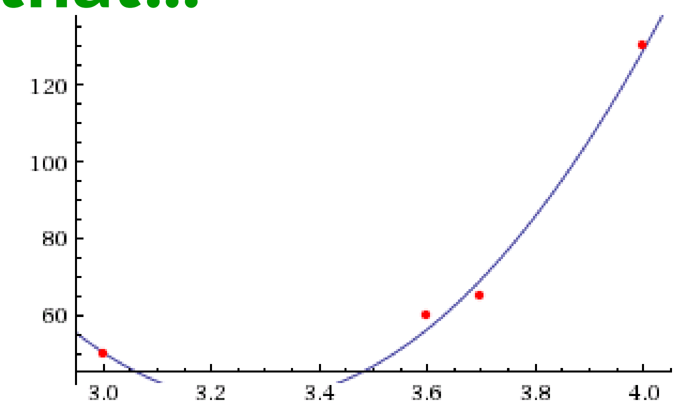
Slides adapted from Carlos Guestrin and Luke Zettlemoyer

Prediction of continuous variables

- Billionaire says: Wait, that’s not what I meant!

- You say: Chill out, dude.
- He says: I want to predict a continuous variable for continuous inputs: I want to predict salaries from GPA.
- You say: **I can regress that…**





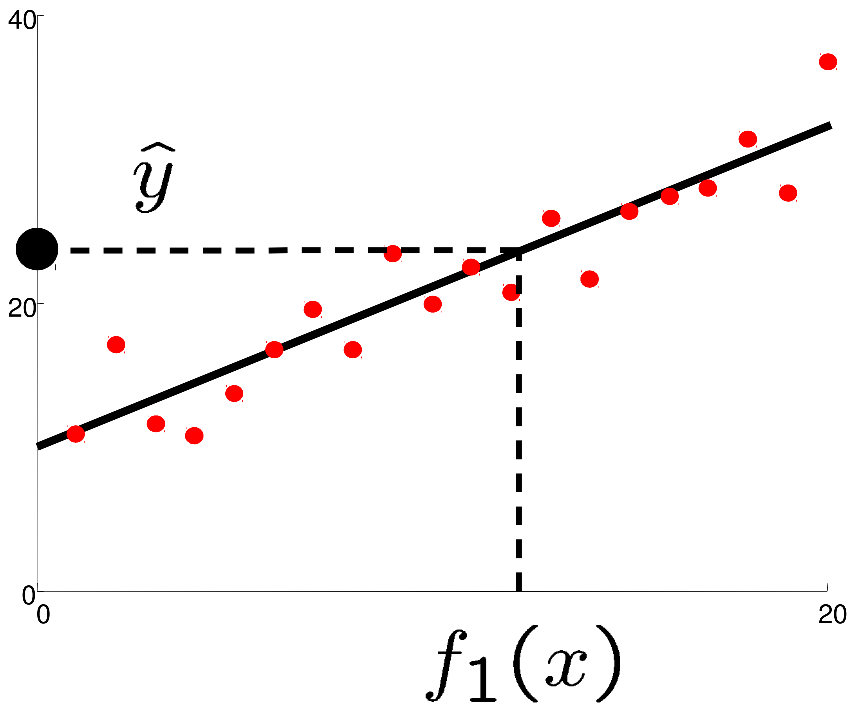
Linear Regression

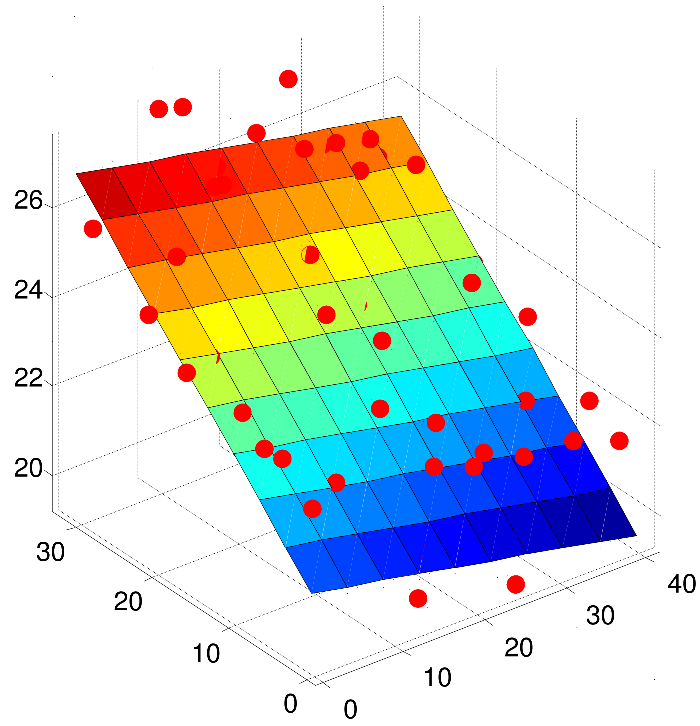
Prediction

$$\hat{y} = w_0 + w_1 f_1(x)$$

Prediction

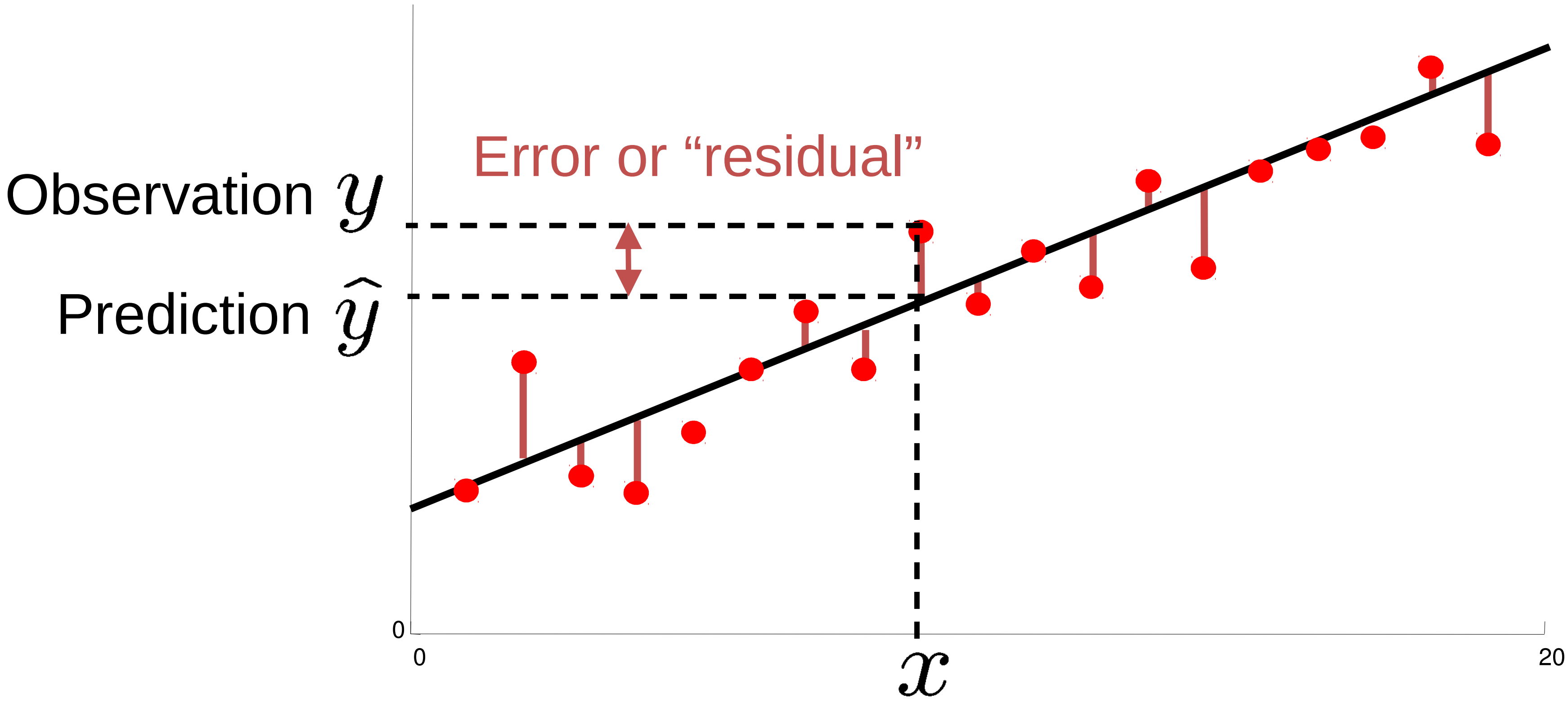
$$\hat{y}_i = w_0 + w_1 f_1(x) + w_2 f_2(x)$$





Ordinary Least Squares (OLS)

$$\text{total error} = \sum_i (y_i - \hat{y}_i)^2 = \sum_i \left(y_i - \sum_k w_k f_k(x_i) \right)^2$$



