Regression

CPS 570
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Supervised Learning

- Given: Training Set
- Goal: Good performance on test set
- Assumptions:
  - Training samples are independently drawn, and identically distributed (IID)
  - Test set is from same distribution as training set

Fitting Continuous Data (Regression)

- Datum i has feature vector: $\phi = (\phi_1(x^{(i)}) \ldots \phi_k(x^{(i)}))$
- Has real valued target: $t^{(i)}$ (row vector)
- Concept space: linear combinations of features:

$$y(\mathbf{x}^{(i)};\mathbf{w}) = \sum_{j=1}^{k} \phi_j(\mathbf{x}^{(i)}) w_j = \phi(\mathbf{x}^{(i)})\mathbf{w} = \phi^{(i)}\mathbf{w}$$

- Learning objective: Search to find "best" w
- (This is standard "data fitting" that most people learn in some form or another.)

Linearity of Regression

- Regression typically considered a *linear* method, but…
- Features not necessarily linear
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- and, BTW, features not necessarily linear

Regression Examples

- Predicting housing price from:
  - House size, lot size, rooms, neighborhood*, etc.
- Predicting weight from:
  - Sex, height, ethnicity, etc.
- Predicting life expectancy increase from:
  - Medication, disease state, etc.
- Predicting crop yield from:
  - Precipitation, fertilizer, temperature, etc.
- Fitting polynomials
  - Features are monomials

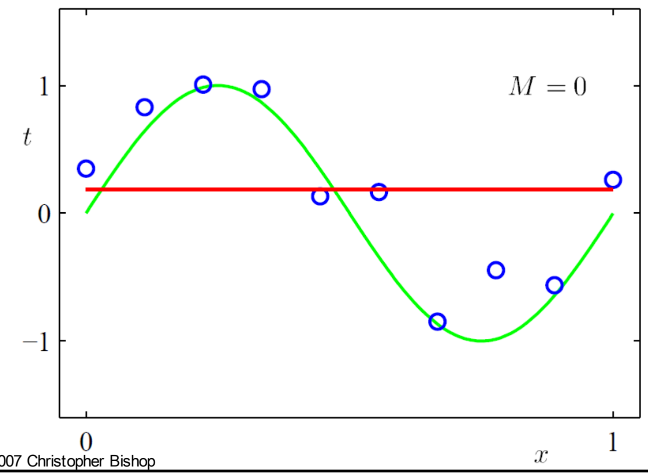
Features/Basis Functions

- Polynomials
- Indicators
- Gaussian densities
- Step functions or sigmoids
- Sinusoids (Fourier basis)
- Wavelets
- Anything you can imagine…

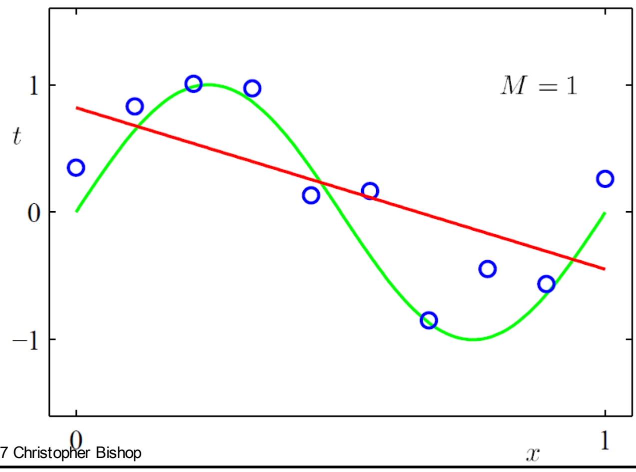
What is "best"?

