Intro to Key Themes in Predictive Modeling

Illustrated through (Generalized) MLR

Readings/Notation: *I'll closely follow Bishop Ch 3.1, 3.2, which uses machine learning notation: parameters are w's (for weights), dependent variable is "t" for target, and model produces output "y".*
(Also see EA:4.6-4.8, KM: 1.2.2)

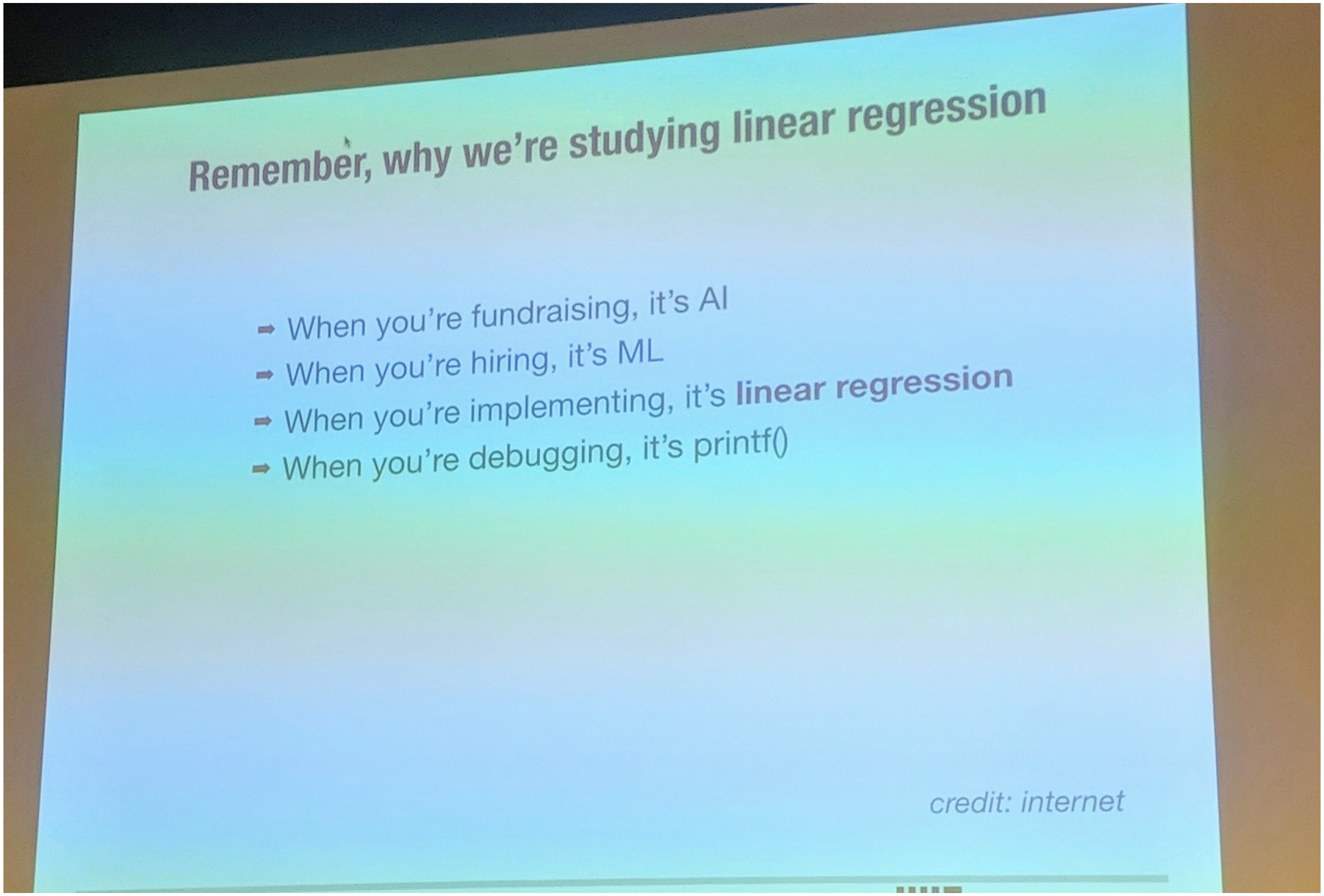
Outline/Objectives

- True Performance (Generalization)
- Overfitting /Underfitting
  - Bias – Variance Tradeoff

All of the above inform Effective Model Choice and Complexity

- Regularization (Ridge and Lasso)

Concepts carry over to classification problems.


Remember, why we're studying linear regression
➡ When you're fundraising, it's AI
➡ When you're hiring, it's ML
➡ When you're implementing, it's linear regression
➡ When you're debugging, it's printf()
credit: internet

Parametric Models

Determine functional form of model (e.g. polynomials, neural nets,…)

- "learn" the parameters (weights) of the model using the training data.

- Example: linear regression

- Generalized linear regression: linear combination of basis functions (basis function expansion)

$$y(x, \mathbf{w}) = \sum_{i=0}^{M} w_i \phi_i(x) = \mathbf{w}^\top \boldsymbol{\phi}(x)$$

  – **Special Case: linear regression**.

  – Special Case: polynomial regression: (with scalar x)

$$y(x, \mathbf{w}) \;=\; w_0 + w_1 x + \ldots + w_M x^M$$

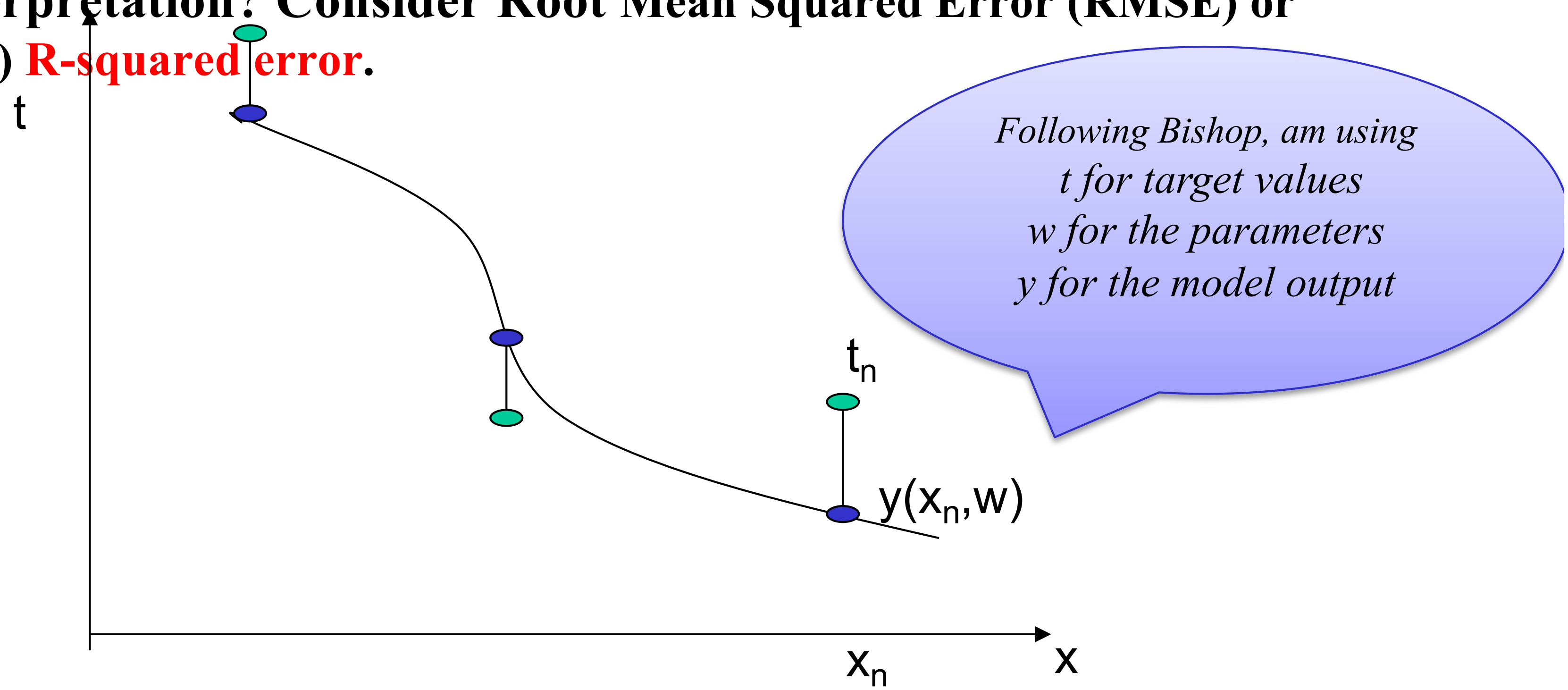
i.e., the basis functions are given by $\phi_i(x) = x^i$

Ordinary Least Squares (OLS)

- Minimize a loss function E(**w**) given by sum-of-squares **error (SSE)** **(t's are the target values)**

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{\mathbf{w}^{\top}\phi(x_n) - t_n\}^2$$

Best interpretation? Consider Root Mean Squared Error (RMSE) or (adjusted) R-squared error.