The regression problem

- Instances: <$\mathbf{x}_j$, t_j>
- Learn: Mapping from x to t($\mathbf{x}$)
- Hypothesis space:
  - Given, basis functions $\{h_1,\ldots,h_k\}$
  - $h_i(\mathbf{x}) \in \mathbb{R}$
  - Find coeffs $\mathbf{w}=\{w_1,\ldots,w_k\}$

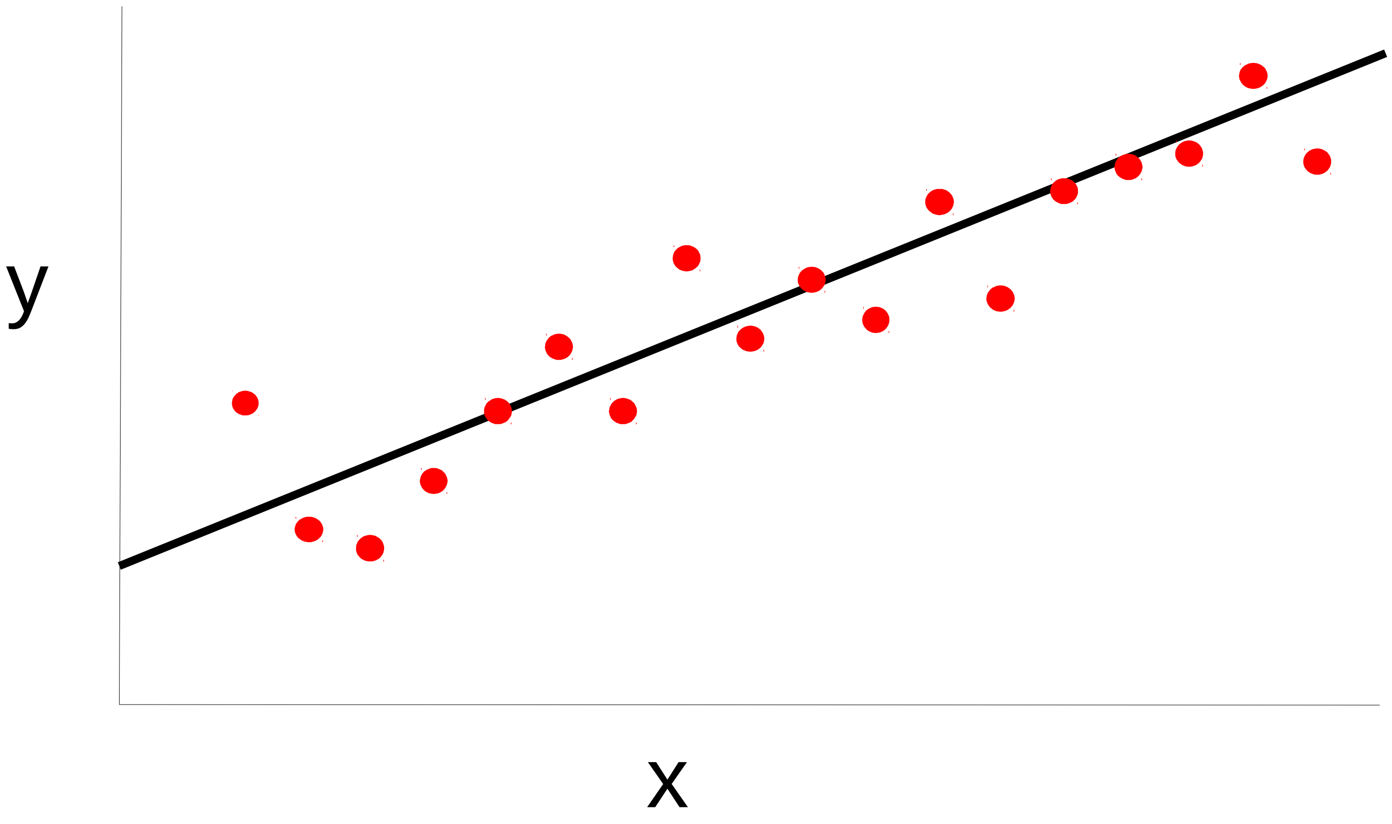
$$H = \{h_1, \ldots, h_K\}$$

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

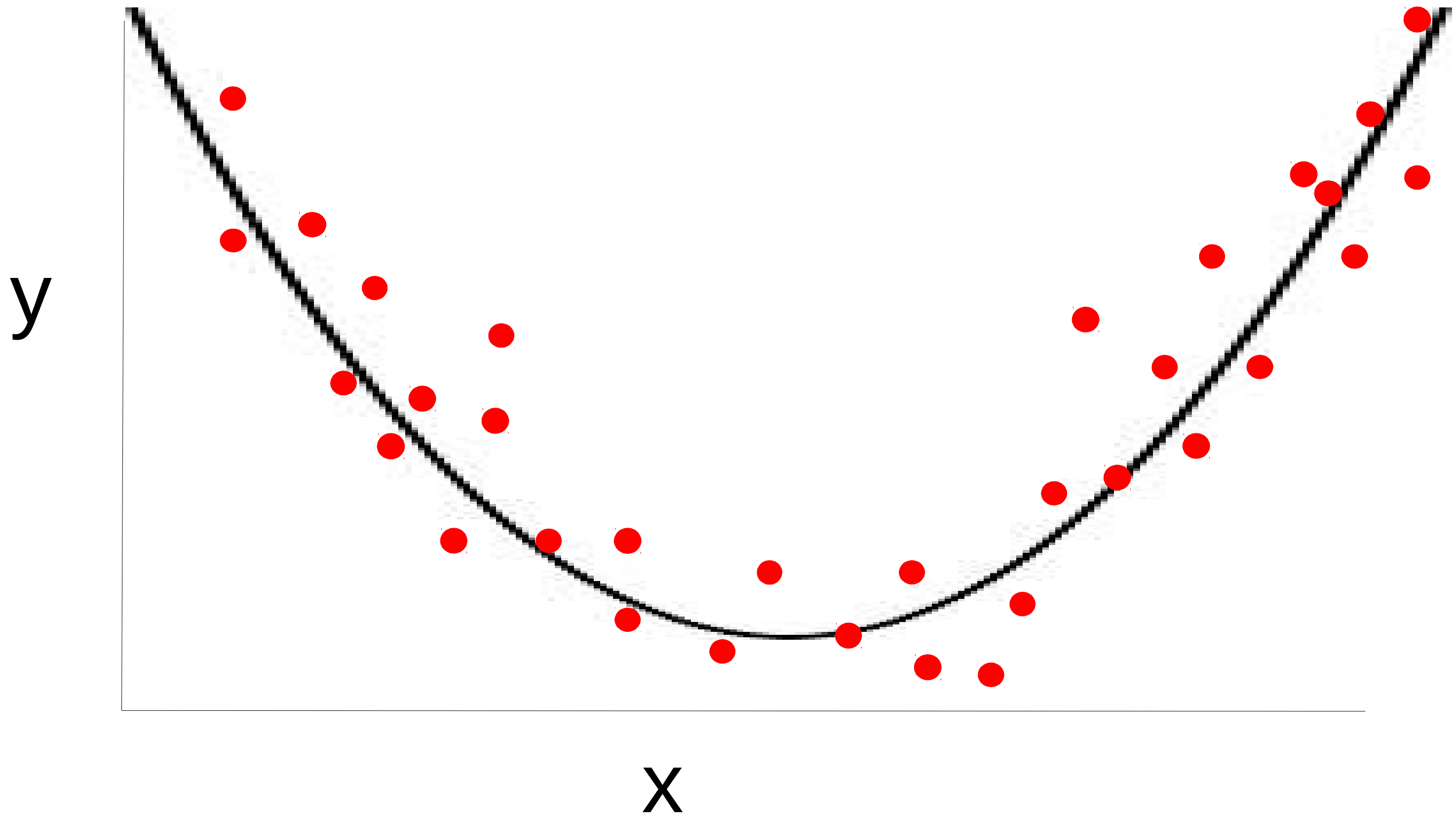
  - Why is this usually called *linear regression*?
    - model is linear in the parameters
    - Can we estimate functions that are not lines???

Linear Basis: 1D input

Need a bias term: $\{h_1(x) = x, h_2(x)=1\}$



- Parabola: $\{h_1(x) = x^2, h_2(x)=x, h_3(x)=1\}$



- 2D: $\{h_1(\mathbf{x}) = x_1^2, h_2(\mathbf{x})= x_2^2, h_3(\mathbf{x})=x_1x_2,\ldots\}$
- Can define any basis functions $h_i(\mathbf{x})$ for n-dimensional input $\mathbf{x}=<x_1,\ldots,x_n>$

The regression problem

- Instances: <$\mathbf{x}_j$, t_j>
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  - Why is this usually called *linear regression*?
    - model is linear in the parameters
    - Can we estimate functions that are not lines???