- No obvious answer to this question
- Three compatible answers:
  - Minimize squared error on training set
  - Maximize likelihood of the data (under certain assumptions)
  - Project data into "closest" approximation
- Other answers possible

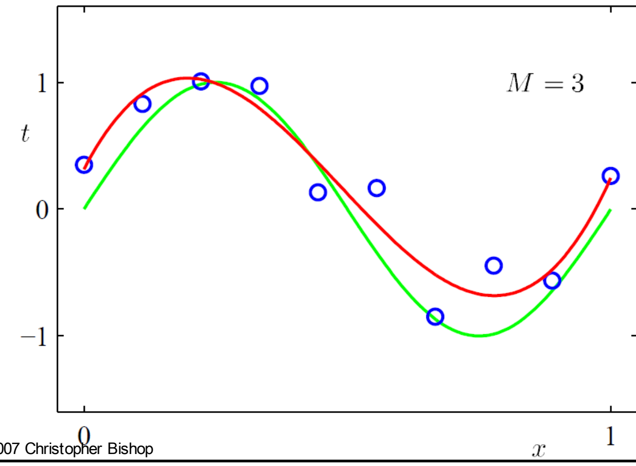
Degree 0 Fit



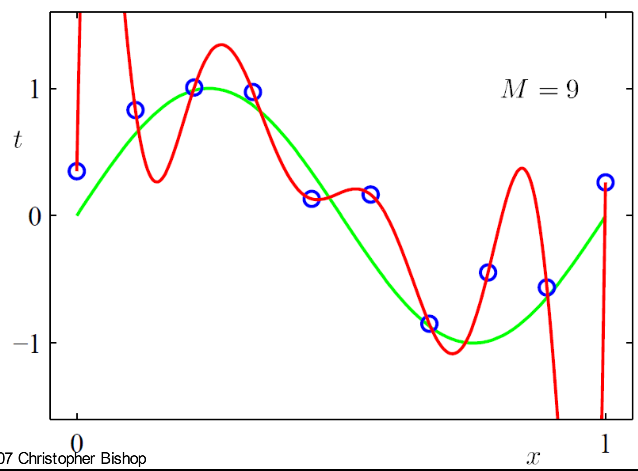
Degree 1 Fit



Degree 3 Fit



Degree 9 Fit



Minimizing Squared Training Set Error

- Why is this good?
- How could this be bad?
- Minimize:

$$E(\mathbf{w}) = \sum_{i=1}^{N}\left(\phi(\mathbf{x}^{(i)})\mathbf{w} - t^{(i)}\right)^2$$

Maximizing Likelihood of Data

- Assume:
  - True model is in H
  - Data have Gaussian noise
- Actually might want:

$$\underset{H}{\operatorname{argmax}} P(H \mid X) = \frac{P(X \mid H)P(H)}{P(X)}$$

- Is maximizing P(X|H) a good surrogate? (maximizing over w)

Maximizing P(X|H)

- Assume: $t^{(i)} = y^{(i)} + \varepsilon^{(i)}$
- Where: $P(\varepsilon^{(i)}) = \frac{1}{\sigma\sqrt{2\pi}} \exp(-\frac{(\varepsilon^{(i)})^2}{2\sigma^2})$

(Gaussian distribution w/mean 0, standard deviation σ)

- Therefore:

$$P(t^{(i)} \mid x^{(i)}, w) = \frac{1}{\sigma\sqrt{2\pi}} \exp(-\frac{(t^{(i)} - \phi(x^{(i)})\mathbf{w})^2}{2\sigma^2})$$

Maximization Continued

- Maximizing over entire data set:

$$\prod_{i=1}^{n} P(t^{(i)} \mid \phi^{(i)}, \theta) = \prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} \exp(-\frac{(t^{(i)} - \phi^{(i)}w)^2}{2\sigma^2})$$

- Maximizing equivalent log formulation: (ignoring constants)

$$\sum_{i=1}^{n} -(t^{(i)} - \phi^{(i)}\mathbf{w})^2$$

- Or minimizing:

$$E = \sum_{i=1}^{n} (t^{(i)} - \phi^{(i)}\mathbf{w})^2$$

Look familiar?

