Nearest Neighbor

Introduction to Nonlinear models!

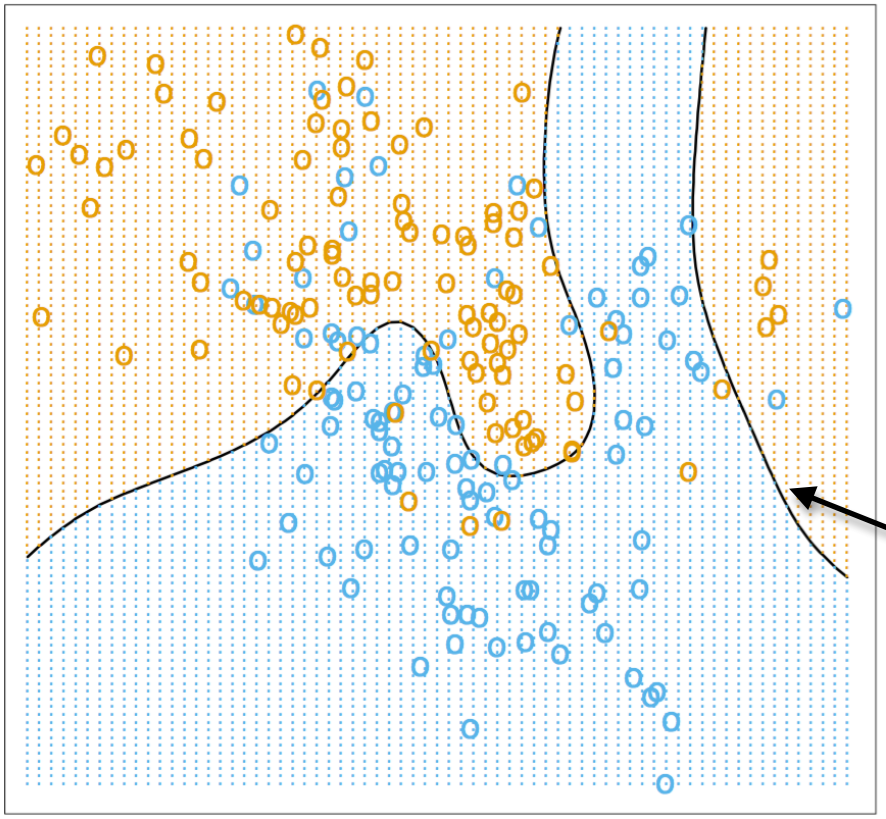
Machine Learning – CSE446

Kevin Jamieson

University of Washington

May 6, 2019

Some data, Bayes Classifier



2D features: i.e. my inputs x = [x_1, x_2] for this figure

Training data:

- True label: +1
- True label: -1

BEST POSSIBLE CLASSIFIER FOR THE DATA.