Least Squares Solution*

- Exact **closed-form** minimizer (ML solution)

$$\mathbf{w}^* = \left(\boldsymbol{\Phi}^\top \boldsymbol{\Phi}\right)^{-1} \boldsymbol{\Phi}^\top \vec{t}$$

where $\vec{t} = (t_1, \ldots, t_N)^\top$
  - "Pseudo-inverse solution"

    and $\boldsymbol{\Phi}$ is the *design matrix* given by

$$\boldsymbol{\Phi} = \begin{pmatrix} \phi_0(\mathbf{x}_1) & \cdots & \phi_M(\mathbf{x}_1) \\ \phi_0(\mathbf{x}_2) & \cdots & \phi_M(\mathbf{x}_2) \\ \vdots & \vdots & \vdots \\ \phi_0(\mathbf{x}_N) & \cdots & \phi_M(\mathbf{x}_N) \end{pmatrix}$$

Takeaways:
- *Direction solution involves inversion of an (M+1)x(M+1) matrix*
- *Computation Linear in data set size, cubic in M*
- *Batch mode training*
- *Explicitly shows collinearity problem*

Collinearity problem: *parameter estimates have high uncertainty if two or more independent variables are highly collinear*

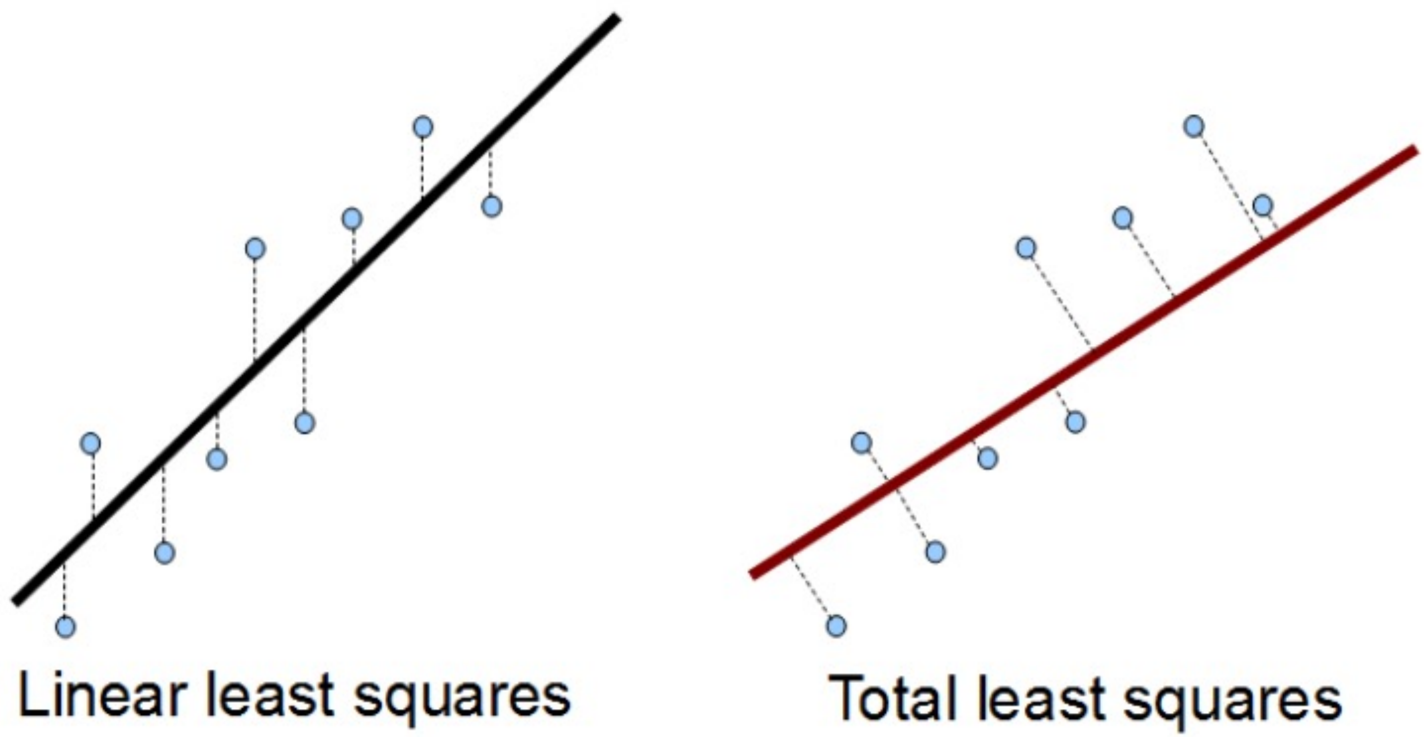
Why OLS?

- Minimizing Mean Squared Error (MSE) on the training data yields the Maximum Likelihood Estimate (MLE) solution of the following (assumed) model:
  - Expected value of *T* given the basis function vector phi is linear in phi.
    - i.e. Conditional mean is linear in the predictors.
  - All distributions around the expected values are assumed to be i.i.d. zero mean Gaussian with constant variance.
  - In stats notation: $Y|X_1 \ldots X_p \sim N(\beta_0 + \beta_1 X_1 \ldots + \beta_p X_p, \sigma^2)$
  - In new notation: (fill in)

(For Proof see **Bishop pg. 140**)

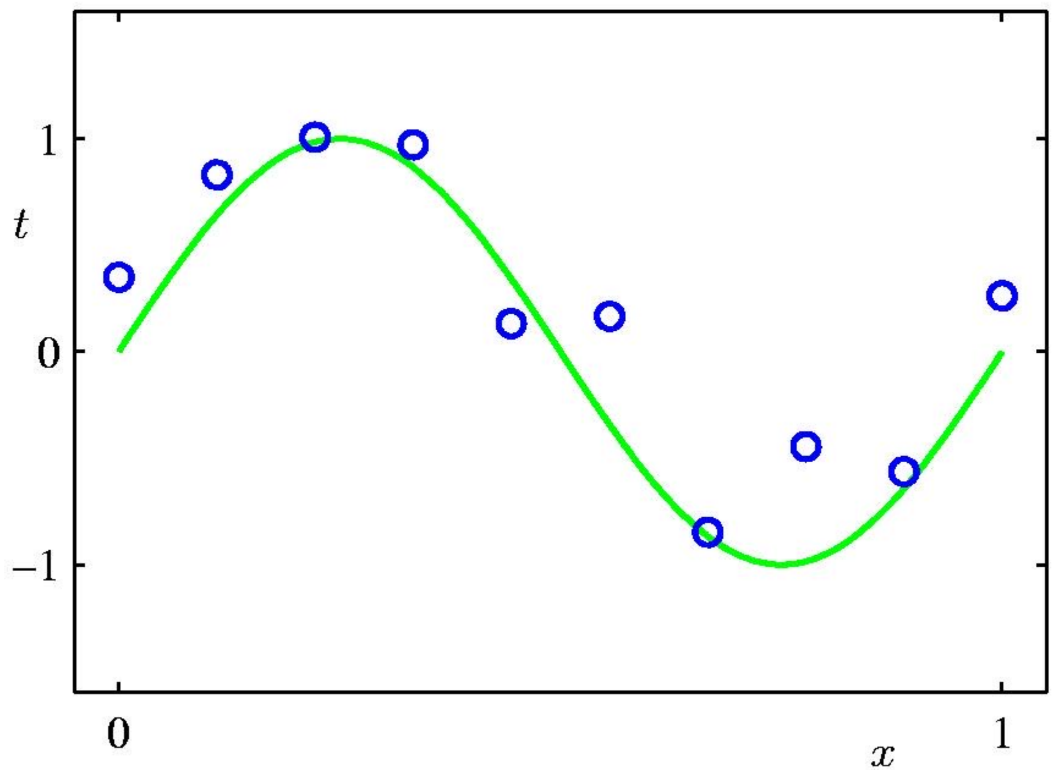
- How can you "verify" that the assumptions seem reasonable?

Total Least Squares (Aside)



Which one is better?
Which one should you choose?

