INTRODUCTION TO DATA SCIENCE

This lecture is
based on course by E. Fox and C. Guestrin, Univ of Washington

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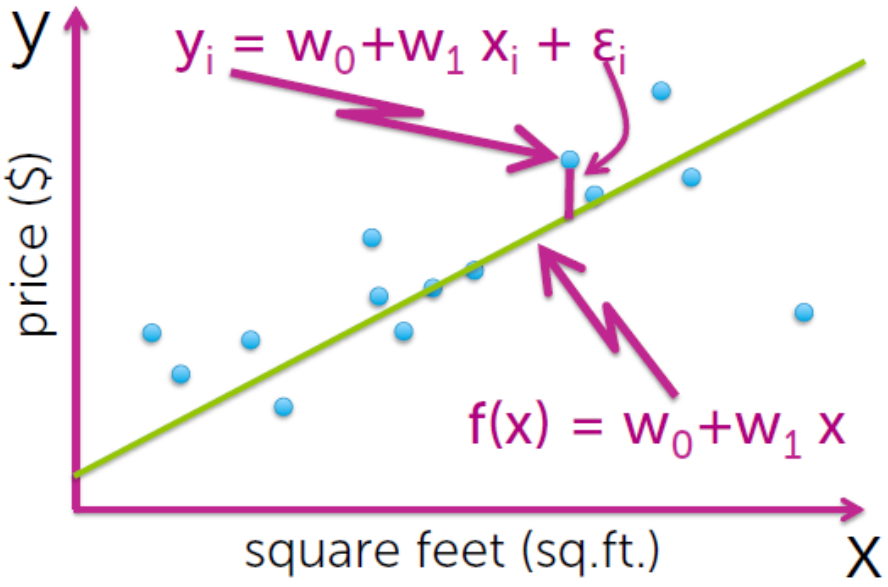
WFAiS UJ, Informatyka Stosowana
II stopień studiów

What we've learned so far

Simple Regression

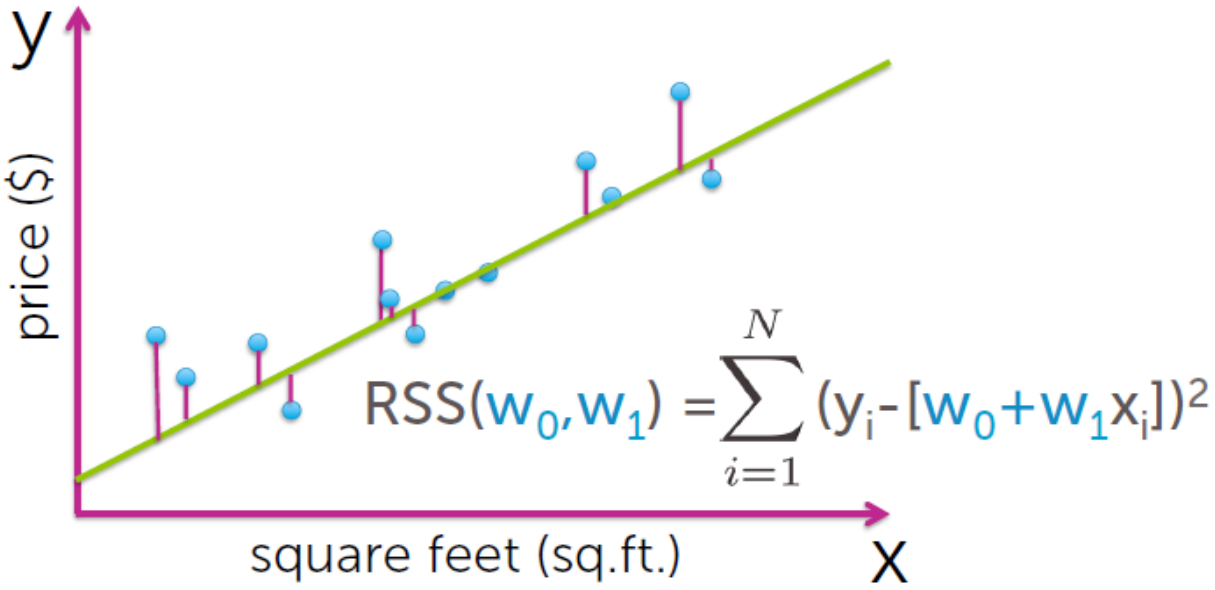
Simple linear regression model

1 input and just fit a line to data

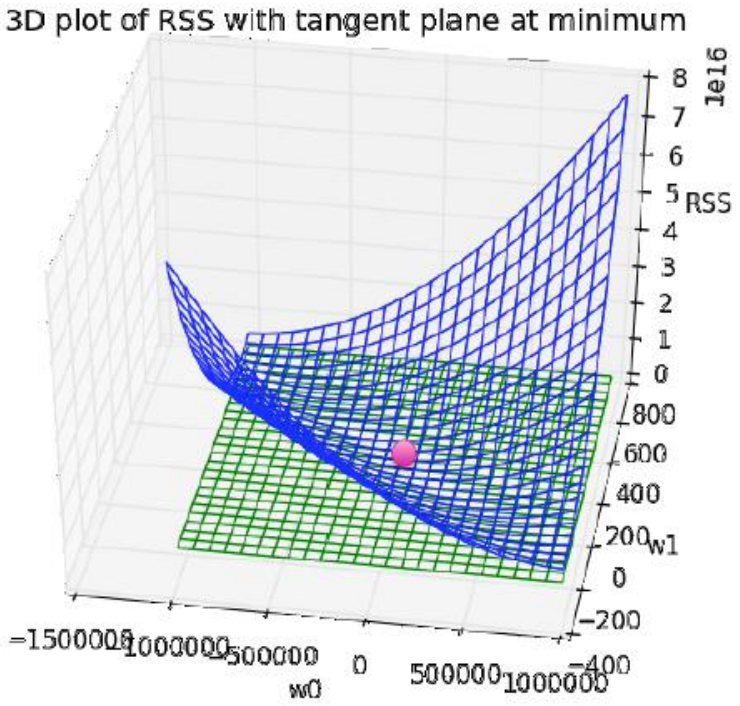


"Cost" of using a given line

Residual sum of squares (RSS)