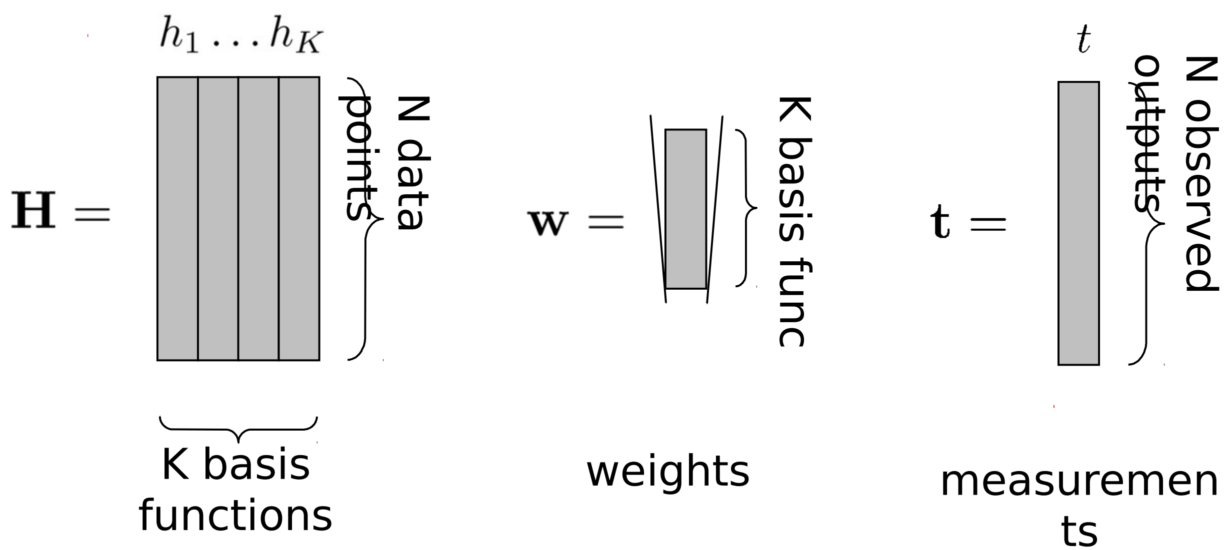
- Precisely, minimize the residual squared error:

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

Regression: matrix notation

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

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



Regression: closed form solution

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

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} (\mathbf{H}\mathbf{w} - \mathbf{t})^T (\mathbf{H}\mathbf{w} - \mathbf{t})$$

$$\mathbf{F}(\mathbf{w}) = (\mathbf{H}\mathbf{w} - \mathbf{t})^T (\mathbf{H}\mathbf{w} - \mathbf{t})$$

$$\nabla_{\mathbf{w}} \mathbf{F}(\mathbf{w}) = \mathbf{0}$$

$$\mathbf{2}\mathbf{H}^T (\mathbf{H}\mathbf{w} - \mathbf{t}) = \mathbf{0}$$

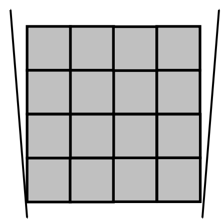
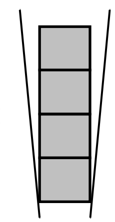
$$\mathbf{H}^T \mathbf{H}\mathbf{w} - \mathbf{H}^T \mathbf{t} = \mathbf{0}$$

$$\boxed{\mathbf{w}^* = (\mathbf{H}^T \mathbf{H})^{-1} \mathbf{H}^T \mathbf{t}}$$

Regression solution: simple matrix math

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

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

where $\mathbf{A} = \mathbf{H}^{\mathrm{T}}\mathbf{H} =$  $\mathbf{b} = \mathbf{H}^{\mathrm{T}}\mathbf{t} =$ 

k×k matrix
for k basis functions

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
  - $t(\mathbf{x}) = \sum_i w_i h_i(\mathbf{x}) + \varepsilon$

- 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 wrt w:

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

$$\arg\max_w \ln \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^N + \sum_{j=1}^{N} \frac{-[t_j - \sum_i w_i h_i(x_j)]^2}{2\sigma^2}$$

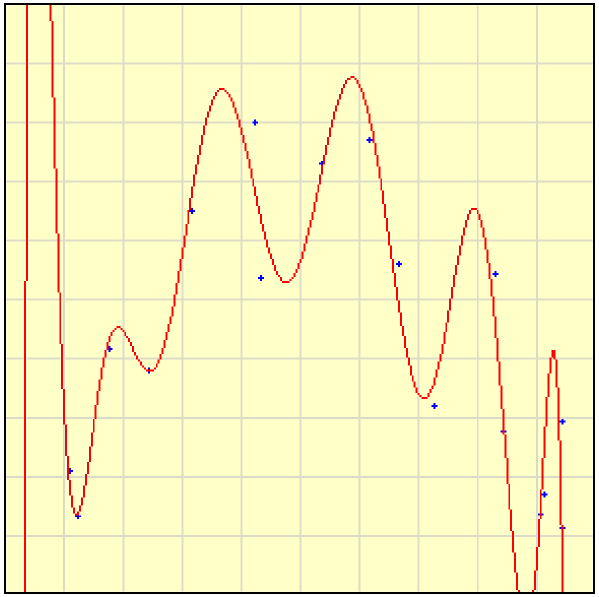
$$= \arg\max_w \sum_{j=1}^{N} \frac{-[t_j - \sum_i w_i h_i(x_j)]^2}{2\sigma^2}$$

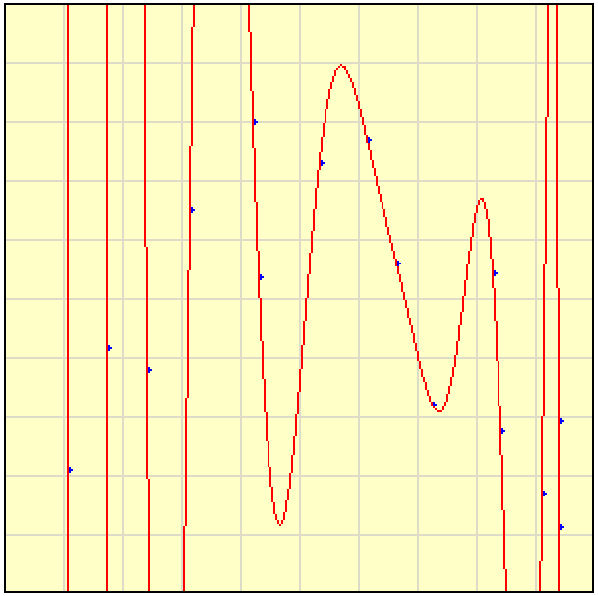
$$= \arg\min_w \sum_{j=1}^{N} [t_j - \sum_i w_i h_i(x_j)]^2$$

$\boxed{\textbf{Least-squares Linear Regression is MLE for Gaussians!!!}}$

Regularization in Linear Regression

- One sign of overfitting: large parameter values!





- *Regularized* or *penalized* regressions modified learning object to penalize large parameters

Ridge Regression

- Introduce a new objective function:

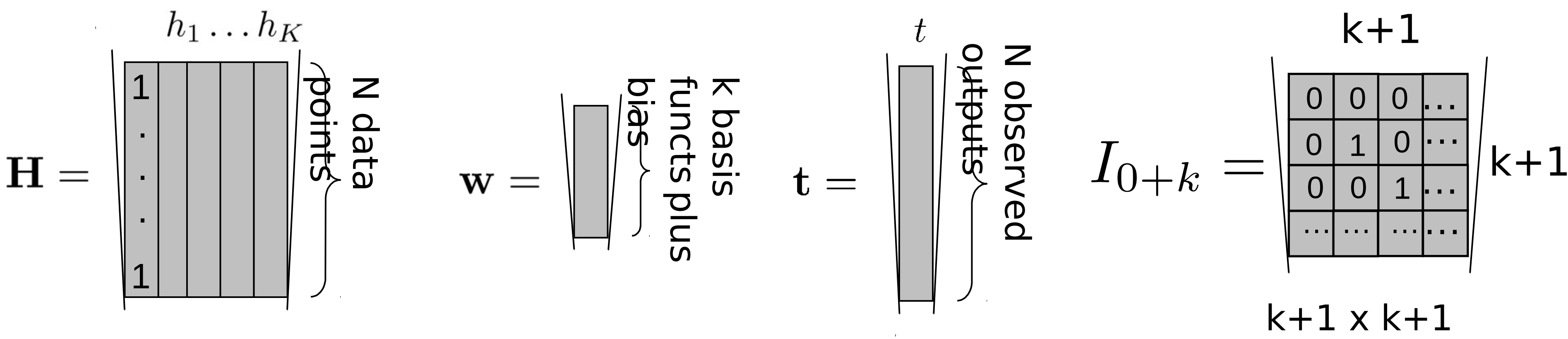
$$\hat{w}_{ridge} = \arg\min_{w} \sum_{j=1}^{N} \left(t(x_j) - (w_0 + \sum_{i=1}^{k} w_i h_i(x_j)) \right)^2$$

  - Prefer low error but also add a squarec
    penalize for large weights
  - λ is hyperparameter that balances tradeoff
  - Explicitly writing out bias feature (essentially h_0=1), which is not penalized

Ridge Regression: matrix notation

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

[redacted] $+ \lambda\, \mathbf{w}^T I_{0+k} \mathbf{w}$



bias column and

k basis functions

weights

measurements

k+1 x k+1 identity matrix, but with 0 in upper left

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

Ridge Regression: closed form solution

[redacted] $+ \lambda\ \mathrm{w}^T I_{0+k} \mathrm{w}$

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

$$\nabla_{\mathbf{w}} \mathbf{F}(\mathbf{w}) = \mathbf{0}$$

$$\mathbf{2H}^T(\mathbf{H}\mathbf{w} - \mathbf{t}) + 2\lambda I_{0+\mathrm{k}} \mathbf{w} = \mathbf{0}$$

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

Regression solution: simple matrix math

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

[redacted] $+ \lambda \, \mathrm{w}^T I_{0+k} \mathrm{w}$

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

Compare to un-regularized regression:

$$\mathbf{w}^* = (\mathbf{H}^T \mathbf{H})^{-1} \mathbf{H}^T \mathbf{t}$$

Ridge Regression

How does varying lambda change w?