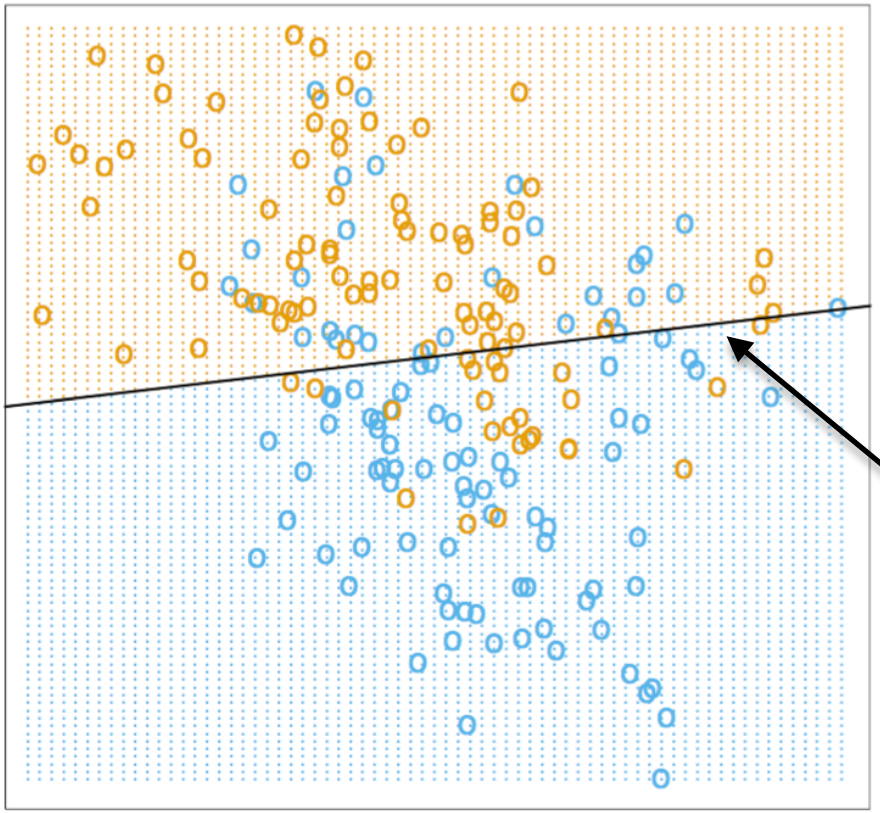
Optimal "Bayes" classifier:

$$\mathbb{P}(Y = 1 | X = x) = \frac{1}{2}$$

- Predicted label: +1
- Predicted label: -1

Figures stolen from Hastie et al

Linear Decision Boundary



Training data:

- True label: +1
- True label: -1

Learned:

No feature maps. Best, linear classifier; poor job of capturing nonlinearities in data.

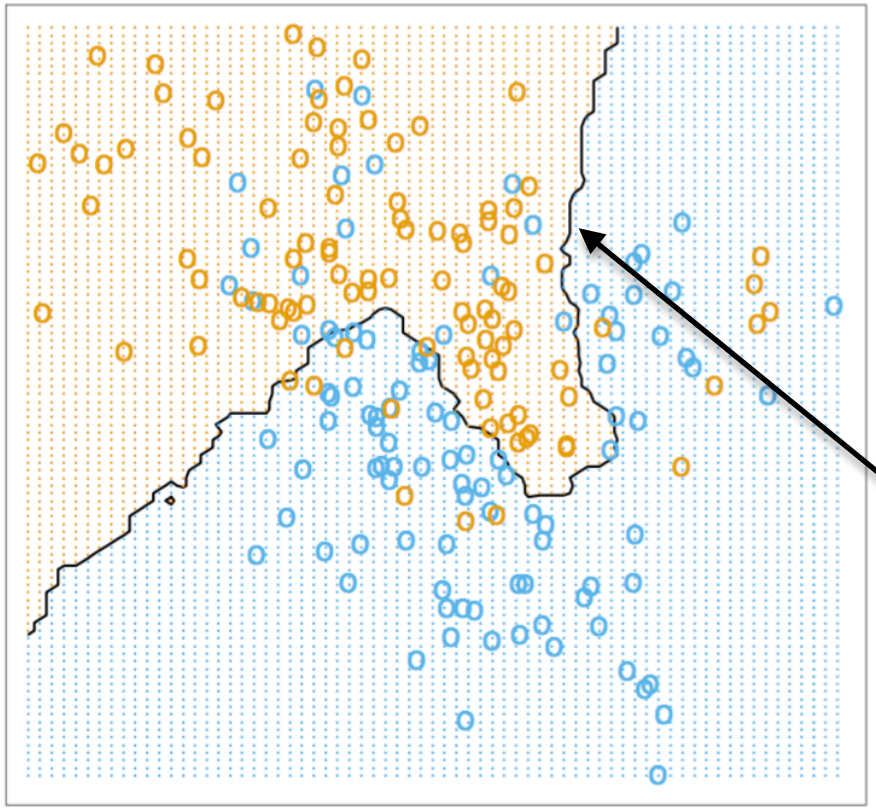
Linear Decision boundary

$$x^T w + b = 0$$

- Predicted label: +1
- Predicted label: -1

Figures stolen from Hastie et al

15 Nearest Neighbor Boundary



Smoother decision boundaries

LABELED!