Minimizing the cost

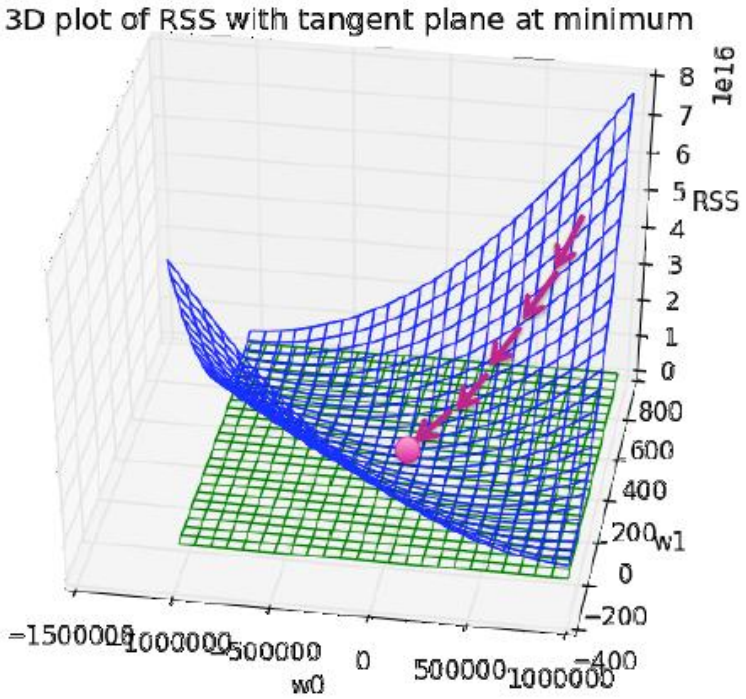


Minimize function over all possible w_0, w_1

$$\min_{w_0, w_1} \sum_{i=1}^{N} (y_i - [w_0 + w_1 x_i])^2$$

$RSS(w_0, w_1)$ is a function of 2 variables

Gradient descent



Algorithm:

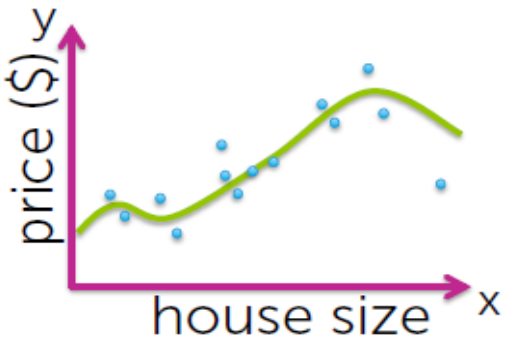
while not converged

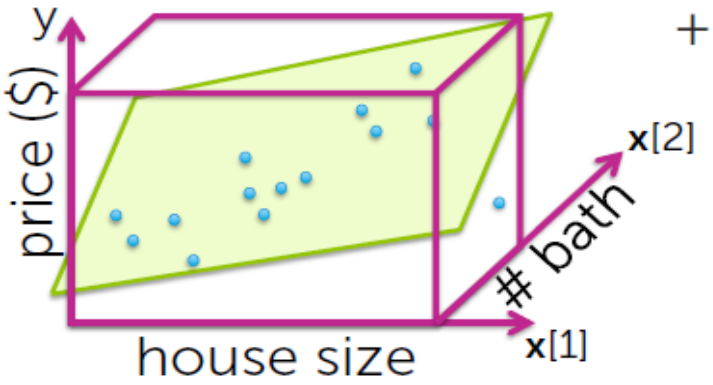
$w^{(t+1)} \leftarrow w^{(t)} - \eta \nabla RSS(w^{(t)})$

What we've learned so far

Multiple Regression

Regression with multiple features





Fit more complex relationships than just a line

Incorporate more inputs + features thereof

- Square feet
- # bathrooms
- # bedrooms
- Lot size
- Year built
- ...

Formally…

Model:

$$y_i = w_0 h_0(\mathbf{x}_i) + w_1 h_1(\mathbf{x}_i) + \ldots + w_D h_D(\mathbf{x}_i) + \varepsilon_i$$

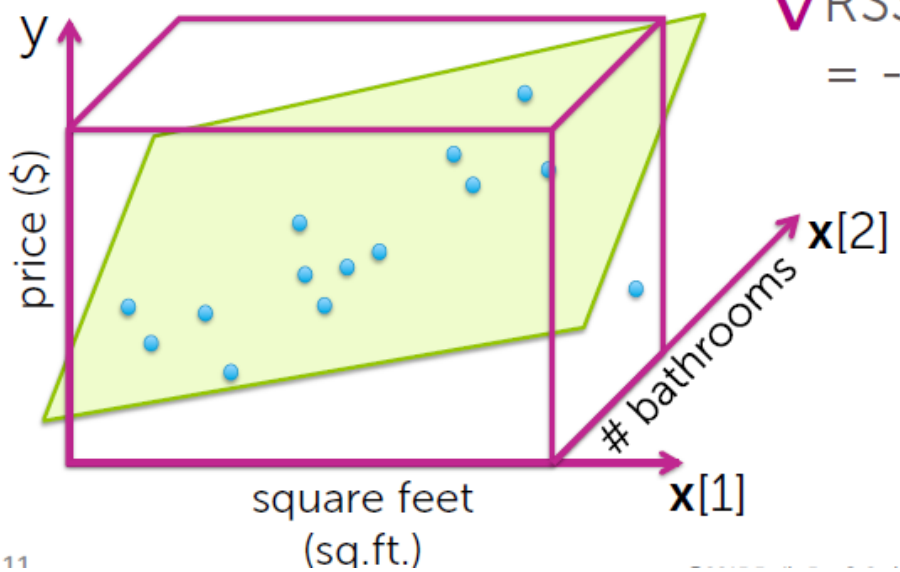
$$= \sum_{j=0}^{D} w_j h_j(\mathbf{x}_i) + \varepsilon_i$$

feature 1 = $h_0(\mathbf{x})$ … e.g., 1
feature 2 = $h_1(\mathbf{x})$ … e.g., $\mathbf{x}$[1] = sq. ft.
feature 3 = $h_2(\mathbf{x})$ … e.g., $\mathbf{x}$[2] = #bath
or, log($\mathbf{x}$[7]) $\mathbf{x}$[2] = log(#bed) x #bath
…
feature D+1 = $h_D(\mathbf{x})$ … some other function of $\mathbf{x}$[1],…, $\mathbf{x}$[d]