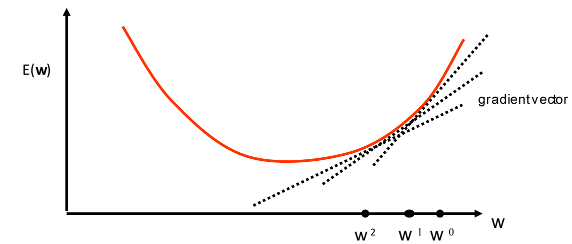
Checkpoint

- So far we have considered:
  - Minimizing squared error on training set
  - Maximizing Likelihood of training set (given model, and some assumptions)
- Different approaches w/same objective!

Solving the Optimization Problem

- Nota bene: Good to keep optimization problem and optimization technique separate in your mind
- Some optimization approaches:
  - Gradient descent
  - Direct Minimization

Minimizing E by Gradient Descent



Start with initial weight vector w_0

Compute the gradient $\nabla_w E = \left(\frac{\partial E(\mathbf{w})}{\partial w_0}, \frac{\partial E(\mathbf{w})}{\partial w_1}, \dots, \frac{\partial E(\mathbf{w})}{\partial w_n}\right)$

Compute $\mathbf{w} \leftarrow \mathbf{w} - \alpha \nabla E$ where α is the step size

Repeat until convergence

(Adapted from Lise Getoor's Slides)

Gradient Descent Issues

- For this particular problem:
  - No local optima
  - Convergence "guaranteed" if done in "batch"
- In general
  - Local optimum only (local=global for lin. regression)
  - Batch mode more stable
  - Incremental possible
    - Can oscillate
    - Use decreasing step size (Robbins-Monro) to stabilize

Solving the Minimization Directly

$$E = \sum_{i=1}^{n} (t^{(i)} - \phi^{(i)}\mathbf{w})^2$$

$$\nabla_w E \propto \sum_{i=1}^{n} (t^{(i)} - \phi^{(i)}\mathbf{w})\phi^{(i)}$$

scalar row vector

Set gradient to 0 to find min:

$$\sum_{i=1}^{n} (t^{(i)} - \phi^{(i)}\mathbf{w})\phi^{(i)} = 0$$

$$\sum_{i=1}^{n} \phi^{(i)} t^{(i)} - \mathbf{w}^T \sum_{i=1}^{n} (\phi^{(i)})^T \phi^{(i)} = 0$$

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

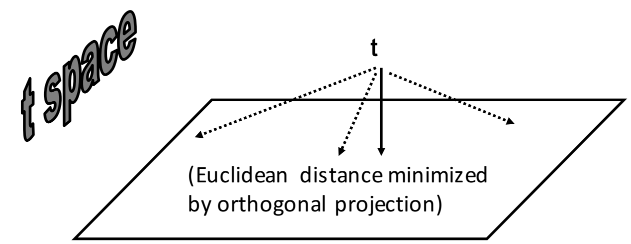
$$\mathbf{w} = \left(\Phi^T \Phi\right)^{-1} \Phi^T \mathbf{t}$$

$$\Phi = \begin{bmatrix} \boldsymbol{\phi}(x^{(1)}) \\ \boldsymbol{\phi}(x^{(2)}) \\ \vdots \\ \boldsymbol{\phi}(x^{(n)}) \end{bmatrix}$$

Geometric Interpretation

- $\mathbf{t}=(t^{(1)}\ldots t^{(n)})$ = point in n-space
- Ranging over $\mathbf{w}$, $\boldsymbol{\Phi}\mathbf{w}$ = H =
  - column space of features
  - subspace of R^n occupied by H
- Goal: Find "closest" point in H to $\mathbf{t}$
- Suppose closeness = Euclidean distance

Another Geometric Interpretation



H space (linear combinations of Φ)

Minimizing Euclidean Distance

- Minimize: $|\mathbf{t}-\Phi\mathbf{w}|_2$
- For n data points:

$$\sqrt{\sum_{i=1}^{n}(t^{(i)}-\phi^{(i)}\mathbf{w})^2}$$

- Equivalent to minimizing:

$$\sum_{i=1}^{n}(t^{(i)}-\phi^{(i)}\mathbf{w})^2$$

Look familiar?