Training data:

- True label: +1
- True label: -1

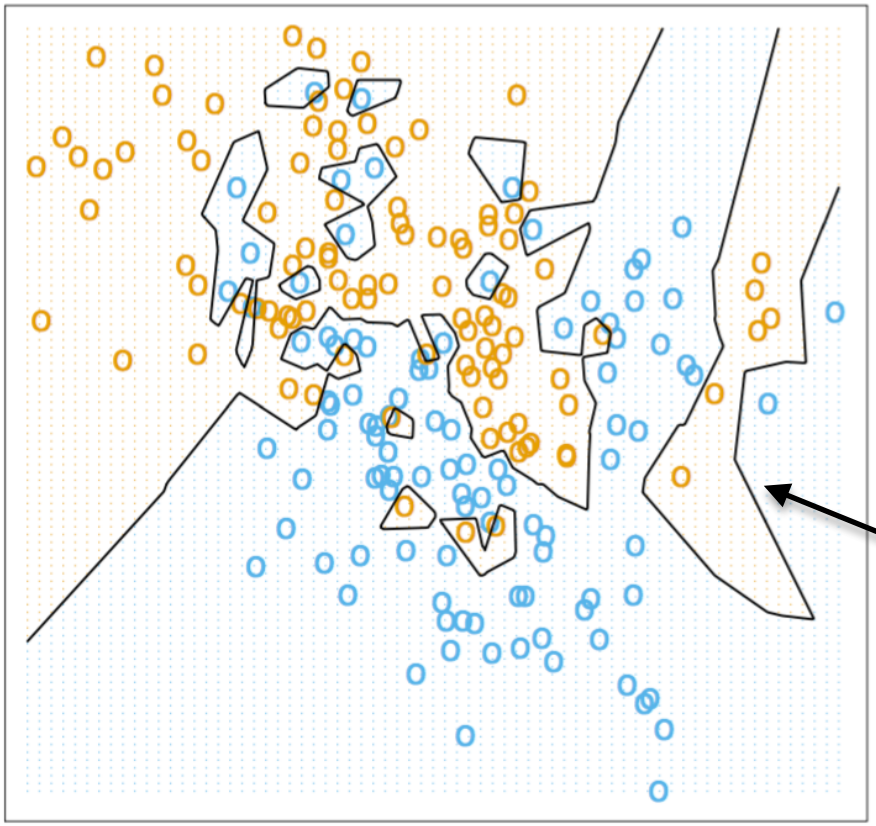
Learned:

For each small dot in the grid, we classify that dot based on the nearest 15 point labels

15 nearest neighbor decision boundary (majority vote)

- Predicted label: +1
- Predicted label: -1

1 Nearest Neighbor Boundary



Overfitting. Just try to get every possible training data point right.

Training data:

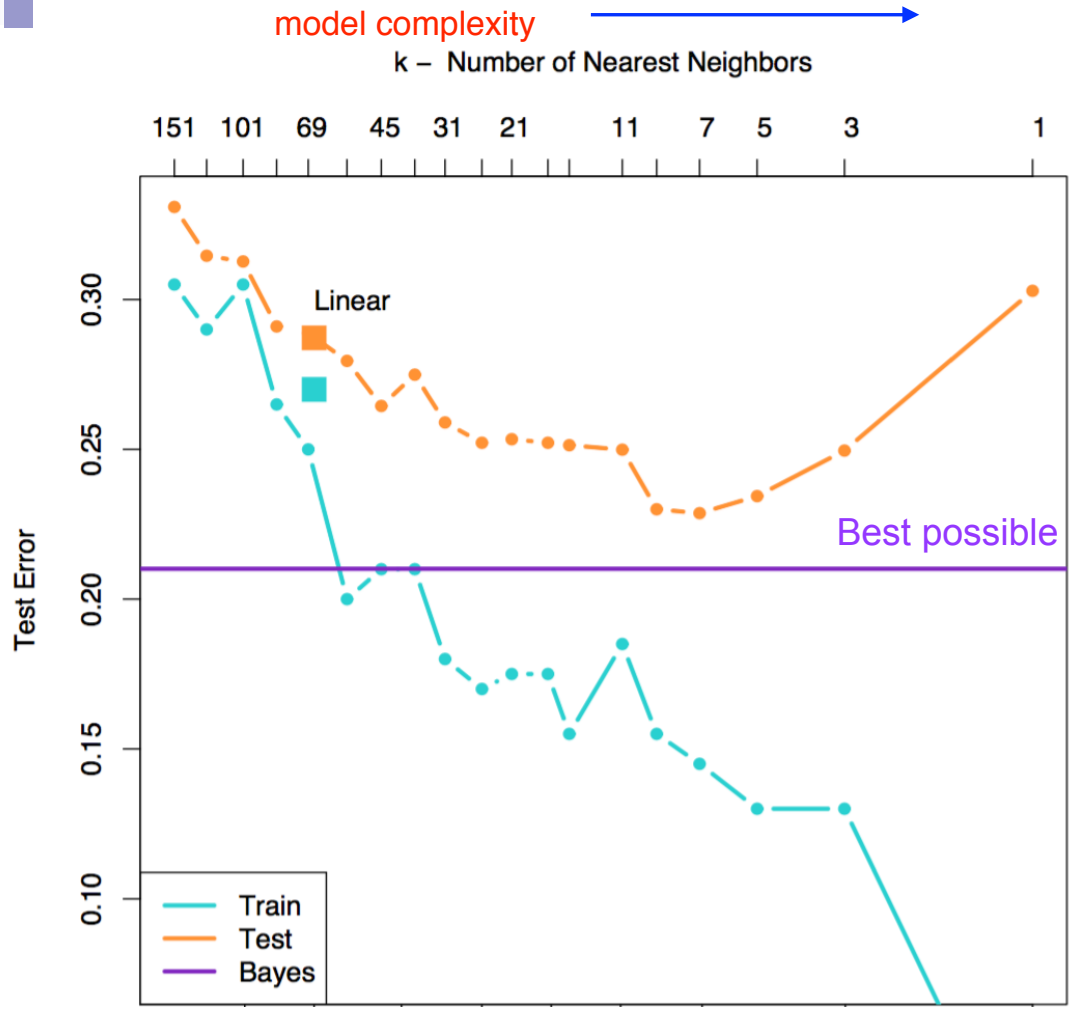
- True label: +1
- True label: -1

Learned:

1 nearest neighbor decision boundary (majority vote)

- Predicted label: +1
- Predicted label: -1

k-Nearest Neighbor Error



As we expect, theres a trade-off between model complexity and bias/variance

Bias-Variance tradeoff

As k->infinity?

Bias: large

Variance: small; essentially averaging over the whole dataset.

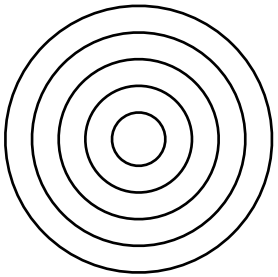
As k->1?