RSS for multiple regression

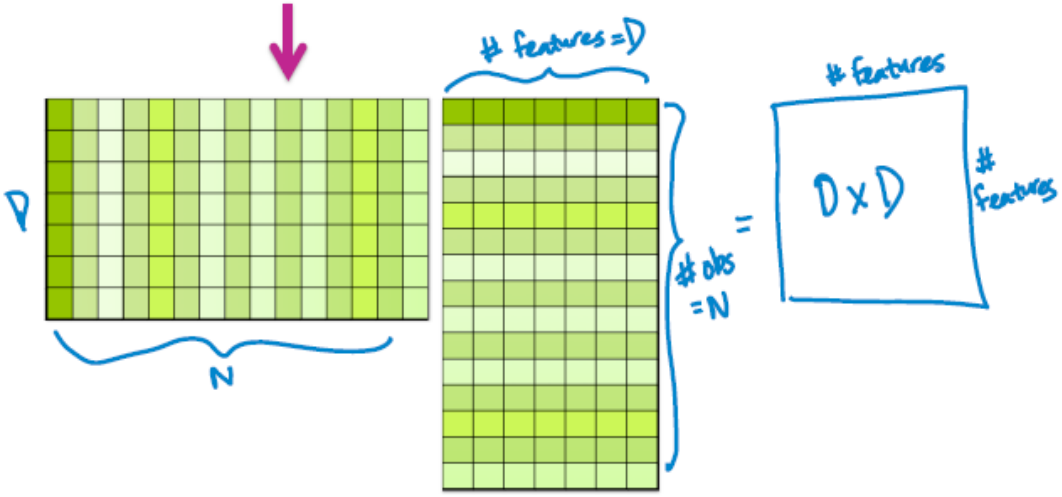
$$RSS(\mathbf{w}) = \sum_{i=1}^{N} (y_i - h(x_i)^T\mathbf{w})^2$$

$$\nabla RSS(\mathbf{w}) = -2\mathbf{H}^T(\mathbf{y} - \mathbf{H}\mathbf{w})$$



Closed-form solution

$$\hat{w} = (H^T H)^{-1} H^T y$$



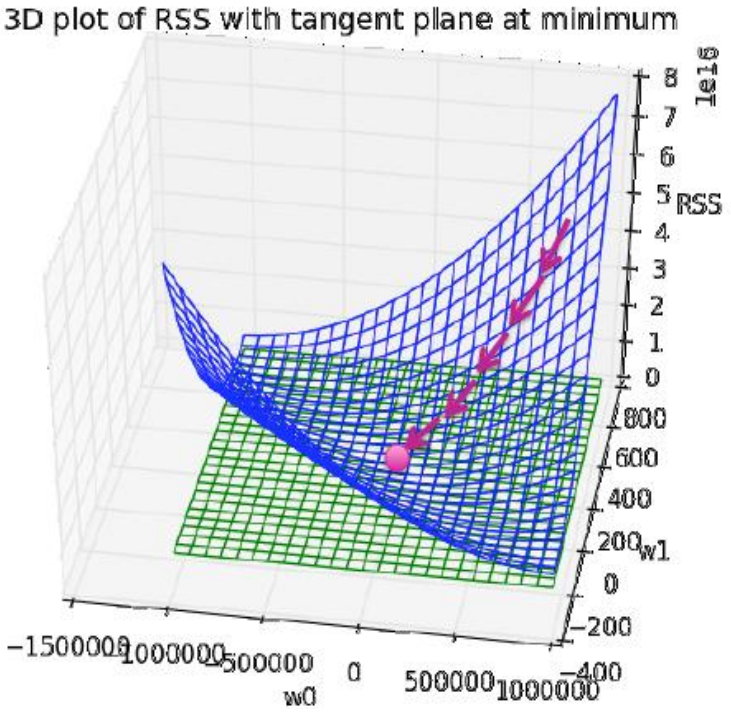
Invertible if: really, # of linearly ind. observations

In most cases is $N > D$

Complexity of inverse:

$O(D^3)$

Gradient descent for multiple regression



init $\mathbf{w}^{(1)}=0$ (or randomly, or smartly), $t=1$

while $||\nabla RSS(\mathbf{w}^{(t)})|| > \varepsilon$

  for $j=0,\ldots,D$

    $partial[j] = -2\sum_{i=1}^{N} h_j(\mathbf{x}_i)(y_i - \hat{y}_i(\mathbf{w}^{(t)}))$

    $\mathbf{w}_j^{(t+1)} \leftarrow \mathbf{w}_j^{(t)} - \eta\ partial[j]$

  $t \leftarrow t + 1$

What we've learned so far

Assessing Performance

Measuring loss

Loss function:

$L(y, f_{\hat{w}}(\mathbf{x}))$

Cost of using ŵ at x when y is true

actual value

$\hat{f}(\mathbf{x})$ = predicted value ŷ

Examples:

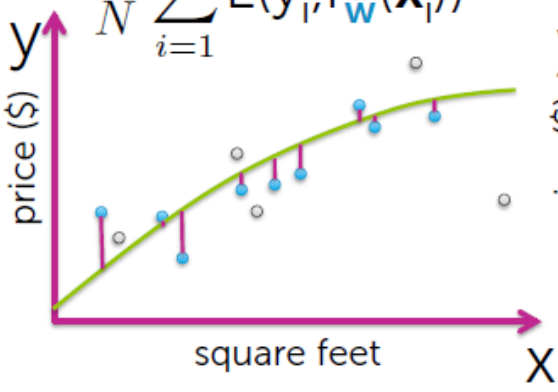
(assuming loss for underpredicting = overpredicting)

Absolute error: $L(y, f_{\hat{w}}(\mathbf{x})) = |y - f_{\hat{w}}(\mathbf{x})|$

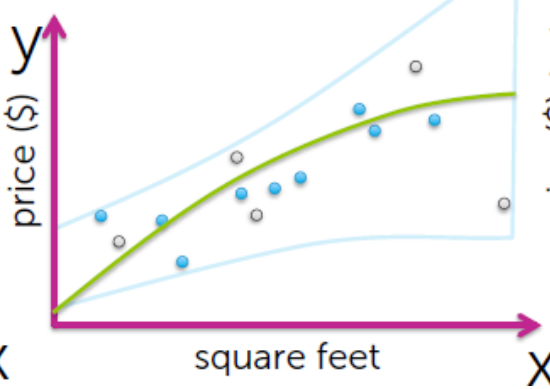
Squared error: $L(y, f_{\hat{w}}(\mathbf{x})) = (y - f_{\hat{w}}(\mathbf{x}))^2$