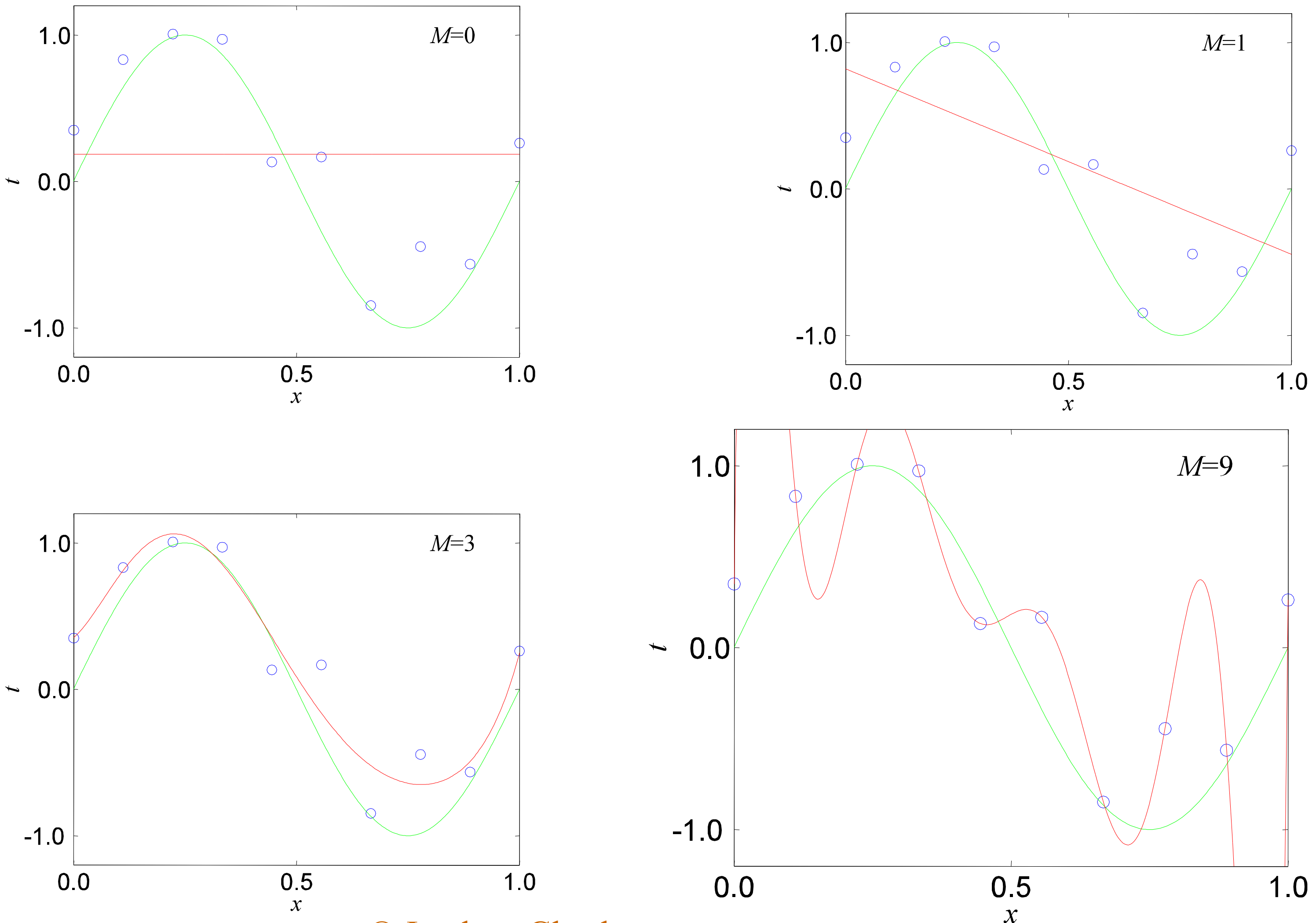
Polynomial Curve Fitting



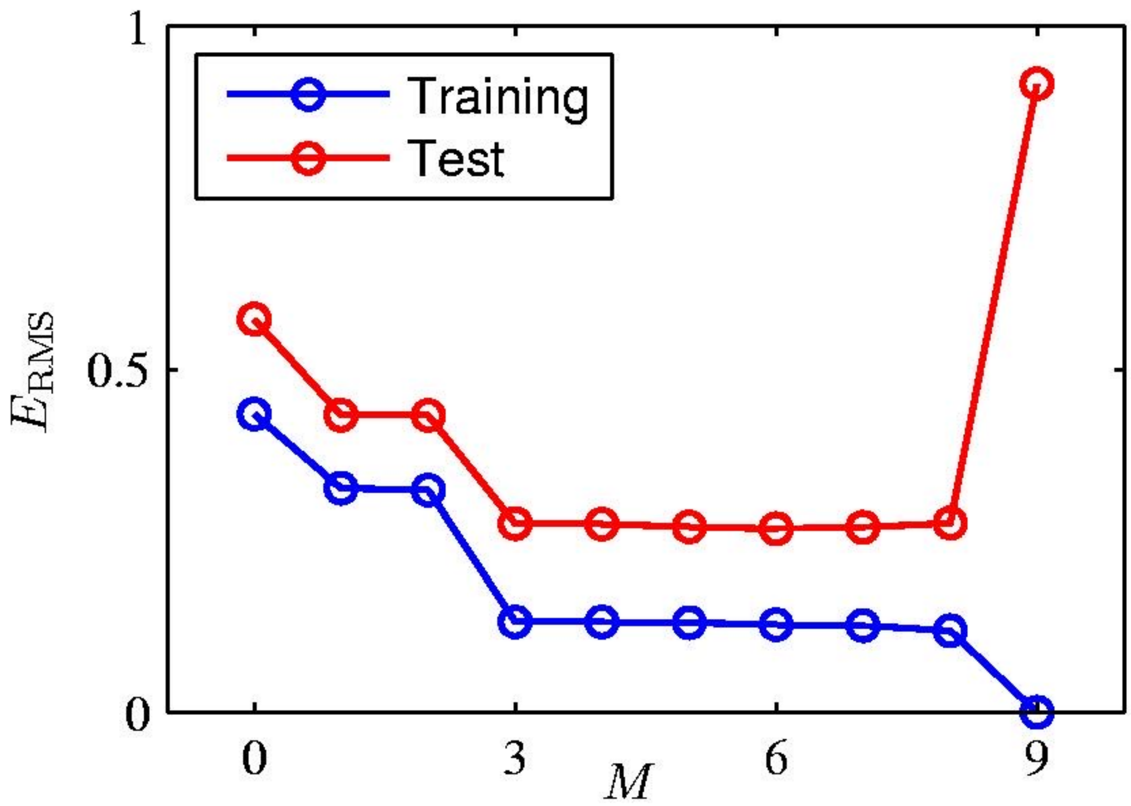
$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

Model Complexity and Overfitting

- "Noisy sine" example from Chris Bishop

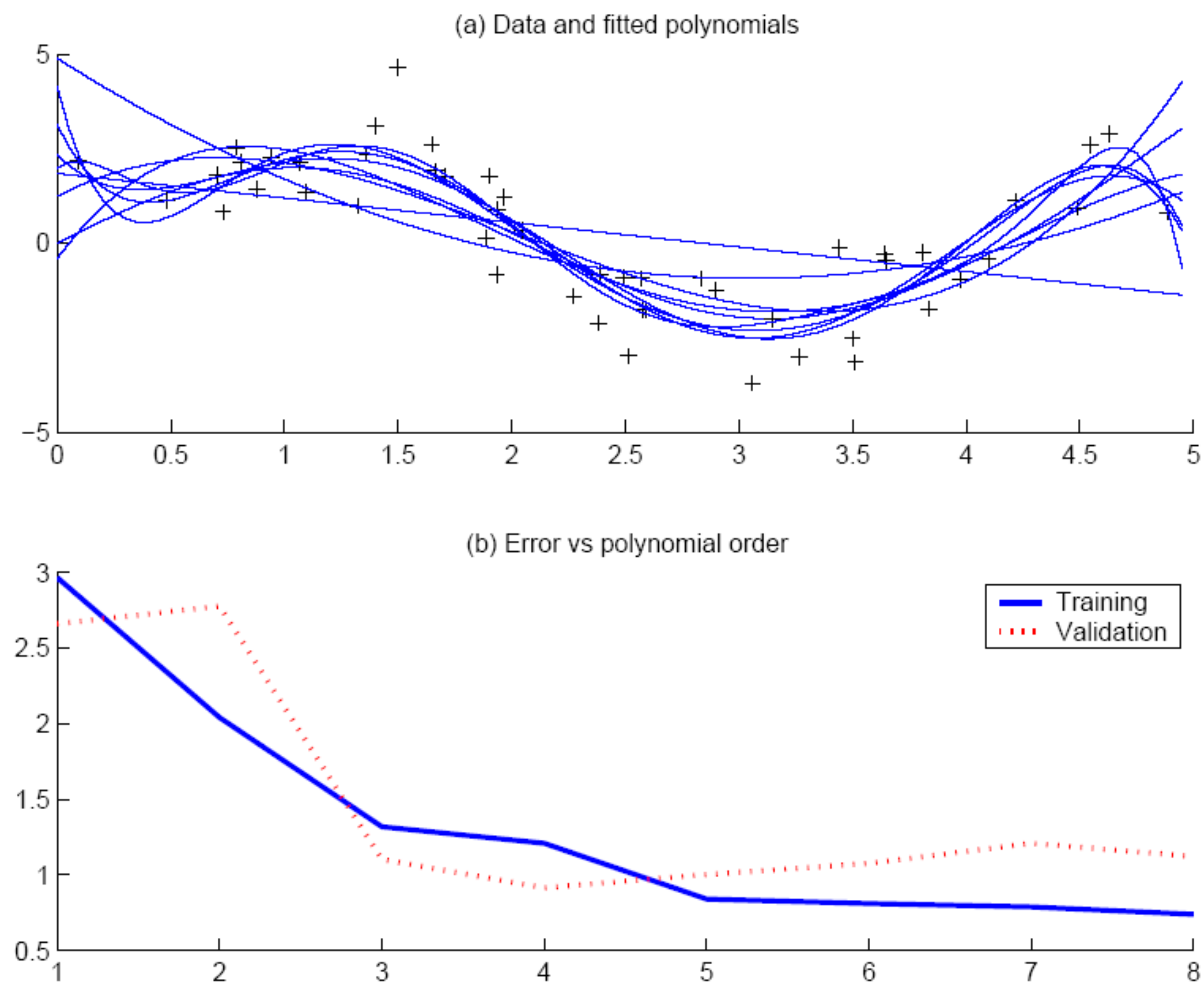


Over-fitting



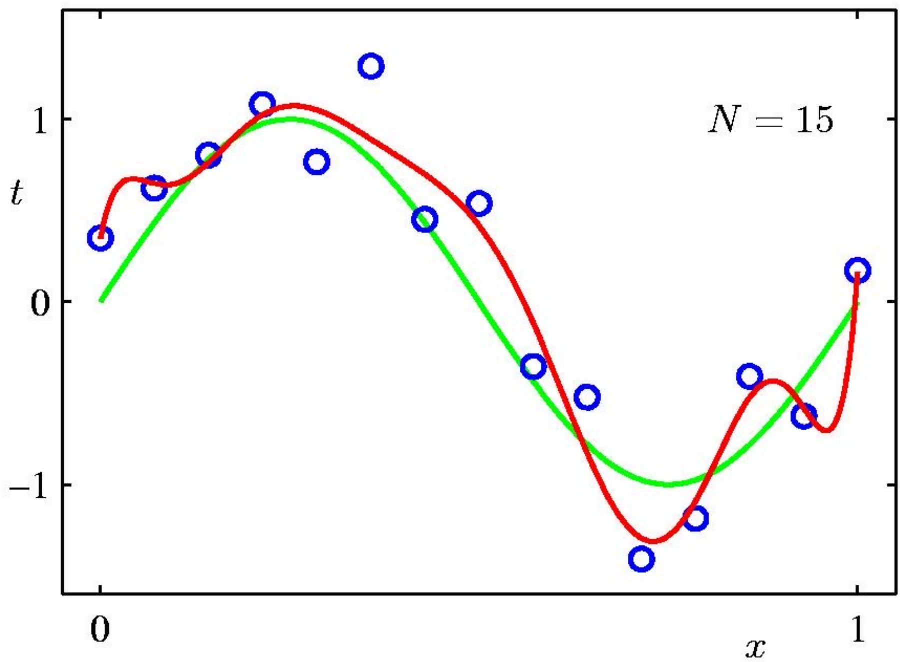
Root-Mean-Square (RMS) Error vs Polynomial order