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

– Larger λ? Smaller λ?

– As λ →0?

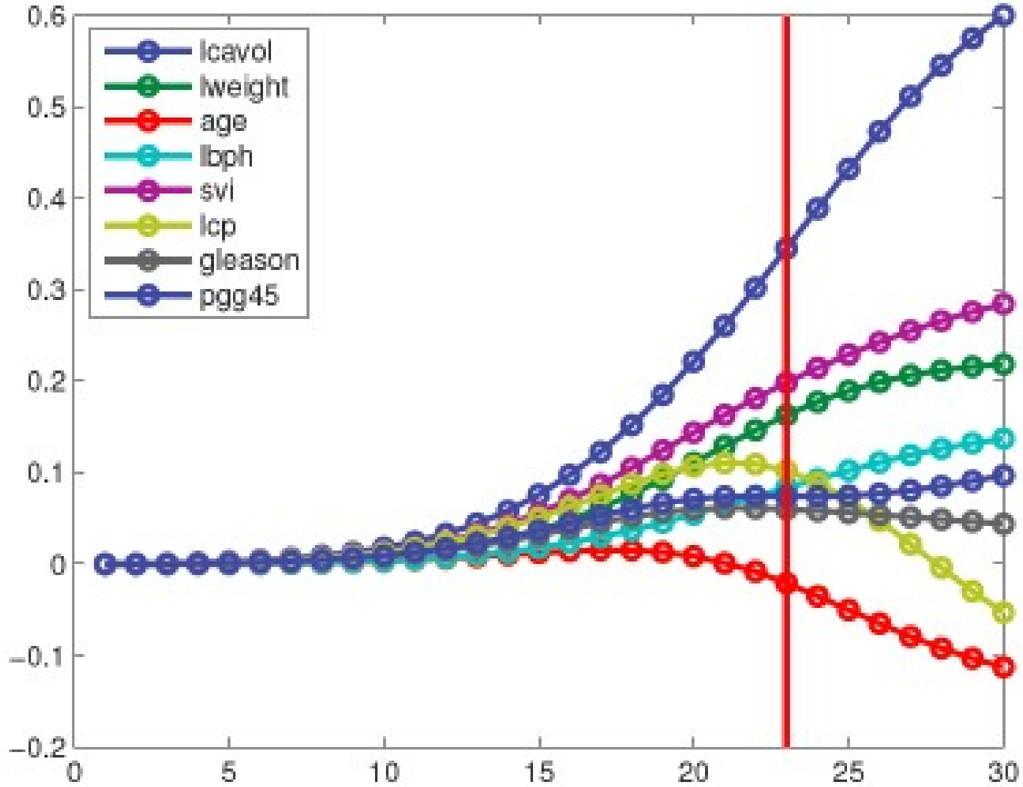
- Becomes same a MLE, unregularized

– As λ →∞?

- All weights will be 0!

Ridge Coefficent Path

Feature Weight

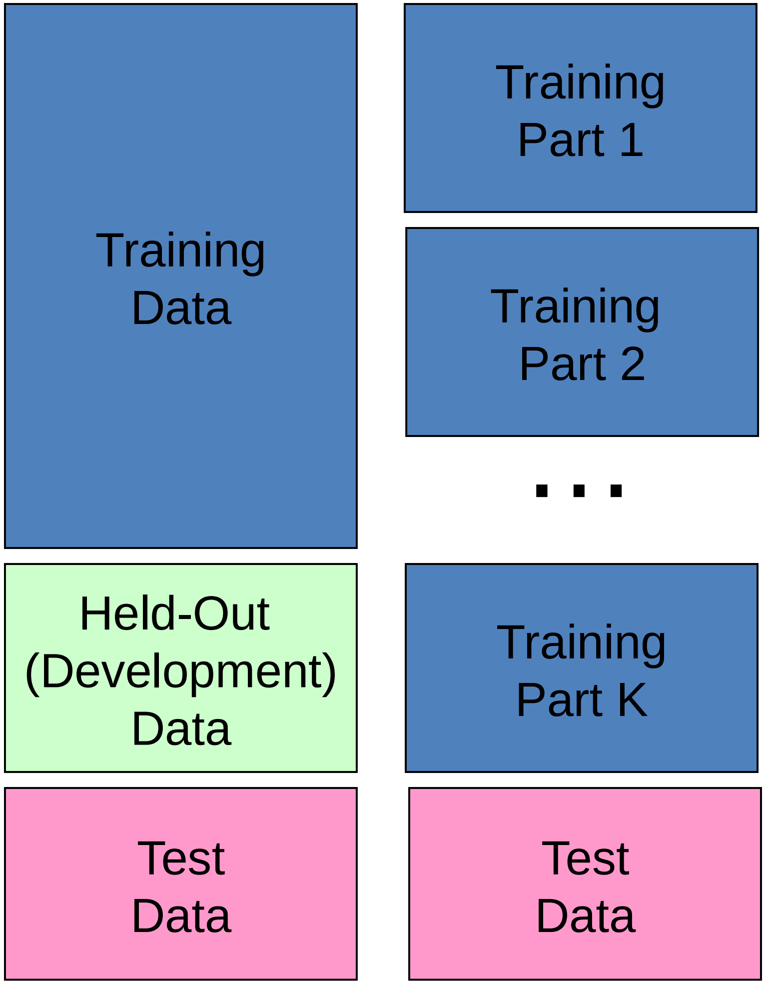


Larger λ $||\hat{w}||_2$ Smaller λ

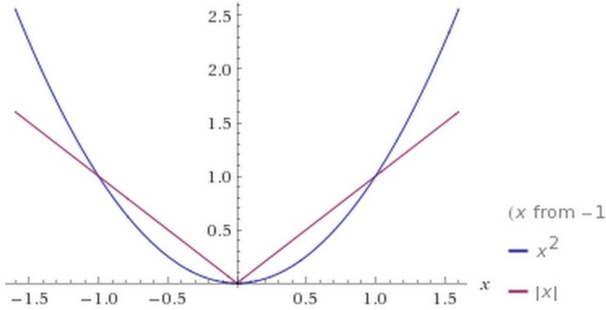
From
Kevin Murphy
textbook

How to pick lambda?

- Experimentation cycle
  - Select a hypothesis *f* to best match training set
  - Tune hyperparameters on held-out set
    - Try many different values of lambda, pick best one
- Or, can do k-fold cross validation
  - No held-out set
  - Divide training set into k subsets
  - Repeatedly train on k-1 and test on remaining one
  - Average the results



Why squared regularization?



- Ridge:

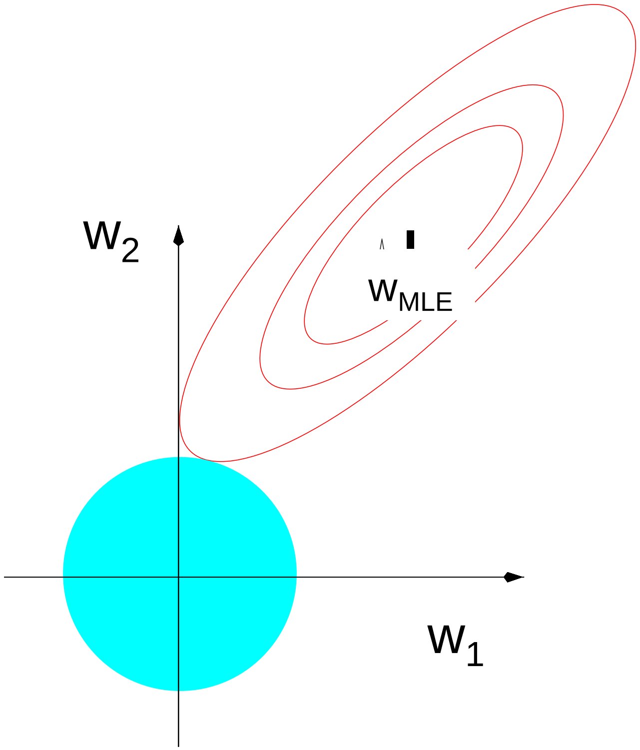
$$\hat{w}_{ridge} = \arg\min_w \sum_{j=1}^{N} \left(t(x_j) - (w_0 + \sum_{i=1}^{k} w_i h_i(x_j)) \right)^2 + \lambda \sum_{i=1}^{k} w_i^2$$