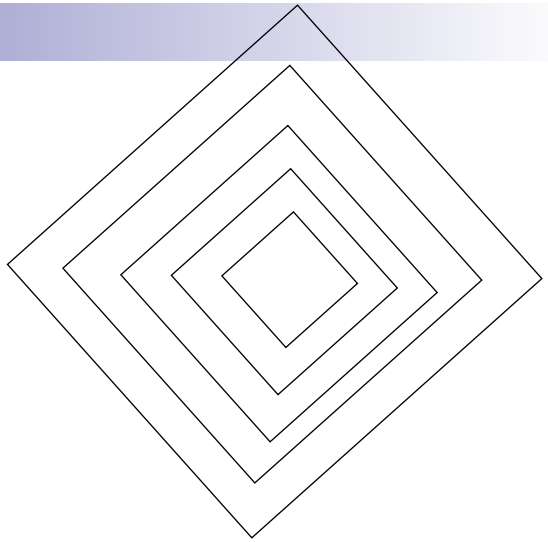
Bias: small

Variance: large; depends a lot of the specific data you saw

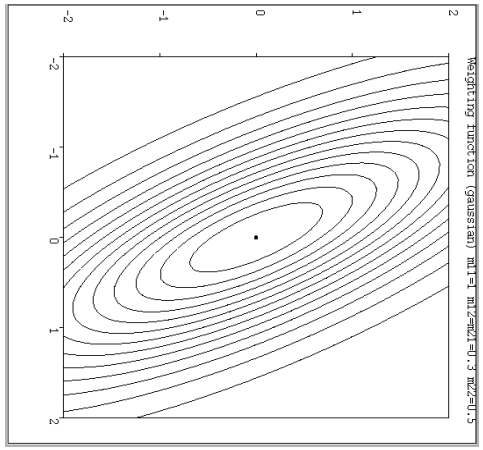
Notable distance metrics (and their level sets)

L_2 norm



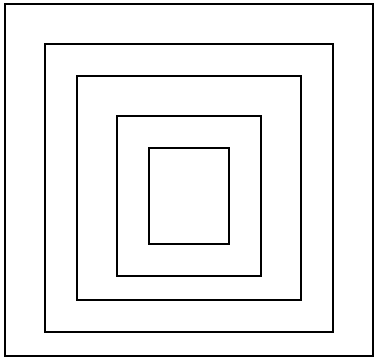


L_1 norm (taxi-cab)



Mahalanobis

xT A x

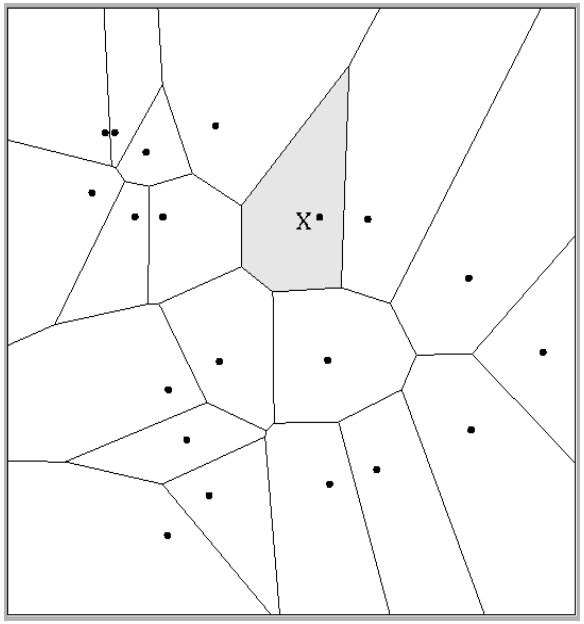


L-infinity *(max) norm*

1 nearest neighbor

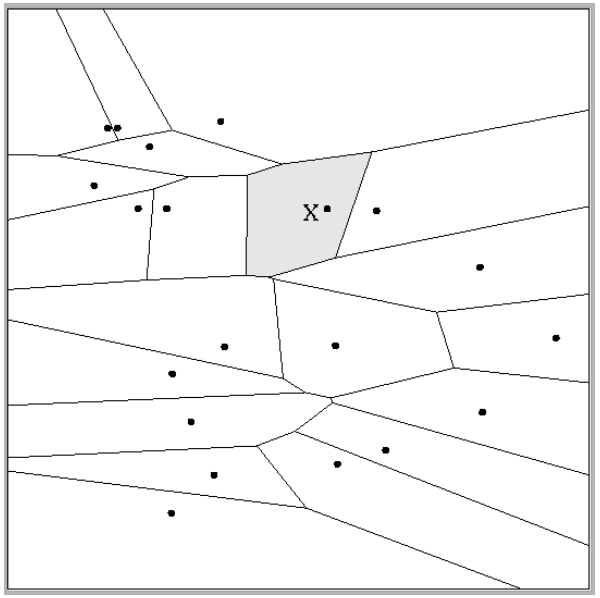
One can draw the nearest-neighbor regions in input space.