Checkpoint

- Three different ways to pick $\mathbf{w}$ in H
  - Minimize squared error on training set
  - Maximize likelihood of training set
  - Distance minimizing projection into H
- All lead to same optimization problem!

$$\underset{\mathbf{w}}{\operatorname{argmin}} E(\mathbf{w})=\sum_{i=1}^{N}\left(\phi^{(i)}\mathbf{w}-t^{(i)}\right)^2$$

Geometric Solution

- Geometric Approach (Strang)
- Let $\mathbf{\Phi}$ be the feature (design) matrix
- Require orthogonality:

$$\forall z : (\Phi z)^T (\Phi \mathbf{w} - \mathbf{t}) = 0$$

Any vector in H

Line from **t** to solution

$$\forall z : z^T [\Phi^T \Phi \mathbf{w} - \Phi^T \mathbf{t}] = 0$$

Direct Solution Continued

- When is this true: $\forall z : z^T [\Phi^T \Phi \mathbf{w} - \Phi^T \mathbf{t}] = 0$
- When:

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

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

Same solution as direct minimization of error

When does the inverse exist?

Hidden Assumption

- Many of our solution methods require that our features (columns of Φ) that are linearly independent
- What if they aren't?
  - Solution isn't unique
  - Can use pseudoinverse (pinv in matlab)
  - Finds solution with minimum 2-norm

What if $t^{(i)}$ is a vector?

- Nothing changes!
- Scalar prediction:

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

- Vector prediction (exercise):

$$\mathbf{W} = (\Phi^T \Phi)^{-1} \Phi^T \mathbf{T}$$

Weight matrix

Target matrix

Checkpoint

- What we have shown:
  - Three different ways of viewing regression as an optimization problem
  - All three lead to the same solution
- What we have not shown
  - How to pick features
  - Whether these views are the "right" objective function

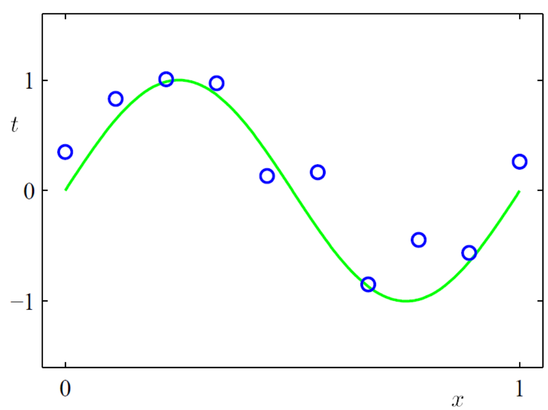
What about other criteria?

- Minimizing worse case (L_∞) loss?

$$\min_{\mathbf{w}} \max_i \left(\phi^{(i)}\mathbf{w} - t^{(i)} \right)$$

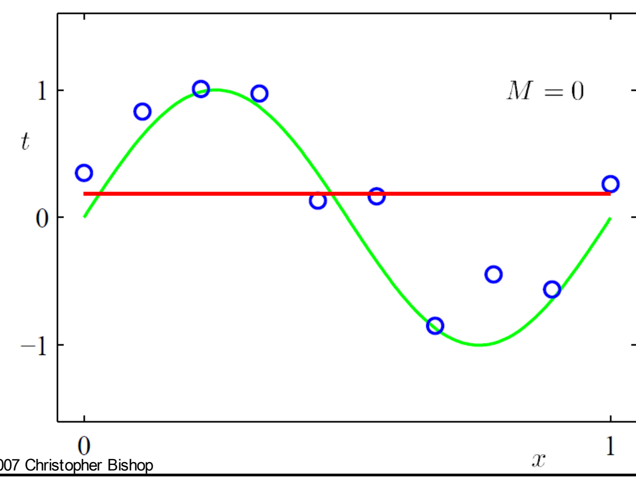
- Solve by linear program…

What is the Best Choice of Features?