- LASSO:

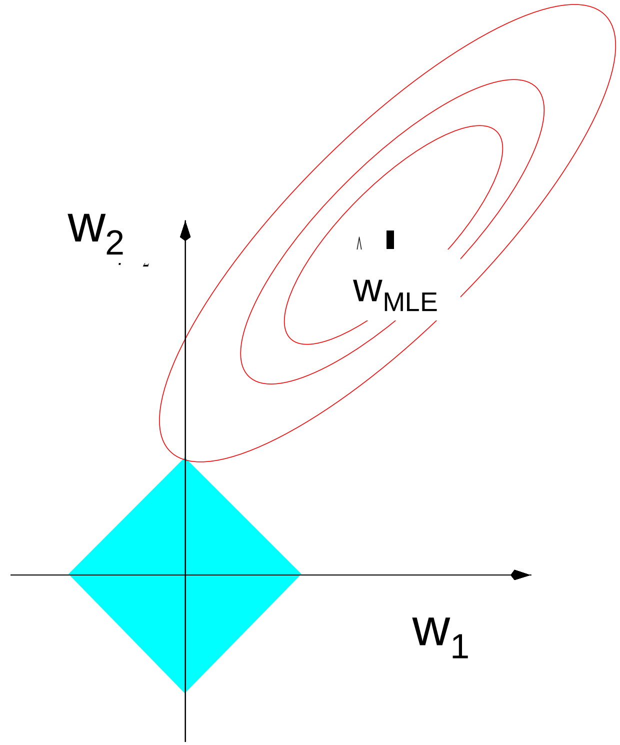
$$\hat{w}_{LASSO} = \arg\min_w \sum_{j=1}^{N} \left(t(x_j) - (w_0 + \sum_{i=1}^{k} w_i h_i(x_j)) \right)^2 + \lambda \sum_{i=1}^{k} |w_i|$$

  – Linear penalty pushes more weights to zero
  – Allows for a type of *feature selection*
  – But, not differentiable and no closed form solution….

Geometric Intuition



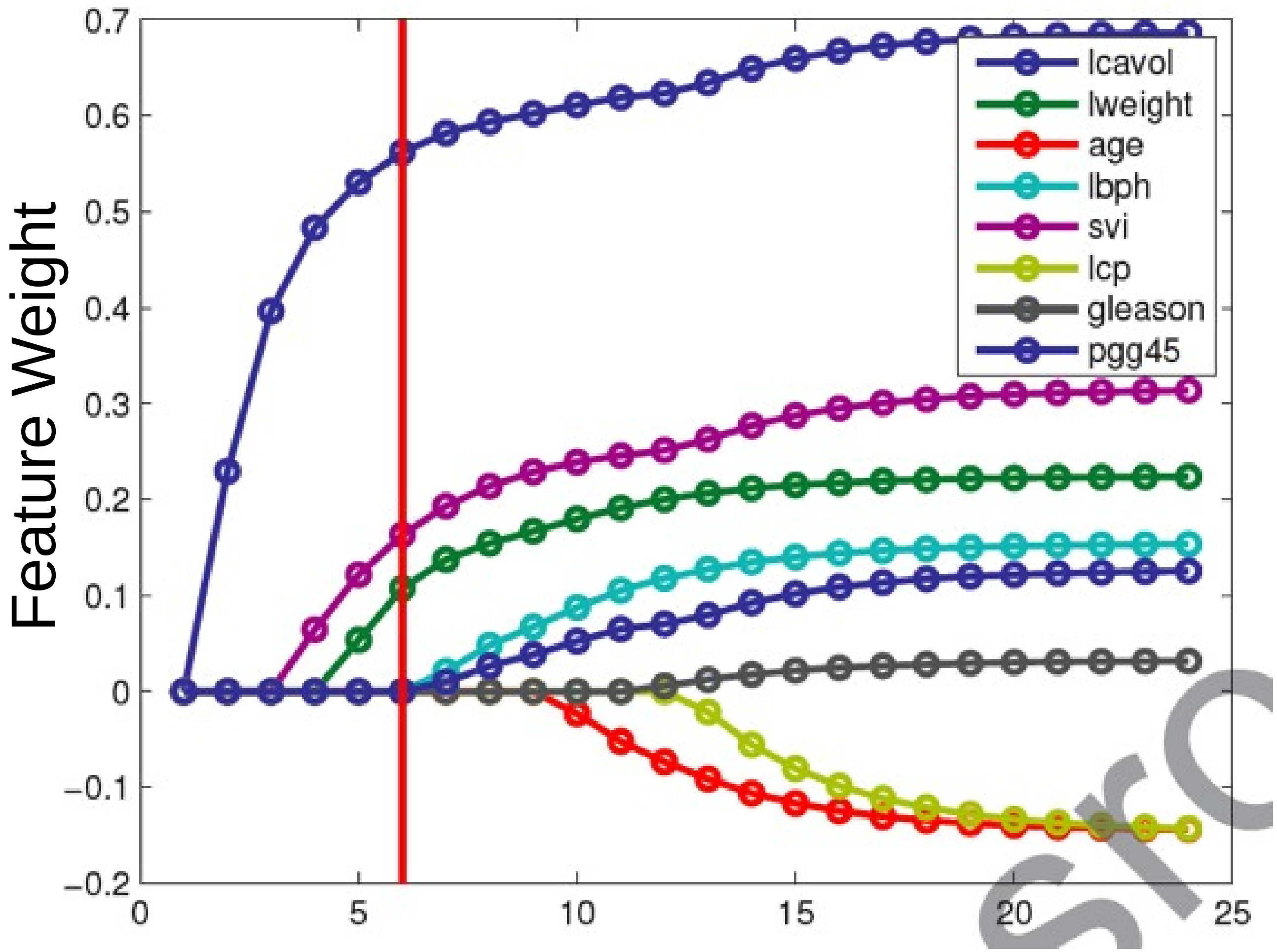
Ridge Regression



Lasso

From
Rob
Tibshirani
slides

LASSO Coefficent Path



From
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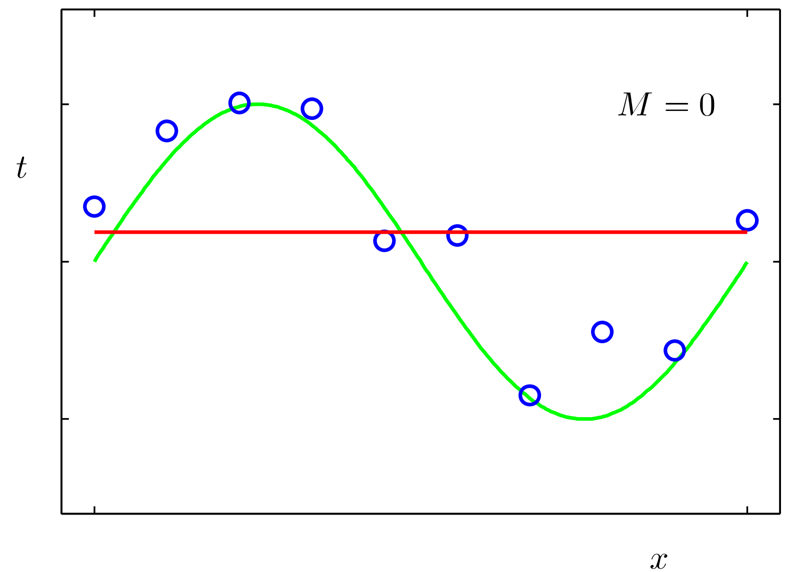
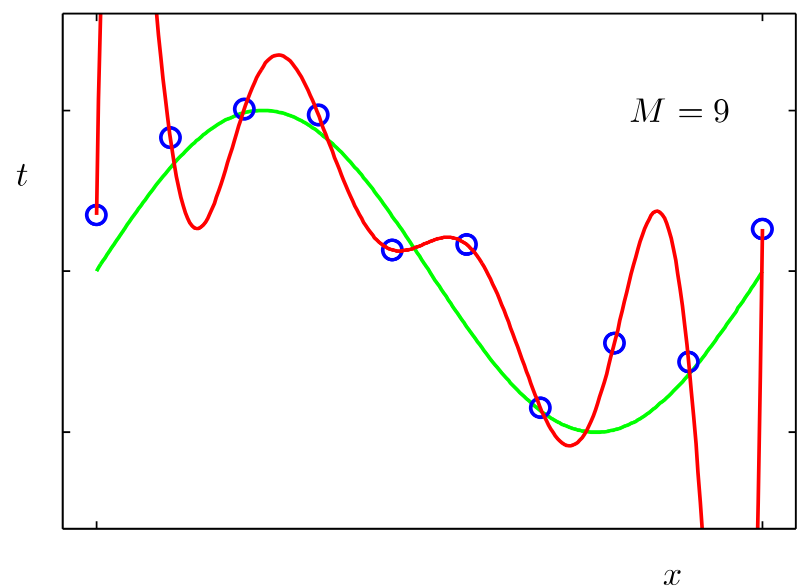
Larger λ $||\hat{w}||_1$ Smaller λ