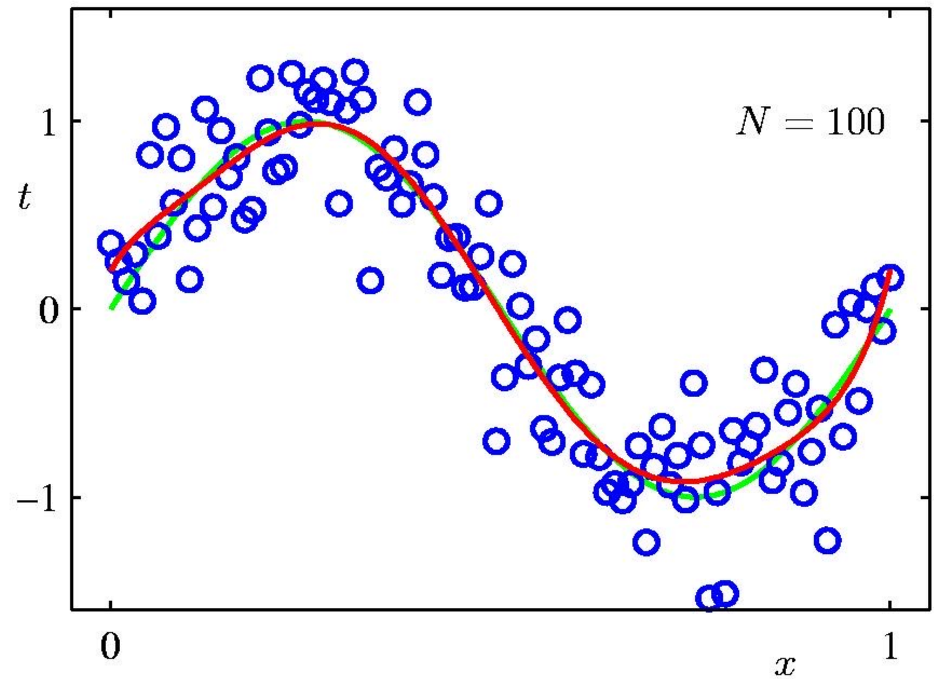
Another Example



Effect of Data Set Size

9^{th} Order Polynomial





$N = 15$ $\qquad$ $N = 100$

Learning Curves

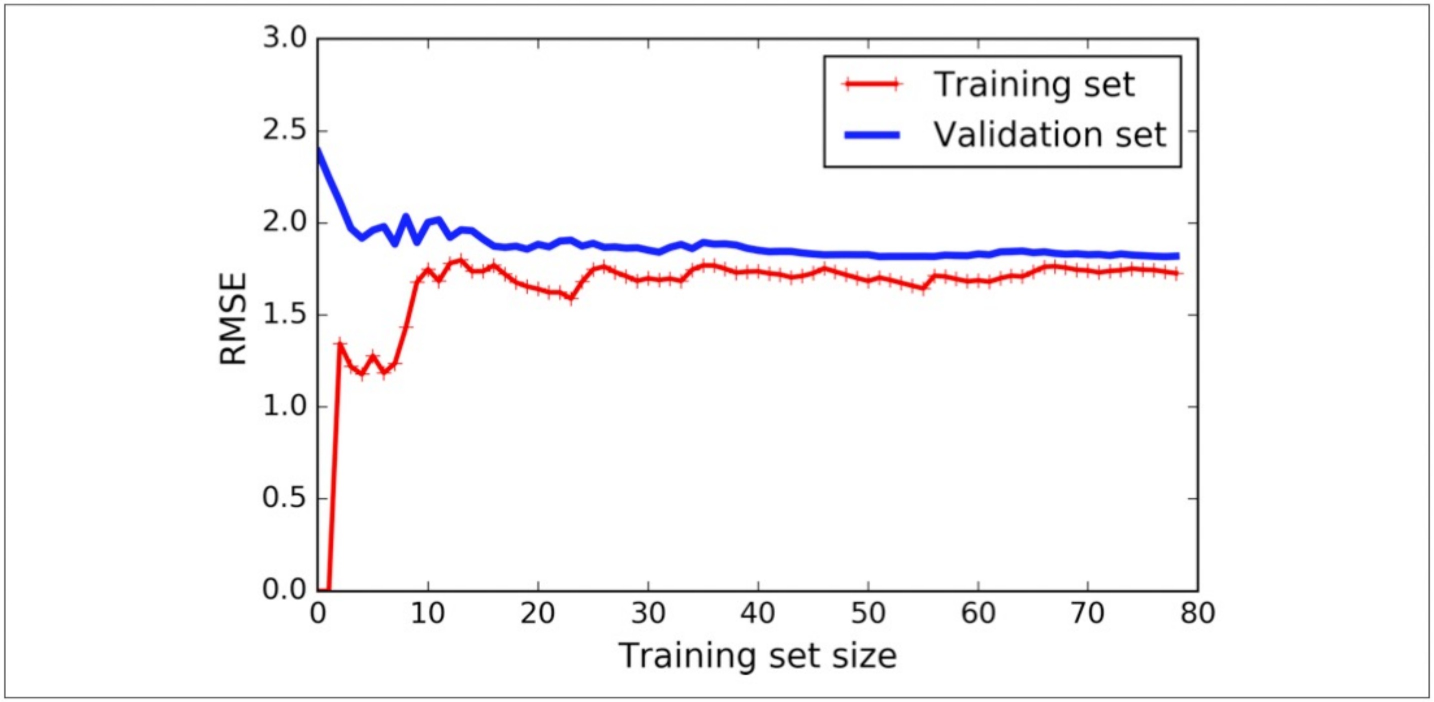


Figure 4-15. Learning curves *(from AG, pg 132)*

- How will these curves look like for different degree polyomials for the ”sine curve” example?
- Understand using bias-variance (later)

Regularization (to avoid overfitting)

- "regularization term" imposes penalty on less desirable solutions
  - Cost = MSE + λ Penalty (f)
    - Scikit uses "alpha" to denote lambda.
  - Regularization Penalty is a functional (maps each function f onto a number)
- Popular Penalties
  - **ridge regression** (sum squared of weights)
  - **Lasso** (sum of |w|; for large λ yields sparse models)
    - **Elastic net:** combines both ridge and Lasso
  - number of non-zero weights
  - smoothness of function

note: 1. "intercept", i.e. w_0, not included in penalties

2. customary to standardize all independent variables first (why?)