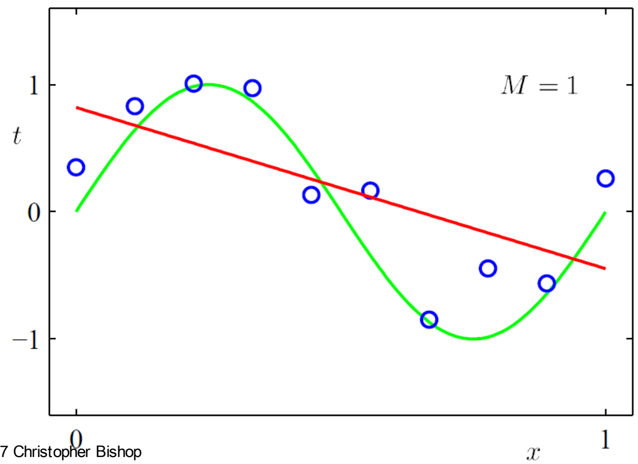


Noisy Source Data

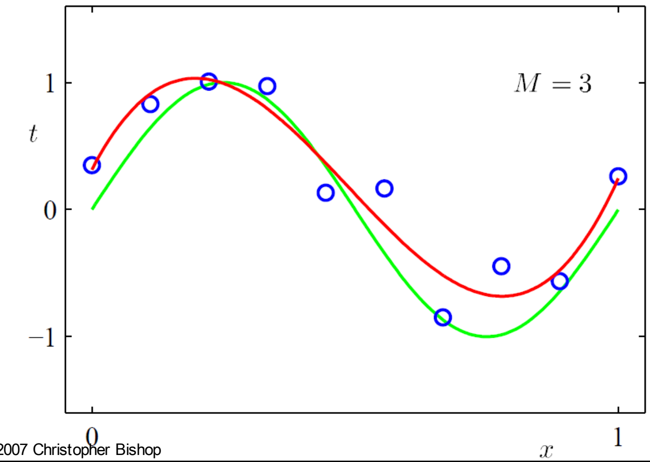
Degree 0 Fit



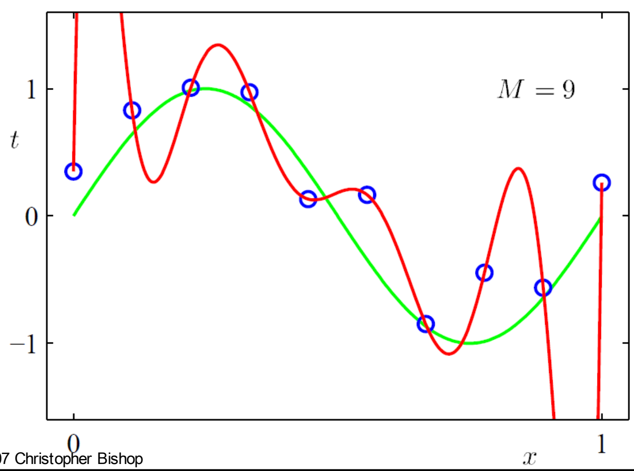
Degree 1 Fit



Degree 3 Fit

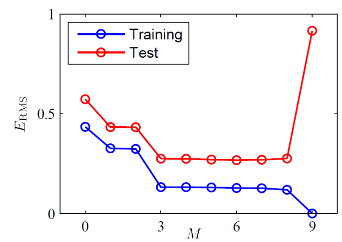


Degree 9 Fit



Observations

- Degree 3 is the best match to the source
- Degree 9 is the best match to the samples
- Performance on test data:



Understanding Loss

- Suppose we have a squared error loss function: L (gets too confusing to use E)
- Define h(**x**)=E[t|**x**]

$$E[L] = \underbrace{\int \{y(\mathbf{x}) - h(\mathbf{x})\}^2 p(\mathbf{x}) d\mathbf{x}}_{\text{Mismatch between hypothesis and target – we can influence this}} + \underbrace{\int \{h(\mathbf{x}) - t\}^2 p(\mathbf{x},t) d\mathbf{x} dt}_{\text{Noise in distribution of targets (nothing we can do)}}$$

Bias and Variance

$$E[L] = \int \{y(\mathbf{x}) - h(\mathbf{x})\}^2 p(\mathbf{x}) d\mathbf{x} + \int \{h(\mathbf{x}) - t\}^2 p(\mathbf{x},t) d\mathbf{x} dt$$

Since y(x) is fit to data, consider expectation over *different draws* of a *fixed size data* set for the part we control

$$E_D\left[\{y(\mathbf{x};D) - h(\mathbf{x})\}^2\right]$$
$$= \underbrace{\{E_D\left[y(\mathbf{x};D) - h(\mathbf{x})\right]\}^2}_{\text{bias}} + \underbrace{E_D\left[\{y(\mathbf{x};D) - E_D\left[y(\mathbf{x};D)\right]\}^2\right]}_{\text{variance}}$$

Understanding Bias

$$\{E_D\left[y(\mathbf{x};D) - h(\mathbf{x})\right]\}^2$$

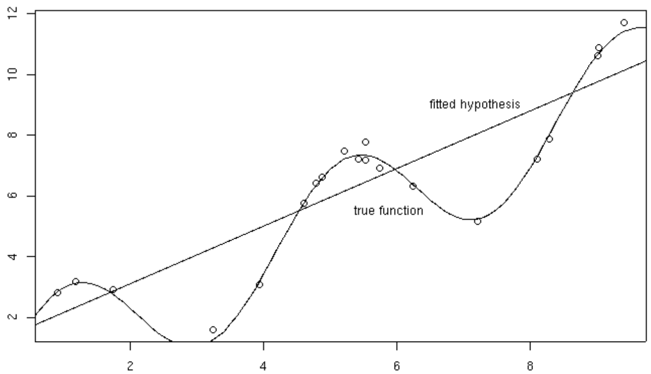
- Measures how well our approximation architecture can fit the data
- Weak approximators (e.g. low degree polynomials) will have high bias
- Strong approximators (e.g. high degree polynomials, will have lower bias)

Understanding Variance

$$E_D\left[\{y(\mathbf{x};D) - E_D\left[y(\mathbf{x};D)\right]\}^2\right]$$

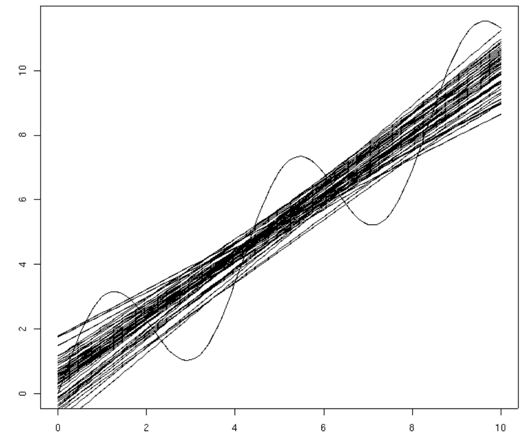
- No *direct* dependence on target values
- For a fixed size D:
  - Strong approximators will tend to have more variance
  - Weak approximators will tend to have less variance
- Variance will typically disappear as size of D goes to infinity