Every point inside each cell, the point in that cell is the closest point



$Dist(\mathbf{x}^i,\mathbf{x}^j) = (x^i_1 - x^j_1)^2 + (x^i_2 - x^j_2)^2$

Nearest neighbors very sensitive to scale.



$Dist(\mathbf{x}^i,\mathbf{x}^j) = (x^i_1 - x^j_1)^2 + (3x^i_2 - 3x^j_2)^2$

The relative scalings in the distance metric affect region shapes

Why does the Nearest Neighbor classifier work so well?

1 nearest neighbor guarantee

$$\{(x_i, y_i)\})_{i=1}^n \qquad x_i \in \mathbb{R}^d, \quad y_i \in \{0, 1\}$$

differentiable up to enough degrees

always nearby points arbitrarily close

As $n \to \infty$ assume the x_i's become *dense* in $\mathbb{R}^d$ and $\mathbb{P}(Y = 1|X = x)$ is *smooth*

As $x_a \to x_b$ we have $\mathbb{P}(Y_a = 1|X_a = x_a) \to \mathbb{P}(Y_b = 1|X_b = x_b)$

As two points get closer together, the probability that x_a is labeled 1 goes to the probability x_b is classified as 1

1 nearest neighbor guarantee

$$\{(x_i, y_i)\})_{i=1}^n \qquad x_i \in \mathbb{R}^d, \quad y_i \in \{0, 1\}$$

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If $p_* = \max_{y=0,1} \mathbb{P}(Y_b = y|X_b = x_b)$ then the Bayes Error $= 1 - p_*$

Lowest possible error rate.

Bayes error rate

1-nearest neighbor error $=$

$$\lim_{n\to\infty} \mathbb{P}(\widehat{f}_{1NN}(x_a) \neq Y_a|X_a = x_a) = \mathbb{P}(Y_b \neq Y_a|X_a = x_b, X_b = x_b)$$

train some model using data hat{f} returns the label of the 1 nearest neighbor.

true label of b does not match true label of a

As the number of data points goes to infinity.

1 nearest neighbor guarantee

$$\{(x_i, y_i)\})_{i=1}^n \qquad x_i \in \mathbb{R}^d, \quad y_i \in \{0, 1\}$$

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As $x_a \to x_b$ we have $\mathbb{P}(Y_a = 1|X_a = x_a) \to \mathbb{P}(Y_b = 1|X_b = x_b)$

If $p_* = \max_{y=0,1} \mathbb{P}(Y_b = y|X_b = x_b)$ then the Bayes Error $= 1 - p_*$

1-nearest neighbor error $=$

true probability.

$$\lim_{n\to\infty} \mathbb{P}(\widehat{f}_{1NN}(x_a) \neq Y_a|X_a = x_a) = \mathbb{P}(Y_b \neq Y_a|X_a = x_b, X_b = x_b)$$
$$= \mathbb{P}(Y_b = 1|X_b = x_b)\mathbb{P}(Y_a = 0|X_a = x_b) + \mathbb{P}(Y_b = 0|X_b = x_b)\mathbb{P}(Y_a = 1|X_a = x_b)$$
$$= 2p_*(1 - p_*) \leq 2(1 - p_*)$$

the best possible classifier

As n->infinity, then 1-NN rule error is at most twice the Bayes error!