3 Measures of error

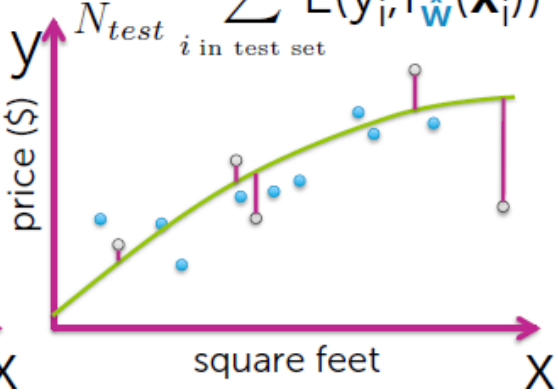
Training error ($\hat{\mathbf{w}}$) = $\frac{1}{N}\sum_{i=1}^{N} L(y_i, f_{\hat{\mathbf{w}}}(\mathbf{x}_i))$



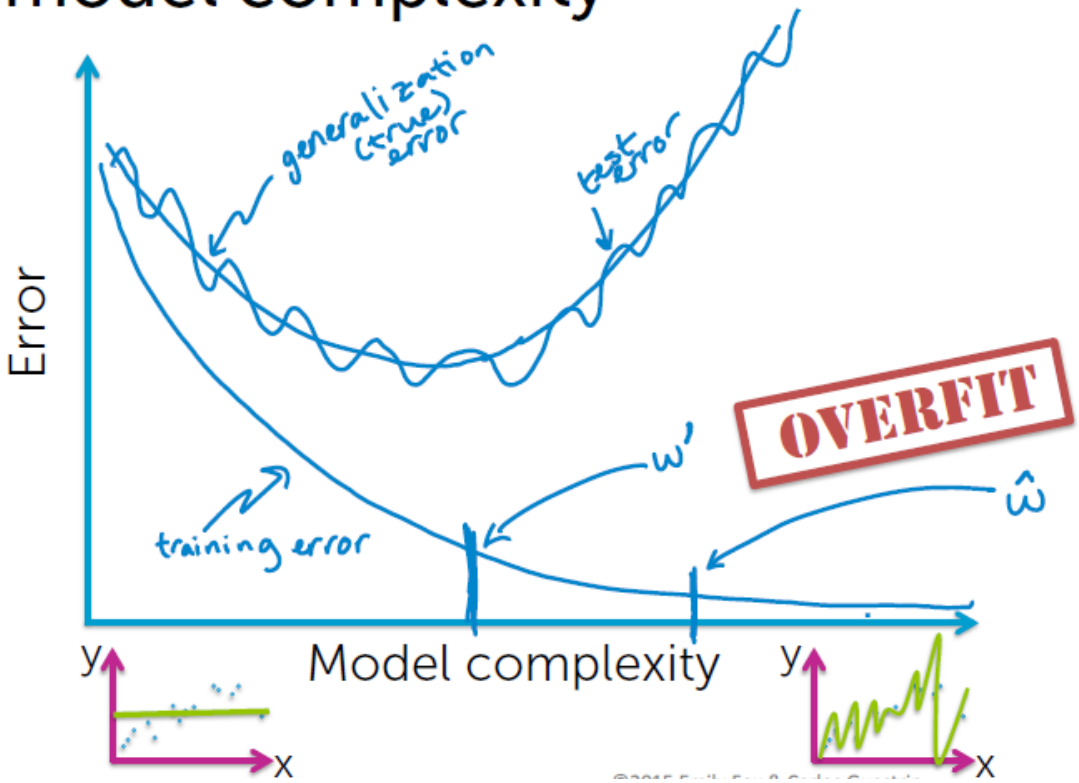
Generalization error ($\hat{\mathbf{w}}$)



Test error ($\hat{\mathbf{w}}$) = $\frac{1}{N_{test}} \sum_{i \text{ in test set}} L(y_i, f_{\hat{\mathbf{w}}}(\mathbf{x}_i))$

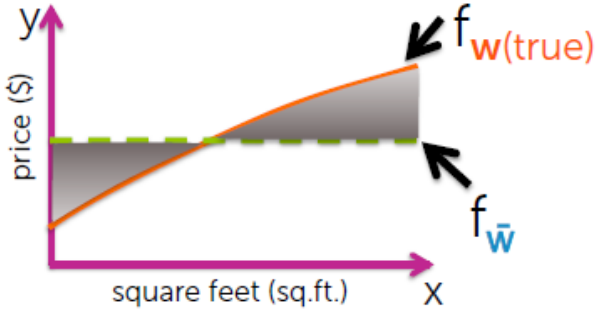


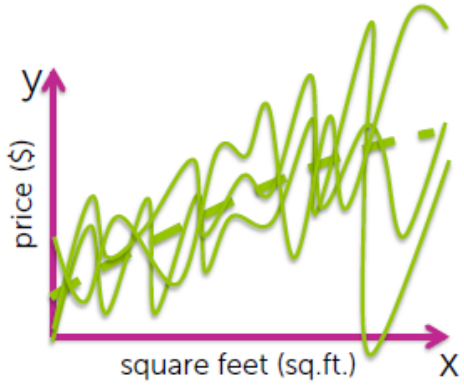
Training, true, & test error vs. model complexity