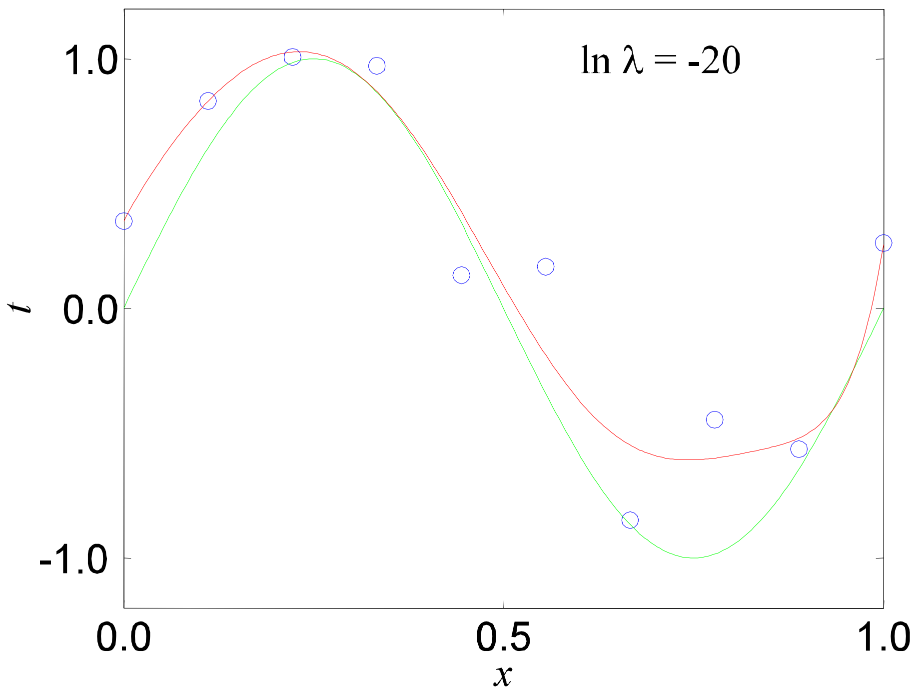
Ridge Regression Example

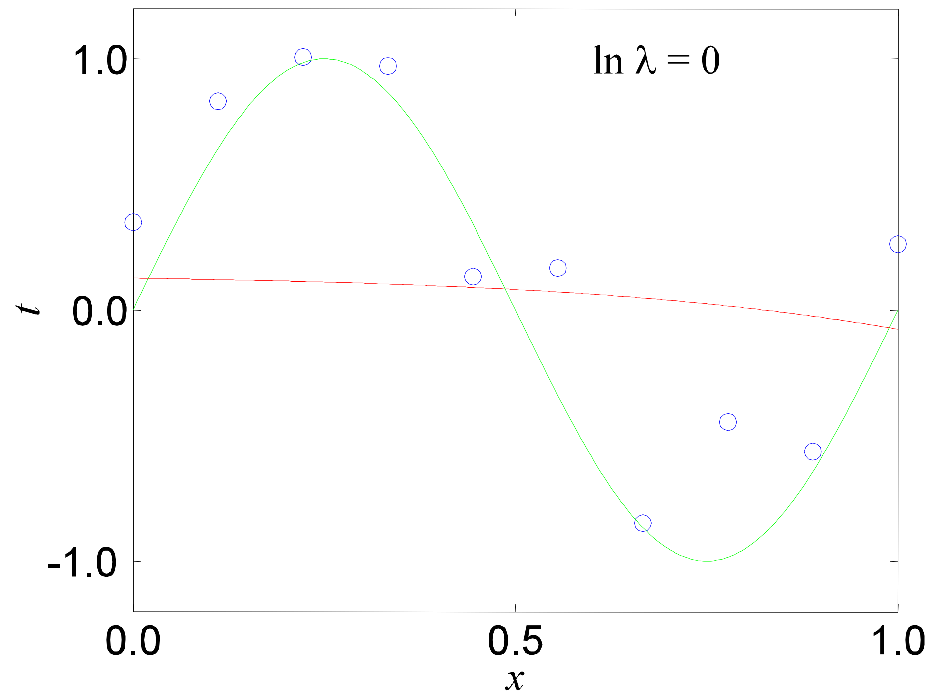
- Discourage large values by adding penalty term to error

$$E(\mathbf{w}) = \sum_{n=1}^{N} \{\mathbf{w}^{\mathsf{T}}\phi(\mathbf{x}_n) - t_n\}^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

- Also called *shrinkage* (stats) or *weight decay (neural nets)*
- The regularization coefficient λ now controls the effective model complexity
- *Closed form solution: $\mathbf{w} = \left(\lambda\mathbf{I} + \mathbf{\Phi}^{\mathrm{T}}\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^{\mathrm{T}}\mathbf{t}.$
  - Leads to numerical stability as well!

Regularized $M = 9$ Polynomial





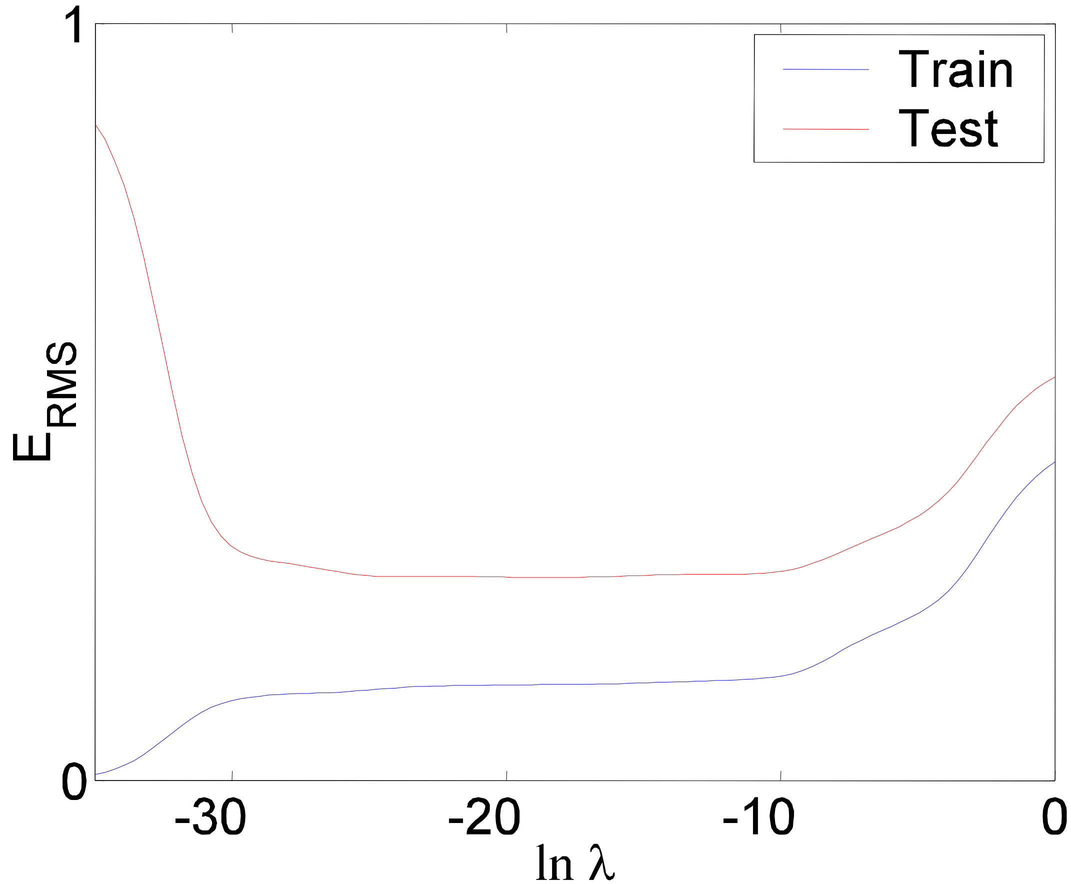
Regularized Parameters

- First col is the unregularized solution

	$\ln \lambda = -\infty$	$\ln \lambda = -20$	$\ln \lambda = 0$
$w_0^\star$	0.35	0.35	0.1273
$w_1^\star$	232.37	5.56	-0.0459
$w_2^\star$	-5321.83	-12.27	-0.0578
$w_3^\star$	48568.31	19.01	-0.0460
$w_4^\star$	-231639.30	-82.58	-0.0321
$w_5^\star$	640042.26	46.49	-0.0201
$w_6^\star$	-1061800.52	141.84	-0.0104
$w_7^\star$	1042400.18	-29.57	-0.0028
$w_8^\star$	-557682.99	-231.55	0.0032
$w_9^\star$	125201.43	142.98	0.0080

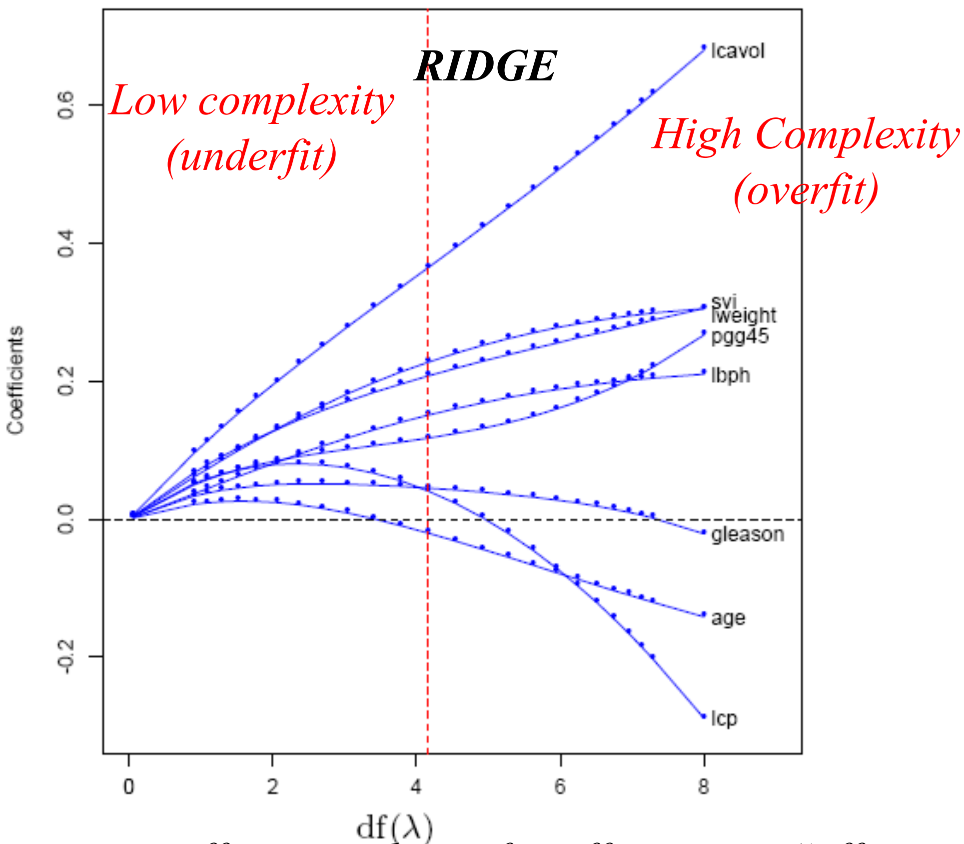
Generalization

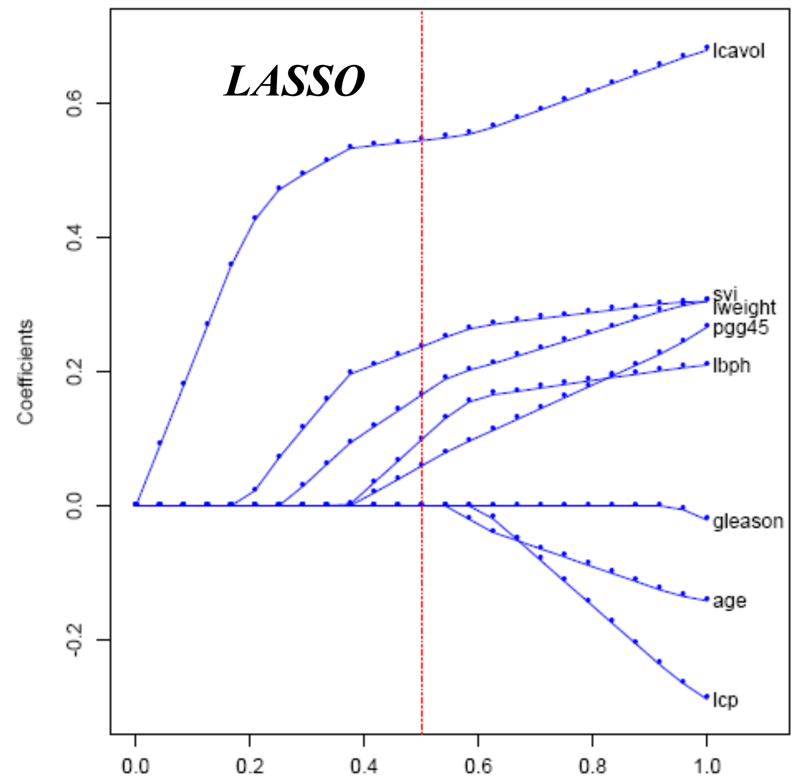
- Noisy sine problem



Ridge vs. Lasso

- HTF figs 3.7, 3.9: Prostate Cancer example. Red line chosen by Cross-validation





Effect on values of coefficients as "effective degrees of freedom (df)" is increased for (a) Ridge regression (left) and (b) Lasso (Right).