Example: 20 points
$y = x + 2\sin(1.5x) + N(0,0.2)$



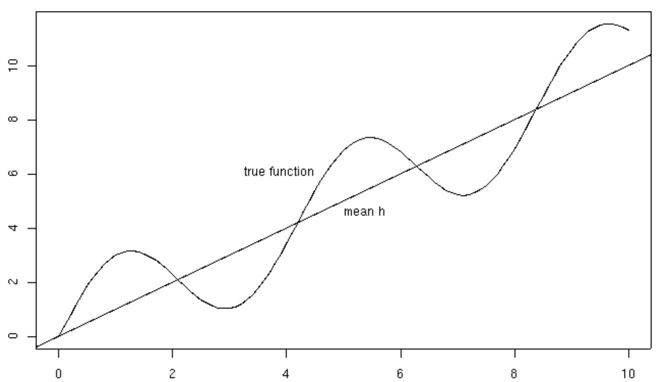
Hypothesis space = linear in x

50 fits (20 examples each)

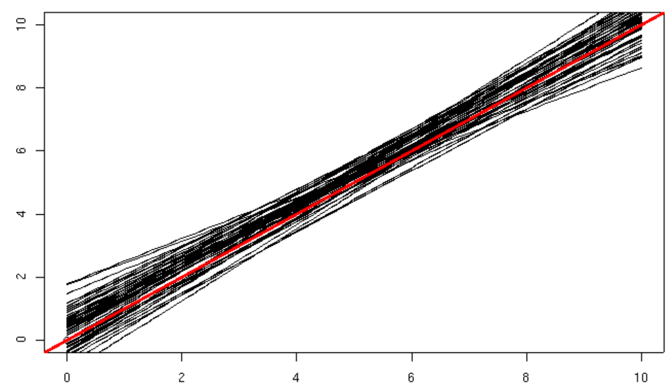


What are we seeing here?

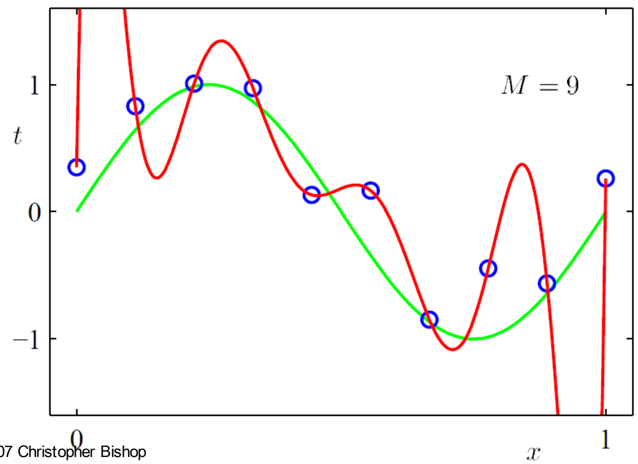
Bias



Variance

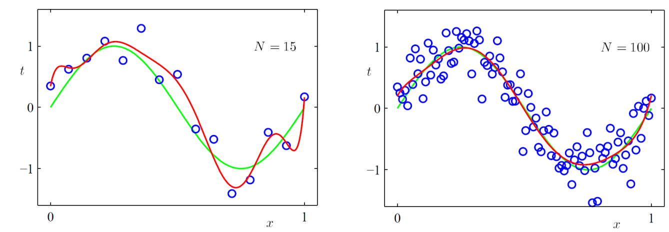


Degree 9 Fit Revisited



Trade off Between Bias and Variance

- Is the problem a bad choice of polynomial?
- Is the problem that we don't have enough data?
- Answer: Yes
- Lower bias -> Higher Variance
- Higher bias -> Lower Variance



Bias and Variance: Lessons Learned

- When data are scarce relative to the "capacity" of our hypothesis space
  - Variance can be a problem
  - Restricting hypothesis space can reduce variance at cost of increased bias
- When data are plentiful
  - Variance is less of a concern
  - May afford to use richer hypothesis space

Concluding Comments

- Regression is the most basic machine learning algorithm
- Multiple views are all equivalent:
  - Minimize squared loss
  - Maximize likelihood
  - Orthogonal projection
- Big question: Choosing features
- First steps towards understanding this:
  Bias and variance trade off