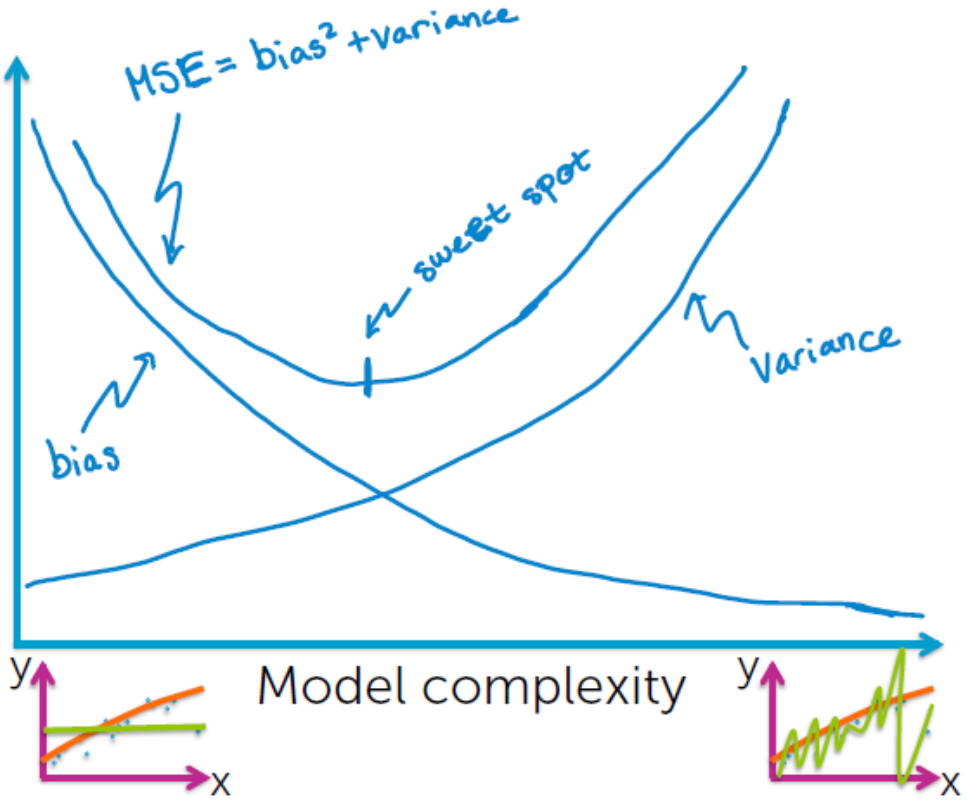
3 Sources of prediction error

1. Noise
2. Bias
3. Variance

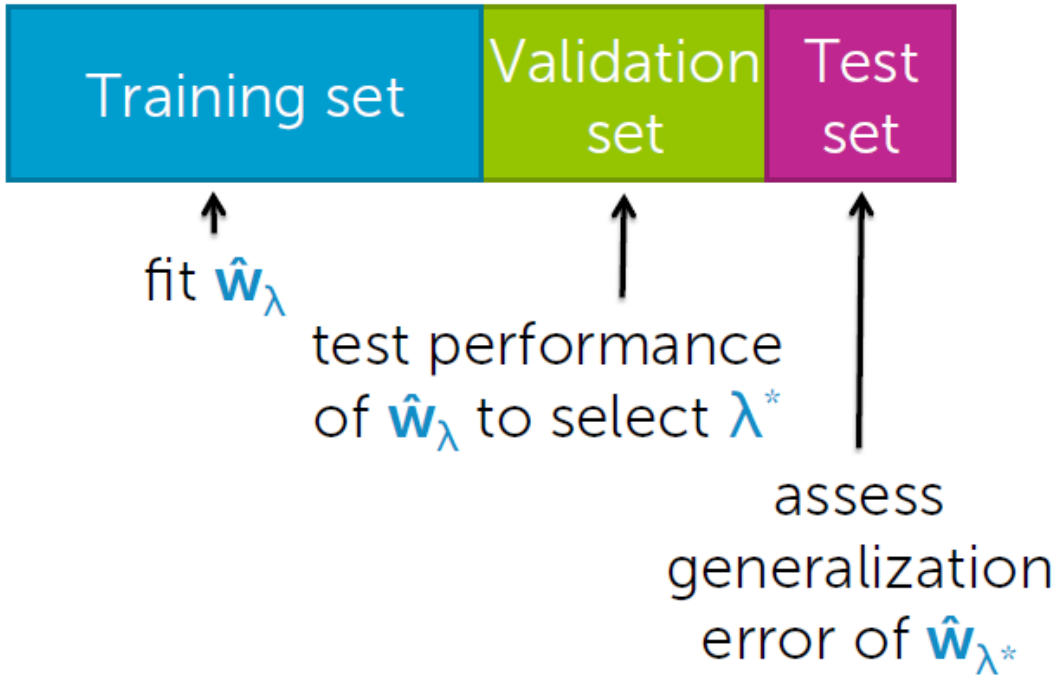




Bias-variance tradeoff



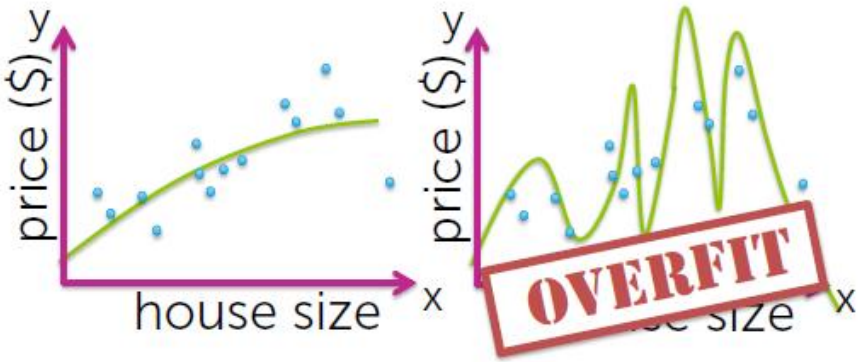
Model selection & assessment



What we've learned so far

Ridge Regression

Balancing fit and model complexity



Ridge total cost =

measure of fit + measure of magnitude of coefficients

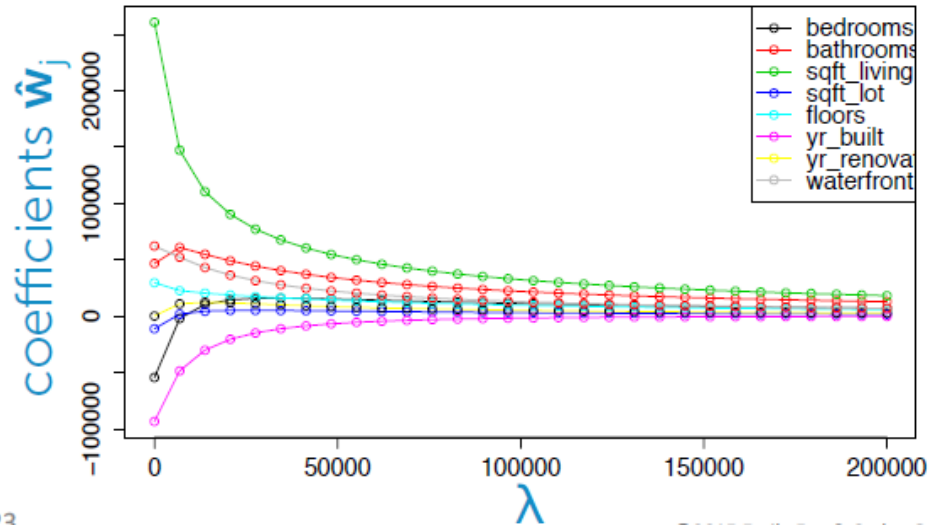
bias-variance tradeoff

Ridge objective function (L_2 regularized regression)