High λ translates to low df, so ***λ is being progressively decreased from left to right along the x-axis.***

Evaluation

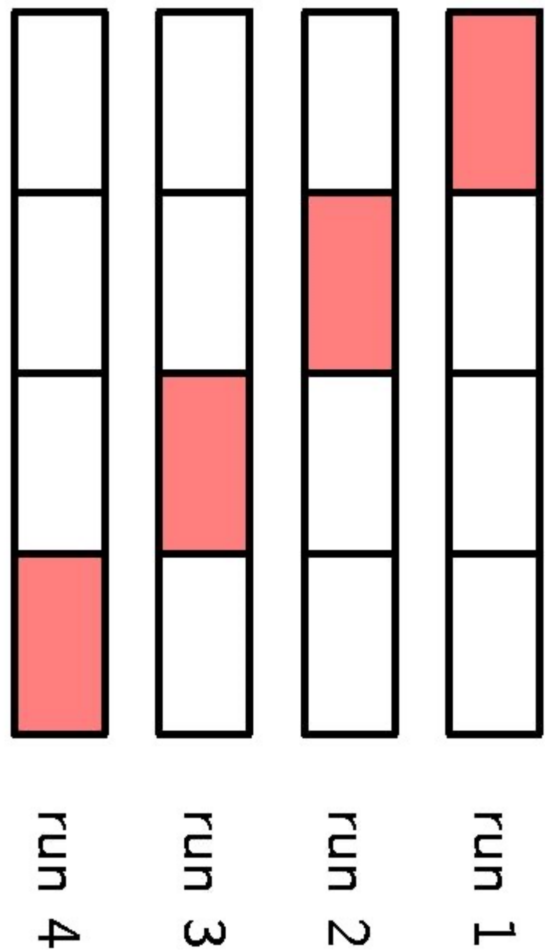
- Quality criterion for regression
  - Mean squared error (MSE) or equivalent, e.g. SSE, RMSE
    - true vs. empirical
    - normalized (R^2 value = % of variance explained)
    - Adjusted R^2

Estimating True Performance (Data Driven)

- enough data? Use "holdout" to estimate
- Moderately large? Use k-fold cross-validation

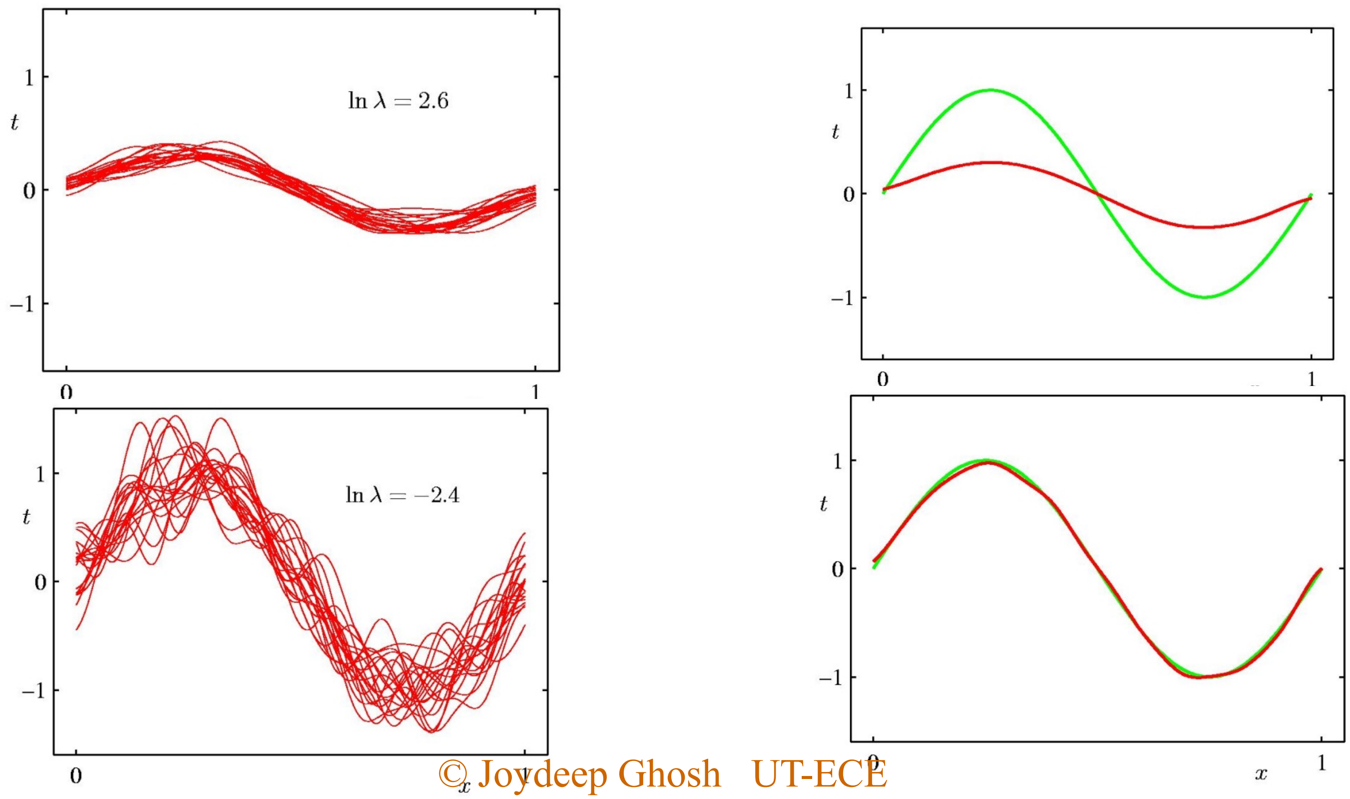
k = 4 example

Shaded subset: validation set for that run



How to evaluate a Regression Model?

- Model = math form + learning method.
  - Will be impacted by given training (and validation) dataset!!
  - Want to evaluate the model irrespective of the specific train/validate dataset used.
    - Need to consider the collection of solutions obtained, not one specific solution.
- Bishop fig 3.5. Compares highly regularized solution (top row) vs. less regularized solution (bottom row). Individual solutions (left), averaged solution (right)



Bias-Variance Dilemma

Usually *measured* output is not a deterministic function of *given* inputs

Assume: t = h (x) + zero-mean noise

- your model gives y (x). The *expected squared loss*,

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

- best predictor: $\mathbb{E}[t \mid x] = h(x)$;

  - MSE_{opt} = variance of the noise inherent in the random variable t. (2nd term on RHS)

- What does the first term comprise of ? $(\text{Model\_bias})^2$ + Model_variance

  Bias: how good the average model is;

  Variance: how sensitive the model is to variations in data.

  Tradeoff between the two terms as function of model complexity

$$\text{expected loss} = (\text{bias})^2 + \text{variance} + \text{noise}$$

Math Details: The Bias-Variance Decomposition*

- Suppose we were given multiple data sets, each of size N. Any particular data set, D, will give a particular function y(x;D).
- For any x, The expected loss (over datasets of size N) is

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

(try to express both terms in words)

The Bias-Variance Decomposition II*

Considering all possible values of x, we can write

$$\text{expected loss} = (\text{bias})^2 + \text{variance} + \text{noise}$$

where

$$(\text{bias})^2 = \int \{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2 p(\mathbf{x})\,\mathrm{d}\mathbf{x}$$

$$\text{variance} = \int \mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}^2\right] p(\mathbf{x})\,\mathrm{d}\mathbf{x}$$

$$\text{noise} = \iint \{h(\mathbf{x}) - t\}^2 p(\mathbf{x}, t)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t$$

Bias: how good the average model is;
Variance: how sensitive the model is to variations in data.

NOTE: the bias and variance concepts here apply to a predictive model, rather than to an estimator of a specific value.