Bias-Variance tradeoff – Intuition

- Model too simple: does not fit the data well
  – A *biased* solution

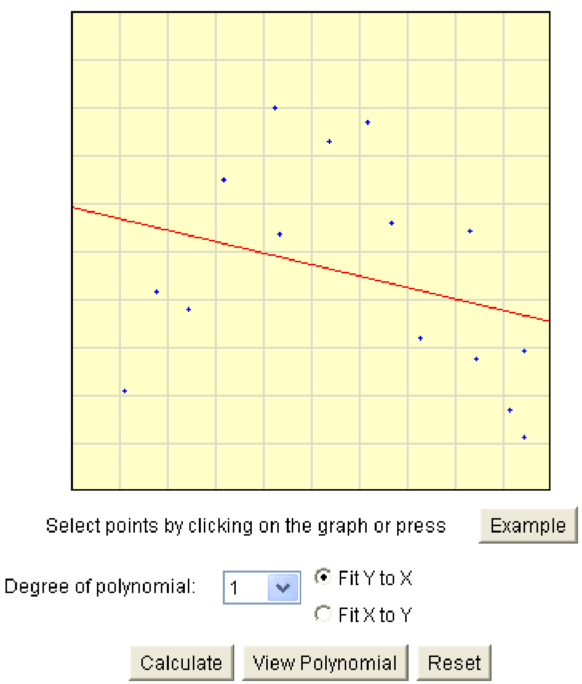


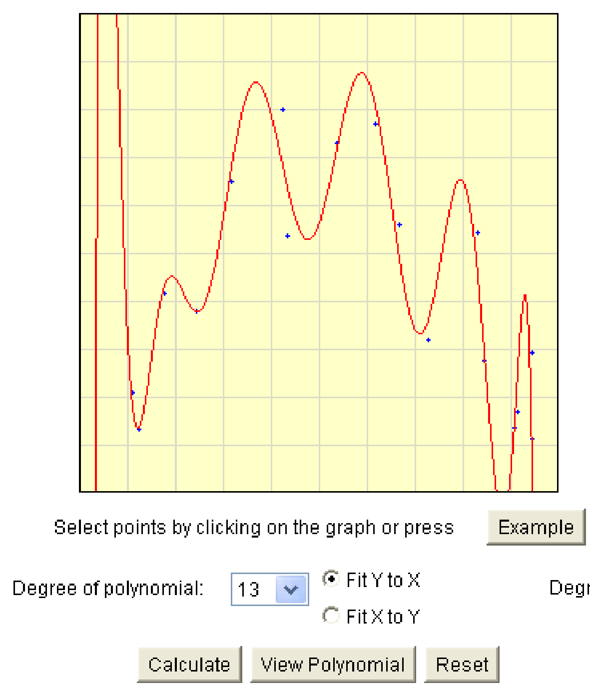
- Model too complex: small changes to the data, solution changes a lot
  – A *high-variance* solution

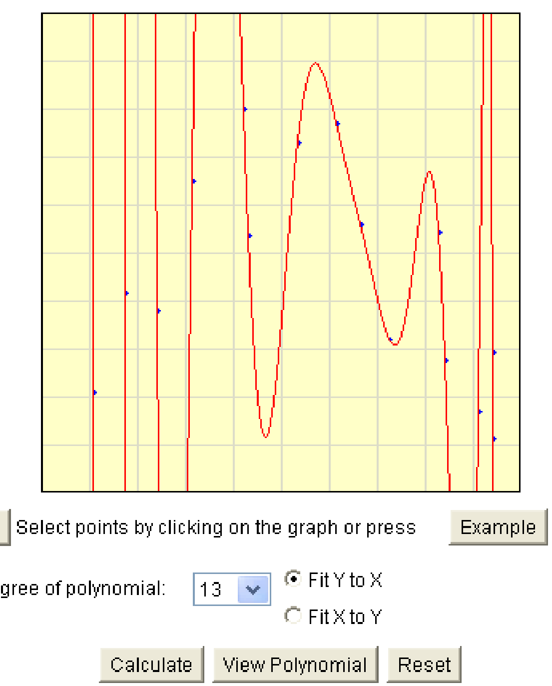


Bias-Variance Tradeoff

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







Training set error

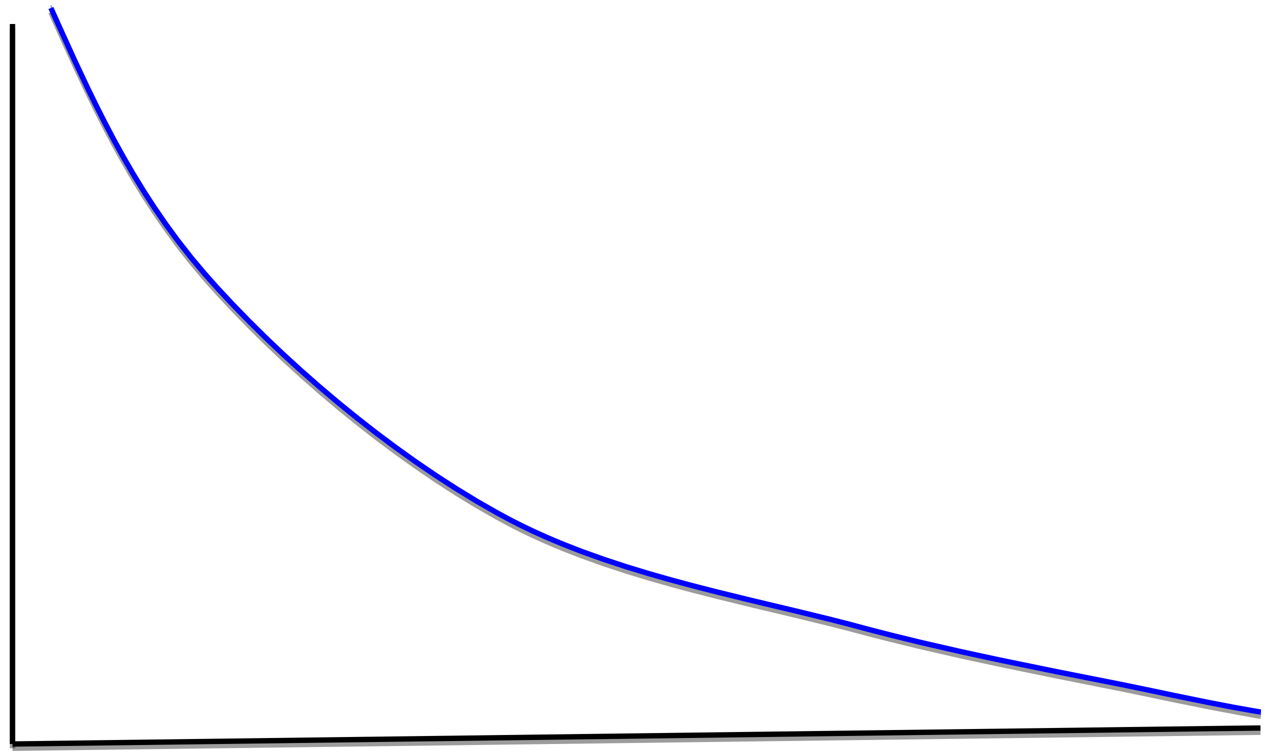
$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \sum_j \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

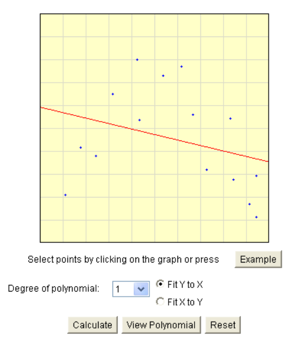
- Given a dataset (Training data)
- Choose a loss function
  - e.g., squared error (L_2) for regression
- Training error: For a particular set of parameters, loss function on training data:

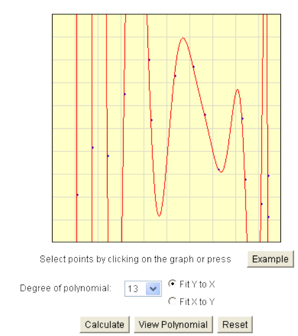
$$error_{train}(\mathbf{w}) = \frac{1}{N_{train}} \sum_{j=1}^{N_{train}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

Training error as a function of model complexity

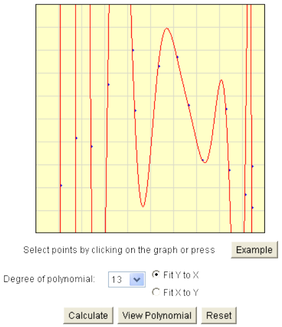
$$error_{train}(\mathbf{w}) = \frac{1}{N_{train}} \sum_{j=1}^{N_{train}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$