$\hat{\mathbf{w}}$ selected to minimize

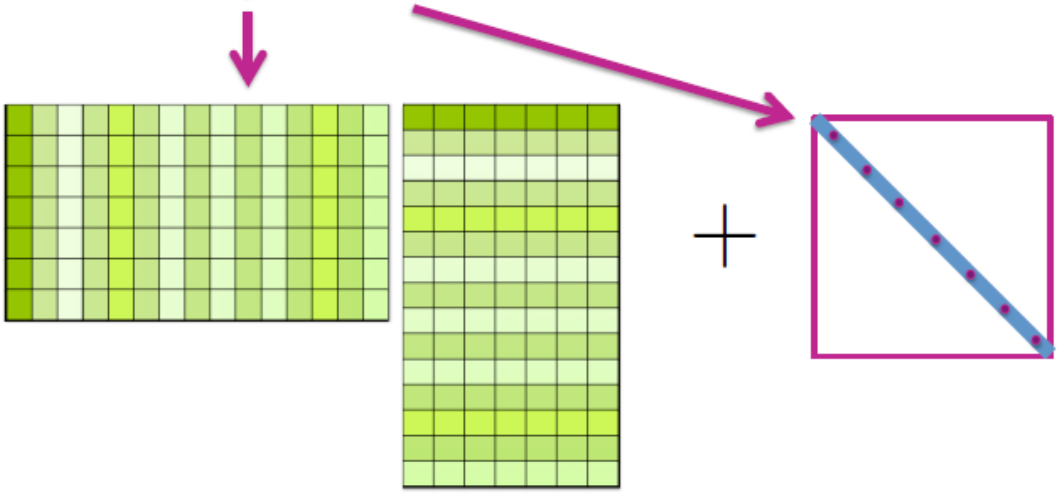
tuning parameter = balance of fit and magnitude

$$\text{RSS}(\mathbf{w}) + \lambda||\mathbf{w}||_2^2$$



Ridge closed-form solution

$$\hat{\mathbf{w}} = (\mathbf{H}^T\mathbf{H} + \lambda\mathbf{I})^{-1}\mathbf{H}^T\mathbf{y}$$



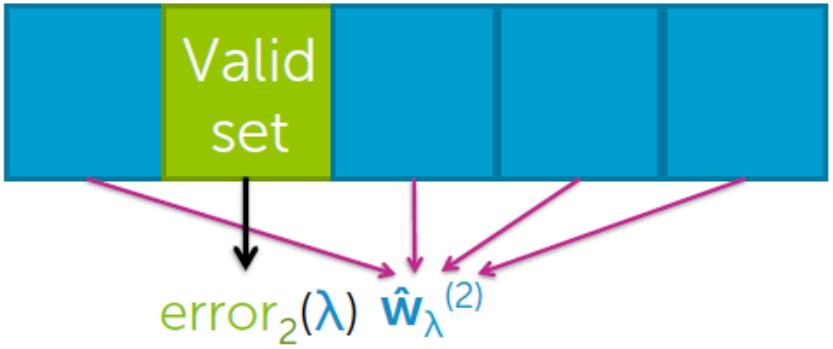
Invertible if:

- Always if $\lambda>0$,
- even if $N < D$

Complexity of inverse:

- $O(D^3)$...
- big for large D!

K-fold cross validation



For k=1,…,K

1. Estimate $\hat{\mathbf{w}}_\lambda^{(k)}$ on the training blocks
2. Compute error on validation block: $\text{error}_k(\lambda)$

Compute average error: $\text{CV}(\lambda) = \frac{1}{K}\sum_{k=1}^{K} \text{error}_k(\lambda)$

What we've learned so far

Lasso Regression

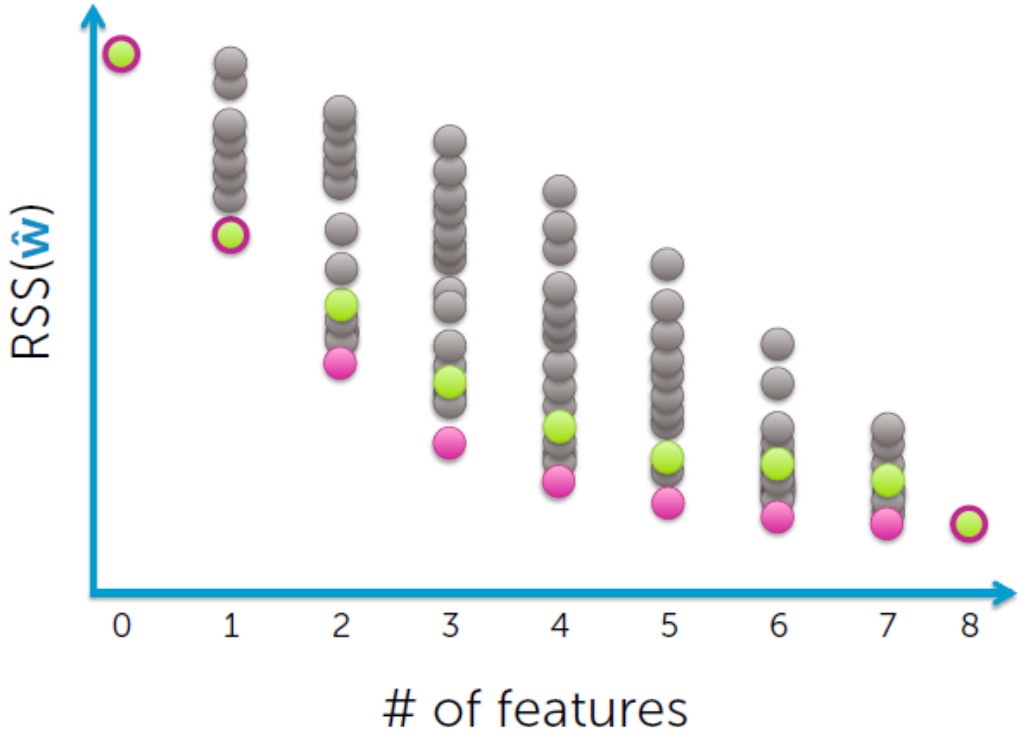
Performing feature selection

Useful for efficiency of predictions and interpretability

Lot size
Single Family
Year built
Last sold price
Last sale price/sqft
Finished sqft
Unfinished sqft
Finished basement sqft
floors
Flooring types
Parking type
Parking amount
Cooling
Heating
Exterior materials
Roof type
Structure style