Extra: Understanding the Bias-Variance Tradeoff

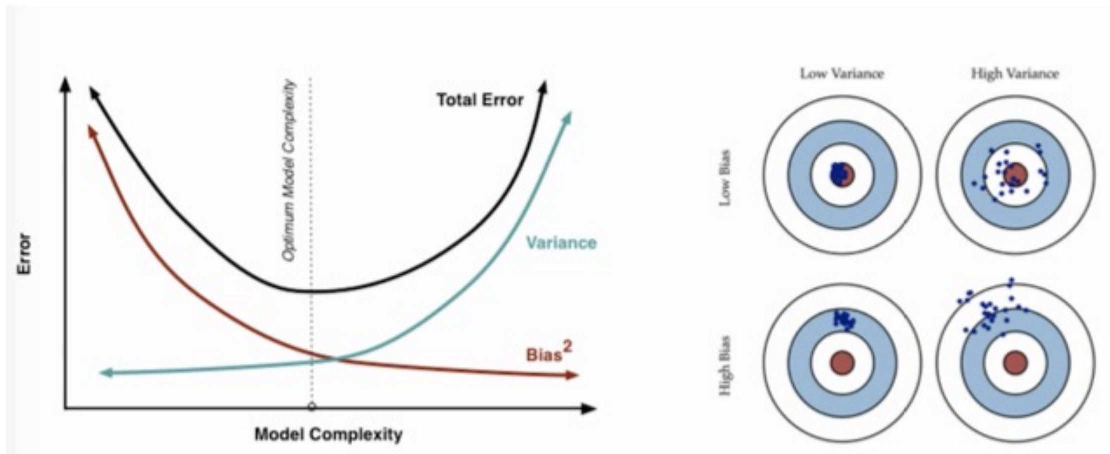
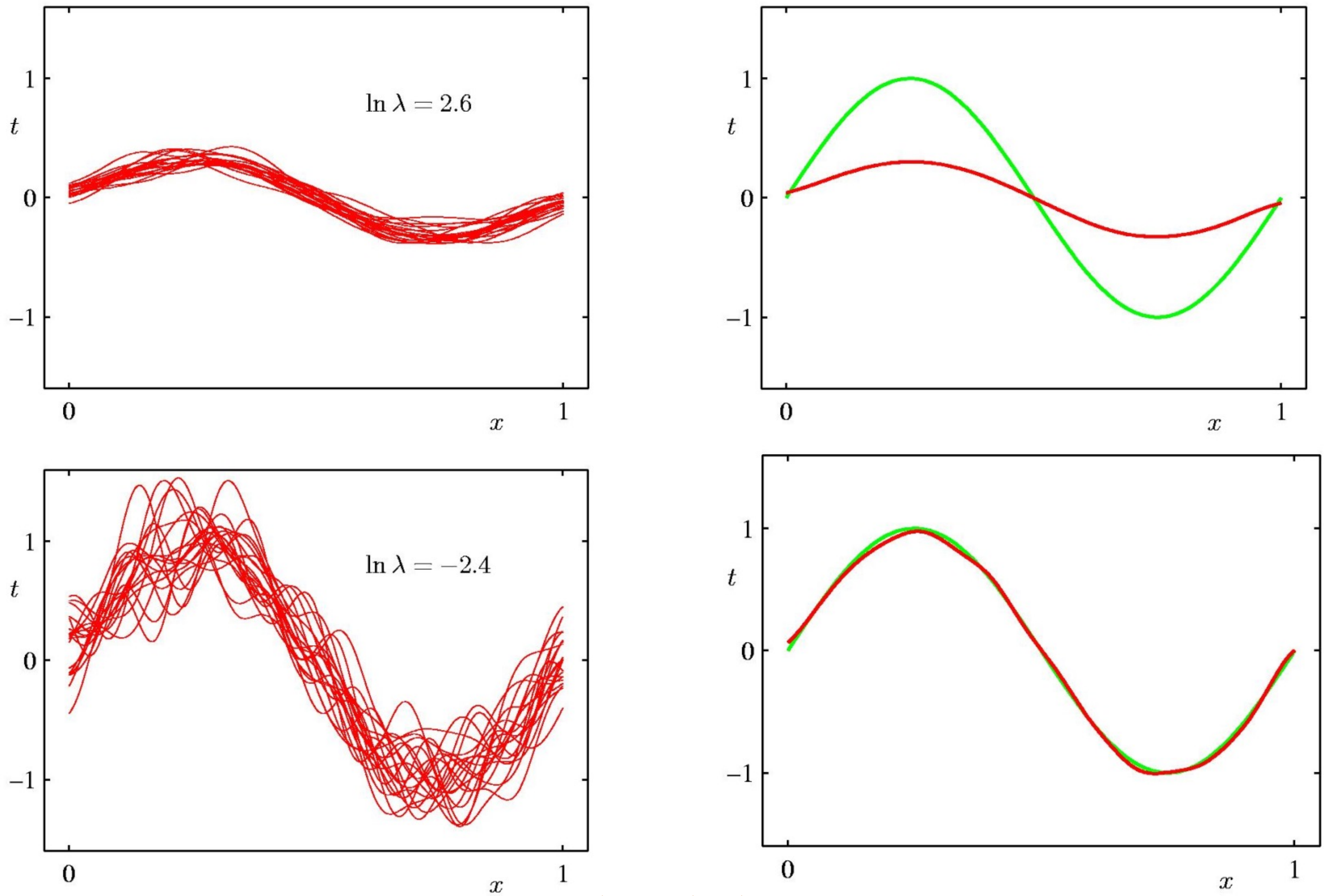


Figure 4.26: Cartoon illustration of the bias variance tradeoff. From `http://scott.fortmann-roe.com/docs/BiasVariance.html`. *Used with kind permission of Scott Fortmann-Roe.*

See a simple video by Andrew Ng
Including how to use the bias-variance tradeoff to diagnose issues with your model, e.g. how much will more data help, etc.

Effect of Regularization on Bias-Variance

- Bishop 06, fig 3.5. Model is sum of 24 gaussians, with ridge regression



Example from KM, pg. 161

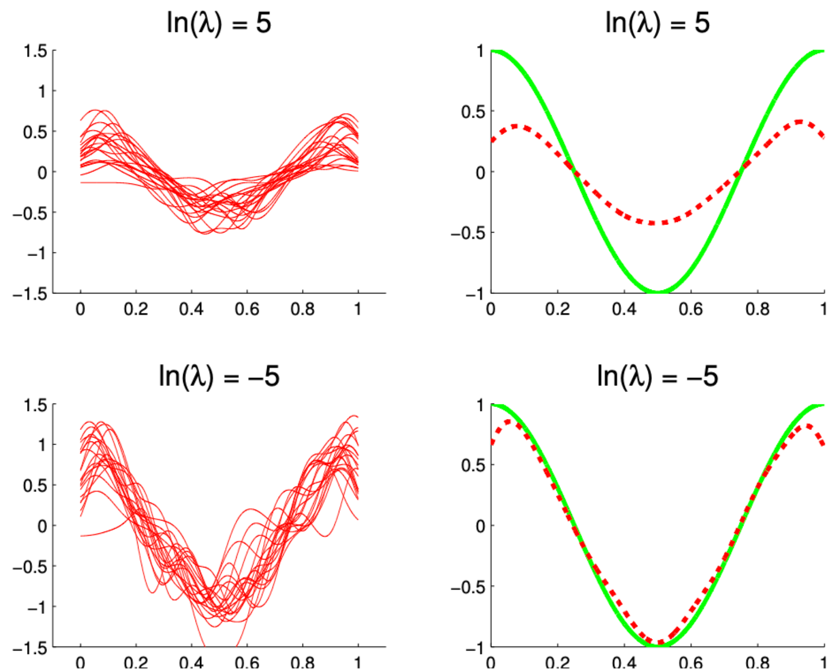
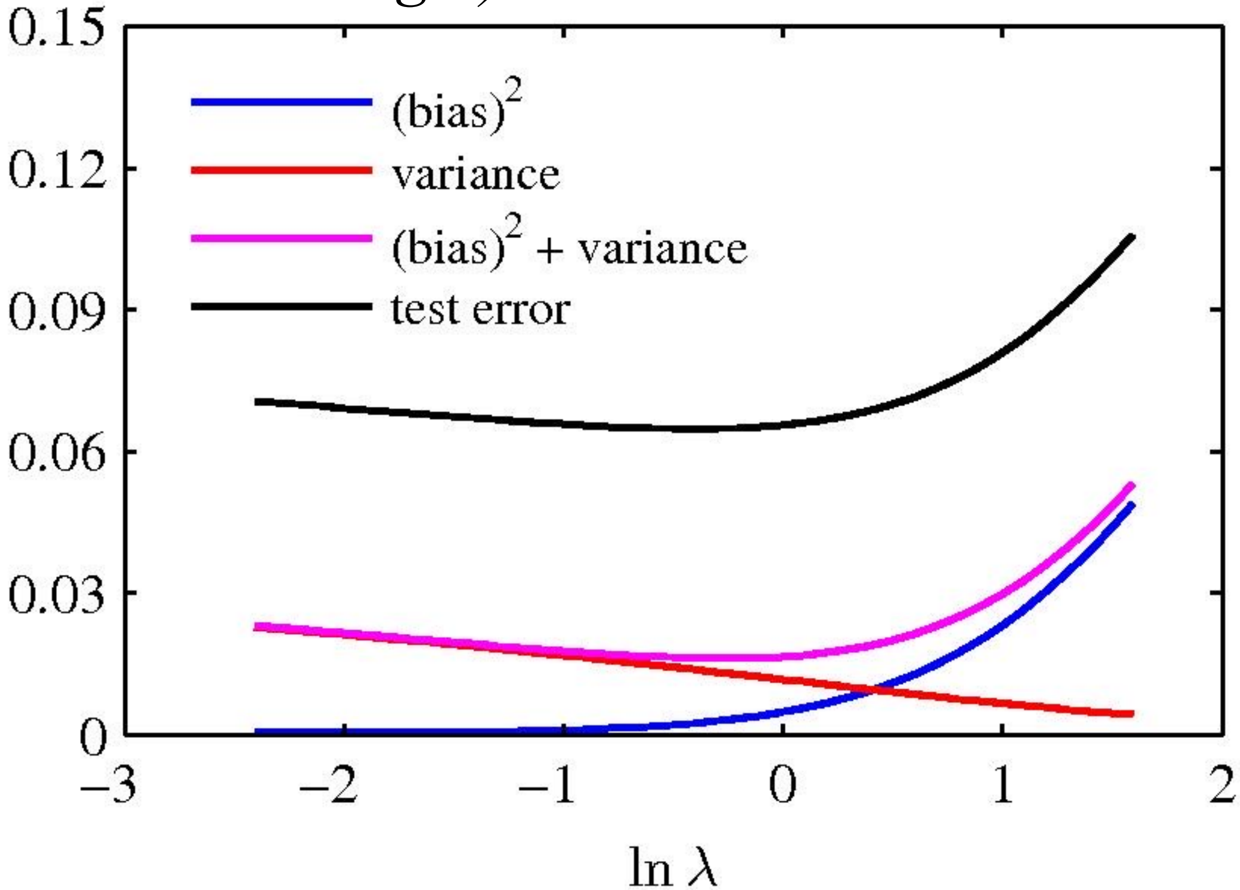