Prediction error



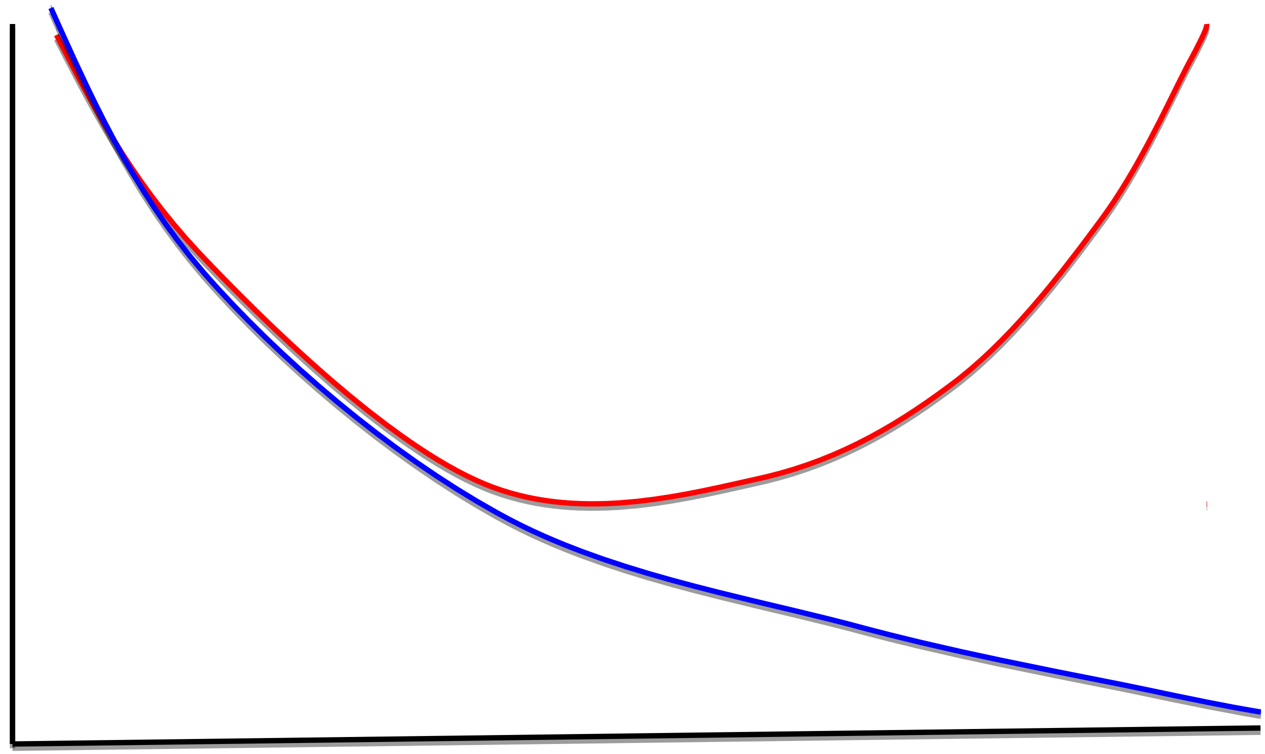
- Training set error can be poor measure of "quality" of solution
- Prediction error (true error): We really care about error over all possibilities:

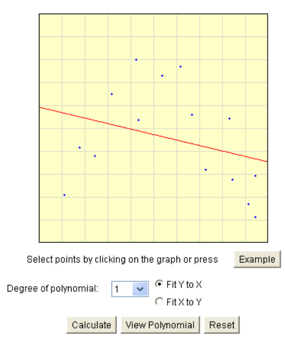
$$
\begin{aligned}
error_{true}(\mathbf{w}) &= E_{\mathbf{x}}\left[\left(t(\mathbf{x}) - \sum_i w_i h_i(\mathbf{x})\right)^2\right] \\
&= \int_{\mathbf{x}} \left(t(\mathbf{x}) - \sum_i w_i h_i(\mathbf{x})\right)^2 p(\mathbf{x})d\mathbf{x}
\end{aligned}
$$

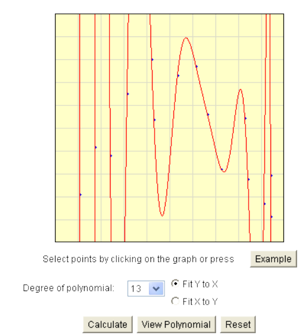
Prediction error as a function of model complexity

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

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







Computing prediction error

- To correctly predict error
  - Hard integral!
  - May not know t(**x**) for every **x**, may not know p(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?

- Sa

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

- Tr

err

- 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 – {$\mathbf{x}_1$,..., $\mathbf{x}_{Ntrain}$}
  - Test data – {$\mathbf{x}_1$,..., $\mathbf{x}_{Ntest}$}
- Use training data to optimize parameters **w**
- Test set error: For the ***final solution*** **w***, evaluate the error using:

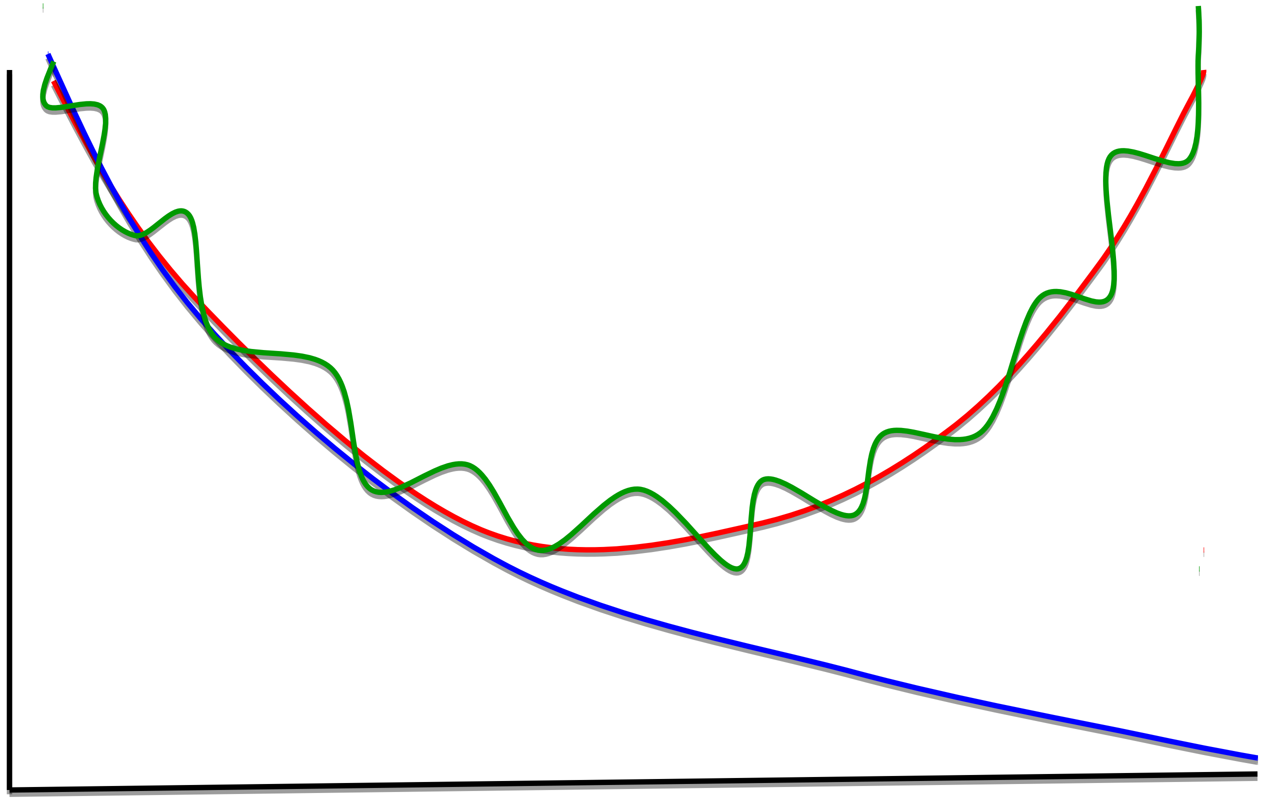
$$error_{test}(\mathbf{w}) = \frac{1}{N_{test}} \sum_{j=1}^{N_{test}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

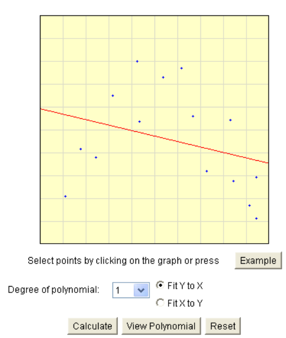
Test set error as a function of model complexity

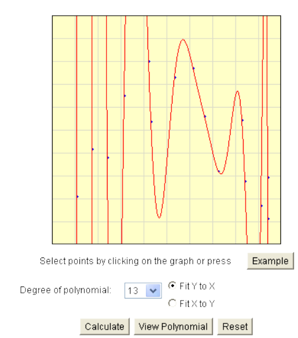
$$error_{train}(\mathbf{w}) = \frac{1}{N_{train}} \sum_{j=1}^{N_{train}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

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

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







Overfitting: this slide is so important we are looking at it again!