Dishwasher
Garbage disposal
Microwave
Range / Oven
Refrigerator
Washer
Dryer
Laundry location
Heating type
Jetted Tub
Deck
Fenced Yard
Lawn
Garden
Sprinkler System
⋮

All subsets vs. greedy



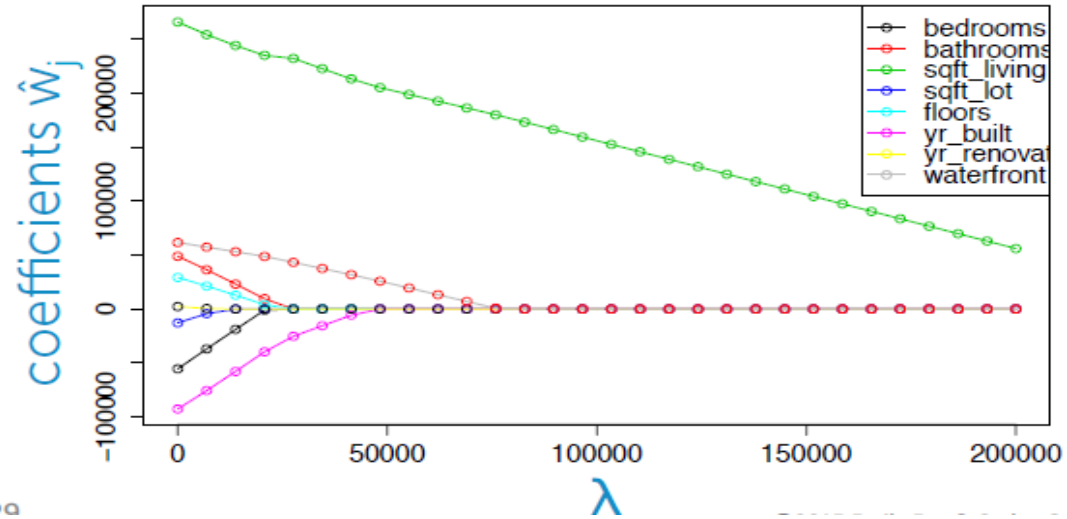
- # bedrooms
- # bathrooms
- sq.ft. living
- sq.ft. lot
- floors
- year built
- year renovated
- waterfront

Lasso objective function (L_1 regularized regression)

$\hat{\mathbf{w}}$ selected to minimize

tuning parameter = balance of fit and **sparsity**

$$\text{RSS}(\mathbf{w}) + \lambda||\mathbf{w}||_1$$



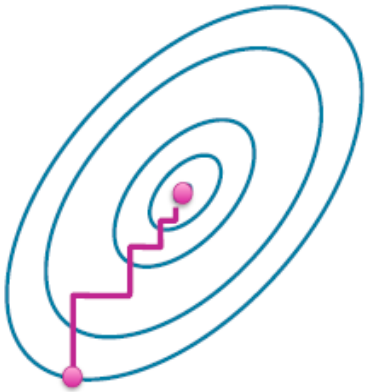
Coordinate descent for lasso

Precompute: $z_j = \sum_{i=1}^{N} h_j(\mathbf{x}_i)^2$

Initialize $\hat{\mathbf{w}} = 0$ (or smartly…)

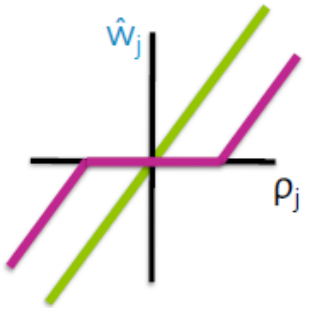
while not converged

for j=0,1,…,D



compute: $\rho_j = \sum_{i=1}^{N} h_j(\mathbf{x}_i)(y_i - \hat{y}_i(\hat{\mathbf{w}}_{-j}))$

set: $\hat{w}_j = \begin{cases} (\rho_j + \lambda/2)/z_j & \text{if } \rho_j < -\lambda/2 \\ 0 & \text{if } \rho_j \text{ in } [-\lambda/2, \lambda/2] \\ (\rho_j - \lambda/2)/z_j & \text{if } \rho_j > \lambda/2 \end{cases}$