Figure 4.25: Illustration of bias-variance tradeoff for ridge regression. We generate 100 data sets from the true function, shown in solid green. Left: we plot the regularized fit for 20 different data sets. We use linear regression with a Gaussian RBF expansion, with 25 centers evenly spread over the $[0, 1]$ *interval. Right: we plot the average of the fits, averaged over all 100 datasets. Top row: strongly regularized: we see that the individual fits are similar to each other (low variance), but the average is far from the truth (high bias). Bottom row: lightly regularized: we see that the individual fits are quite different from each other (high variance), but the average is close to the truth (low bias). Adapted from [Bis06] Figure 3.5. Generated by code.probml.ai/book1/4.25.*

Bias-Variance vs. Regularization Amount

- *What happens to the curves as amount of training data increases ? (note: effective model complexity is decreasing towards the right)*



Bias-Variance Tradeoff

- **Your task: qualitatively plot bias^2 and variance in fig 2.11**
- Change model type? Affect bias
- More training data: decrease variance
  - "consistent estimators" converge to ideal solution as $|D| \rightarrow$ infinity
  - For small data sets, lower complexity models may be preferred.
- **Ideal solution: suitable model type & complexity**

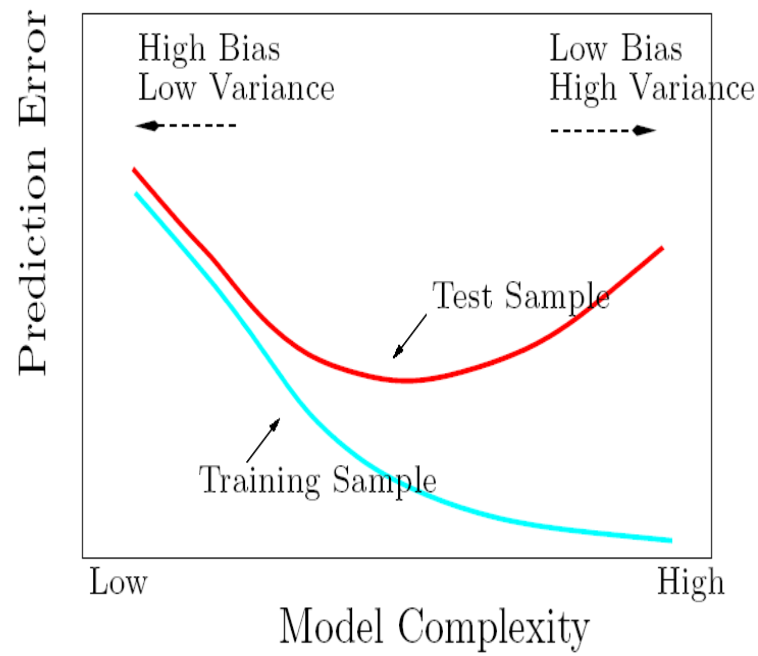


Figure 2.11: *Test and training error as a function of model complexity.*

Bias –variance tradeoff in encountered in many situations
Example: determining # of bins for a histogram.

Application: How do you improve your model?

- Get more training data
- Change complexity (e.g. via regularization)
- Change optimization method
- Change Model type

- Still not acceptable?
  - Change feature space

Extras

Function Approximation / Regression/Prediction

- A predictive modeling technique
  - Given:
    - A set of input (AI) /independent (math)/ explanatory or predictor (stats) variables X
    - corresponding (set of) output/dependent/response variables T
  - Think of training/test datasets as i.i.d. samples from an underlying joint distribution p(X,T)

  - Build: a model relating X to T
    - single value for T given X (most common)
      - e.g. E[T |X], the "regression of t on X.
      - Assumes T = function of X + (zero-mean, symmetric) noise
      - Add Confidence Interval (e.g. based on the Normally distributed noise term in MLR)
    - (Arbitrary) Distribution of T given X

Geometry of Least Squares*

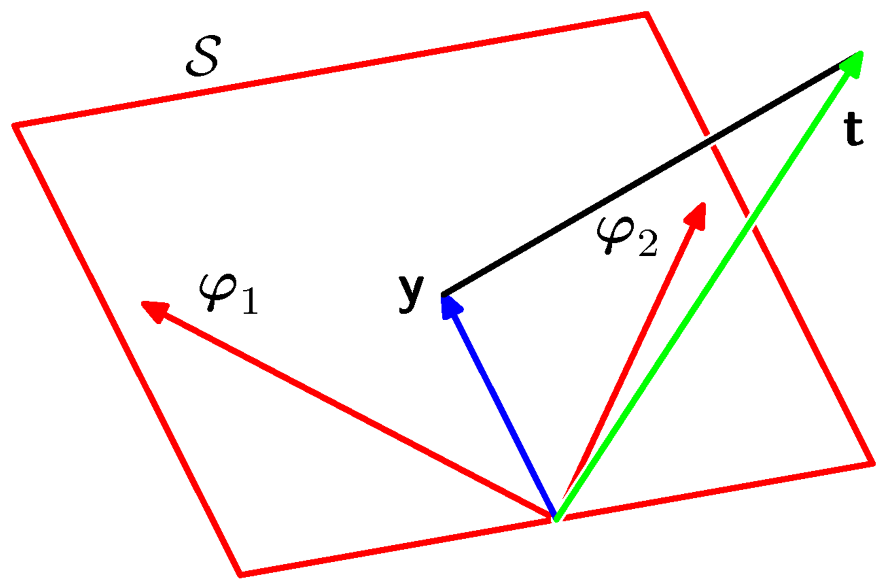
•Consider

$$\mathbf{y} = \mathbf{\Phi}\mathbf{w}_{\mathrm{ML}} = [\boldsymbol{\varphi}_1, \ldots, \boldsymbol{\varphi}_M]\, \mathbf{w}_{\mathrm{ML}}.$$

$$\mathbf{y} \in \mathcal{S} \subseteq \mathcal{T} \qquad \mathbf{t} \in \mathcal{T}$$

N-dimensional

M-dimensional



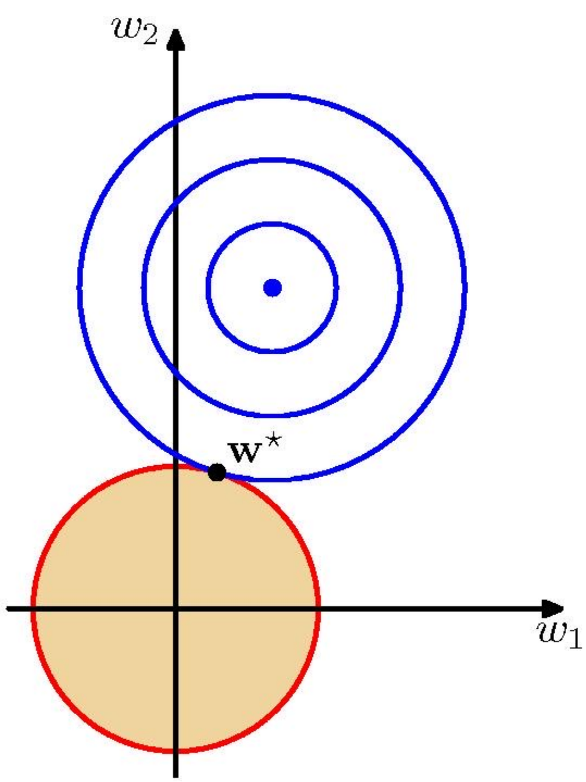
•S is spanned by $\boldsymbol{\varphi}_1, \ldots, \boldsymbol{\varphi}_M$.

•$\mathbf{w}_{\mathrm{ML}}$ minimizes the distance between t and its orthogonal projection on S, i.e. y.

Takeaway: You are restricted by your choice of the features

Comparing Shrinkage Methods B06: fig 3.4

- ridge regression (Regularization Penalty = sum squared of weights)
  vs
- **Lasso ((Regularization Penalty = sum of |w|)**
  red: constant penalty contour; blue: unregularized error contours



Estimating True Performance (Formula Driven)*

- true mean squared error (MSE = SSE/N) = empirical error + complexity term
  - complexity term = f (model type, # of parameters, # of training points)
    - e.g. linear regression with N samples, P parameters
      Akaike's Final Prediction error = $MSE_{empirical} (N+P) / (N - P)$
    - for nonlinear models, find "effective number of parameters" and plug into linear formulae

Takeaway: Formula Driven Estimates of True Performance specialized for linear models. Not so relevant in data mining context

Breaking News (2019)

- Variance can actually go down in the highly over-parameterized regime (going beyond interpolation)!!
  - Figure below from M. Belkin, D. Hsu, S. Ma, and S. Mandal, “Reconciling modern machine learning practice and the bias-variance trade-off,” *Proceedings of the National Academy of Sciences*, vol. 116, no. 32, pp. 15849–15854, 2019.