- Assume:
  - Data generated from distribution $D(X,Y)$
  - A hypothesis space H
- Define: errors for hypothesis $h \in H$
  - Training error: $error_{train}(h)$
  - Data (true) error: $error_{true}(h)$

- We say h ***overfits*** the training data if there exists an $h' \in H$ such that:

$$error_{train}(h) < error_{train}(h')$$

and

$$error_{true}(h) > error_{true}(h')$$

Summary: error estimators

- Gold Standard:

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

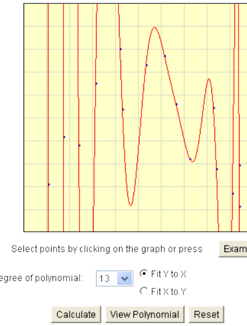
- Training: optimistically biased

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

- Test: our final measure

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

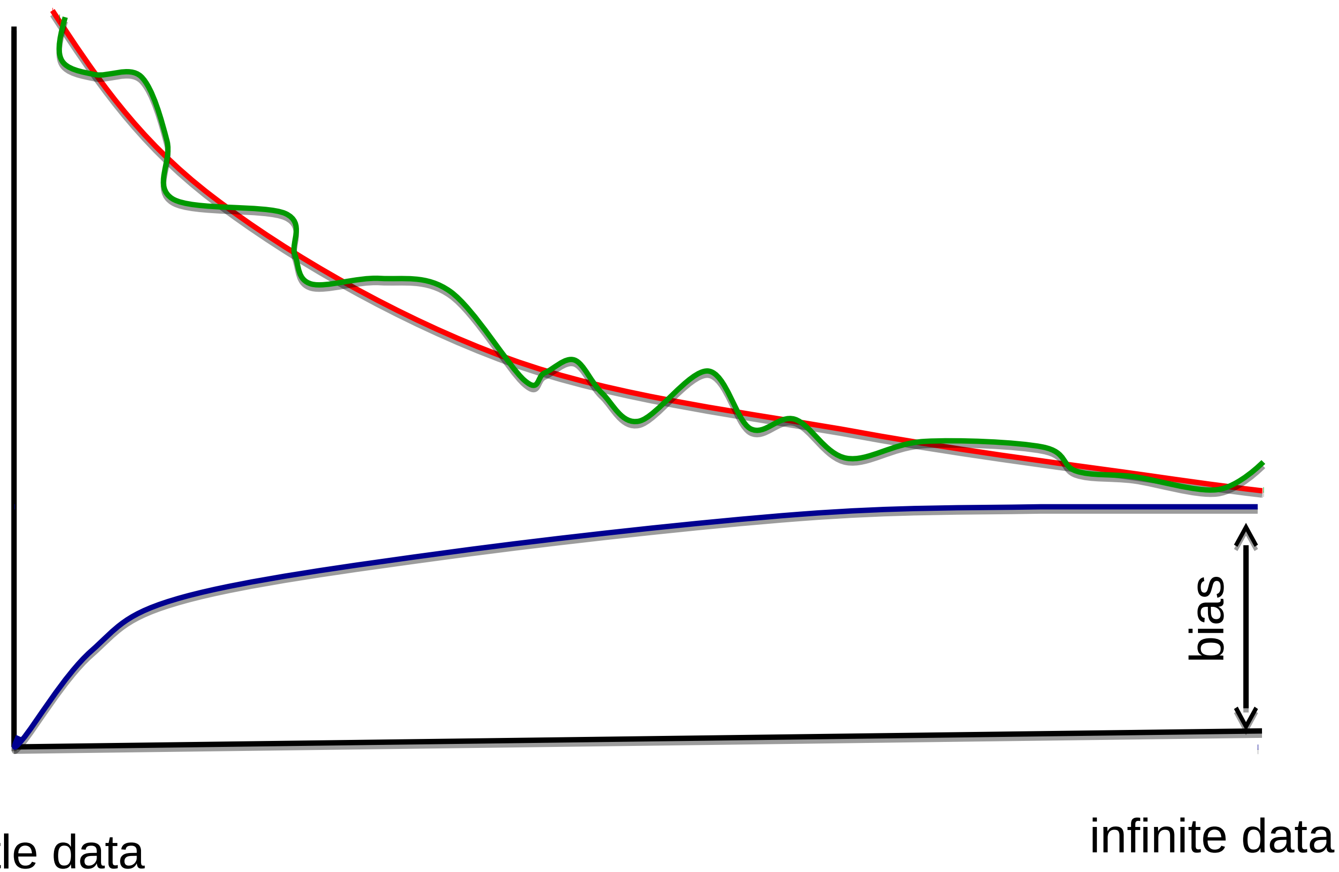
Error as a function of number of training examples for a fixed model complexity



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

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

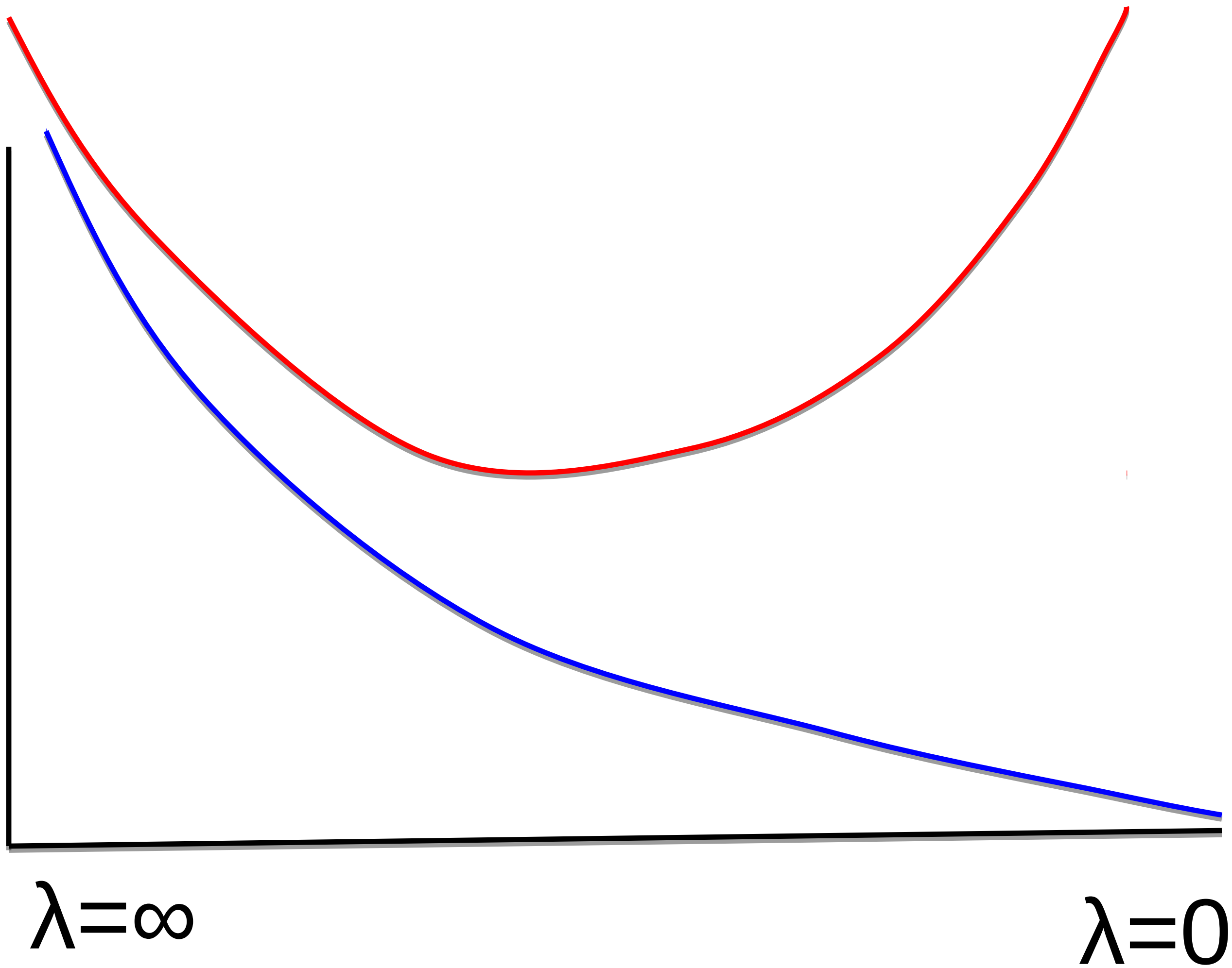
$$error_{test}(\mathbf{w}) = \frac{1}{N_{test}} \sum_{j=1}^{N_{test}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$



Error as function of regularization parameter, fixed model complexity

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

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



Summary: error estimators

- Ge
- Tr
- Te

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

- Regression
  - Basis function = features
  - Optimizing sum squared error
  - Relationship between regression and Gaussians
- Regularization
  - Ridge regression math
  - LASSO Formulation
  - How to set lambda
- Bias-Variance trade-off