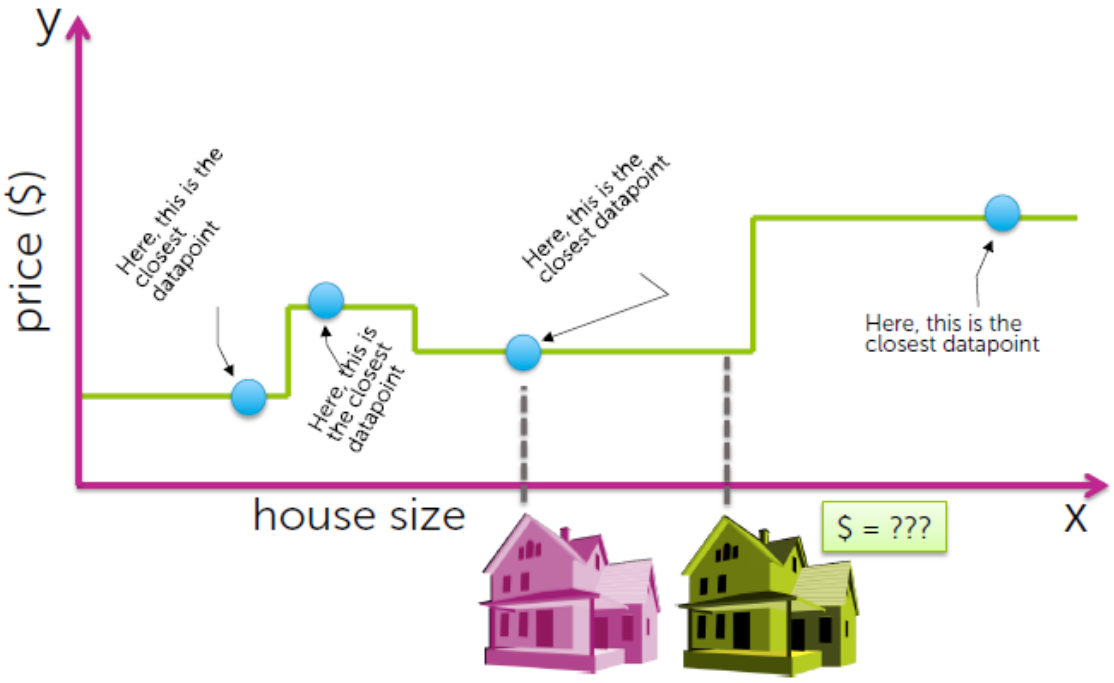
What we've learned so far

Nearest Neighbor

&

Kernel Regression

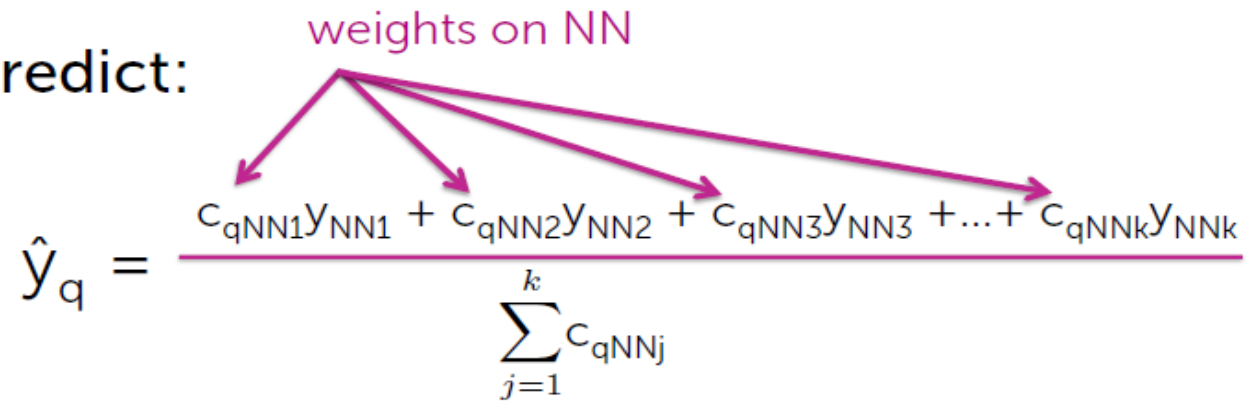
1-Nearest neighbor regression



Weighted k-NN

Weigh more similar houses more than those less similar in list of k-NN

Predict:



Kernel regression

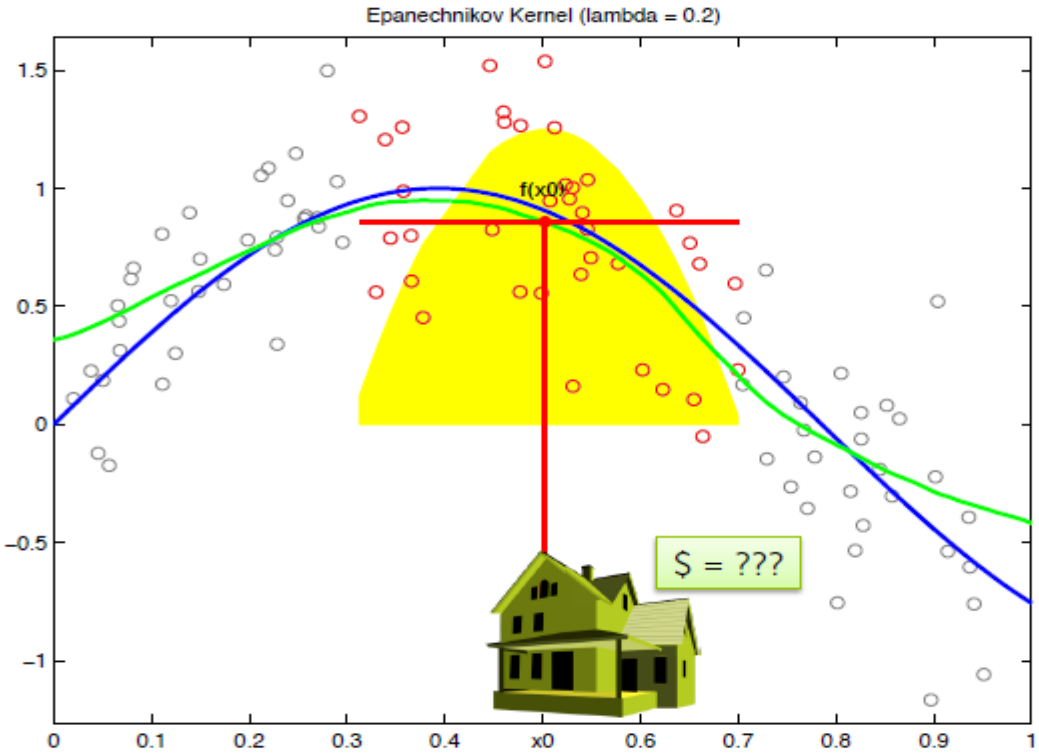
Instead of just weighting NN, weight *all* points

Predict:

weight on each datapoint

$$\hat{y}_q = \frac{\sum_{i=1}^{N} c_{qi} y_i}{\sum_{i=1}^{N} c_{qi}} = \frac{\sum_{i=1}^{N} \text{Kernel}_\lambda(\text{distance}(\mathbf{x}_i, \mathbf{x}_q)) * y_i}{\sum_{i=1}^{N} \text{Kernel}_\lambda(\text{distance}(\mathbf{x}_i, \mathbf{x}_q))}$$

Visualizing kernel regression



Summary of what we have learned

Models

- Linear regression
- Regularization: Ridge (L2), Lasso (L1)
- Nearest neighbor and kernel regression

Algorithms

- Gradient descent
- Coordinate descent

Concepts

- Loss functions, bias-variance tradeoff, cross-validation, sparsity, overfitting, model selection, feature selection