[Cover, Hart, 1967]

Curse of dimensionality Ex. 1

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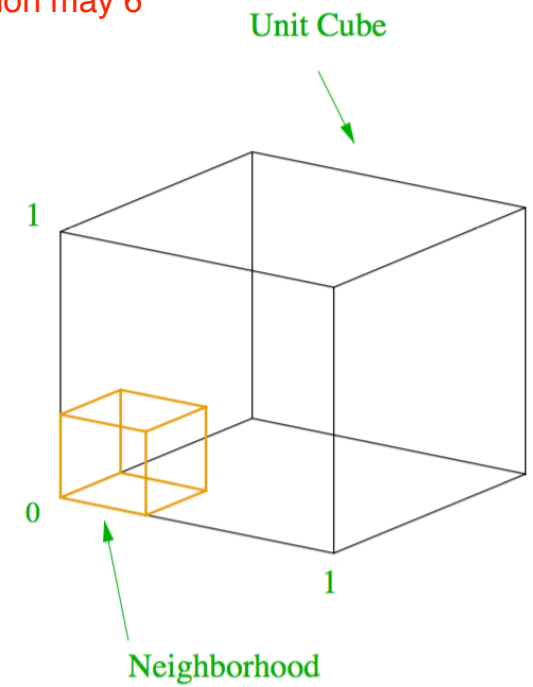
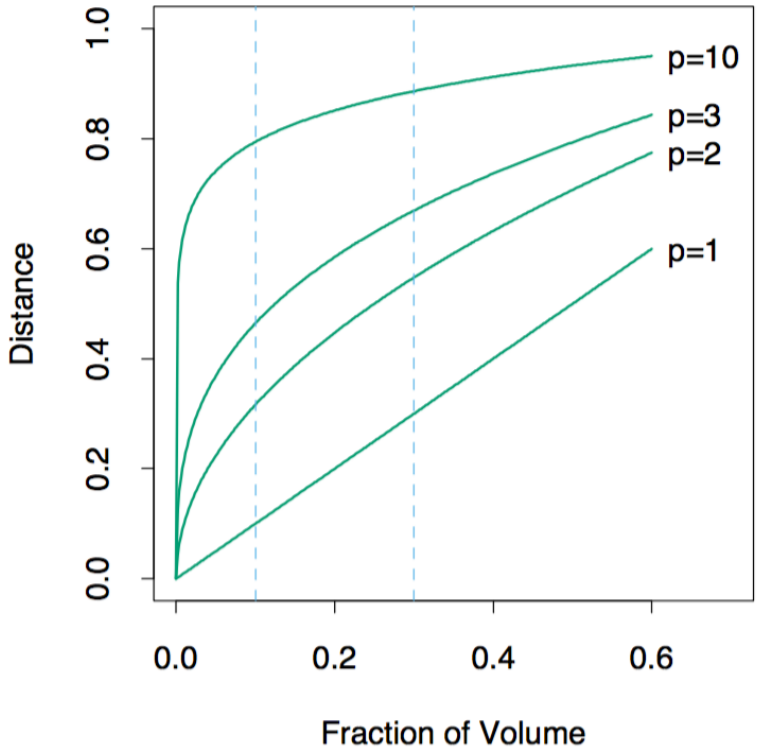


side length r

if you want to



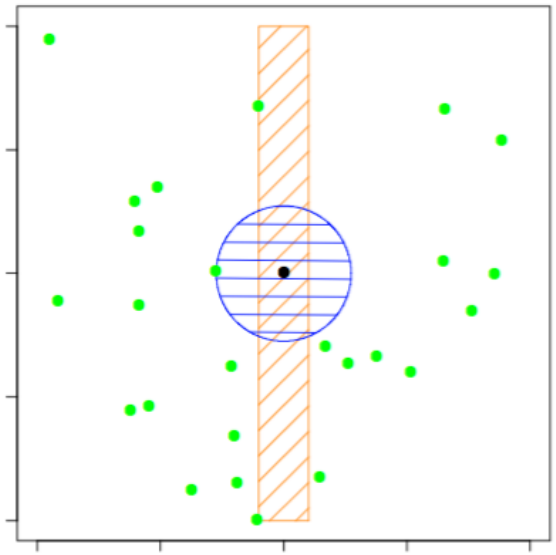
X is uniformly distributed over $[0,1]^p$. What is $\mathbb{P}(X \in [0,r]^p)$?

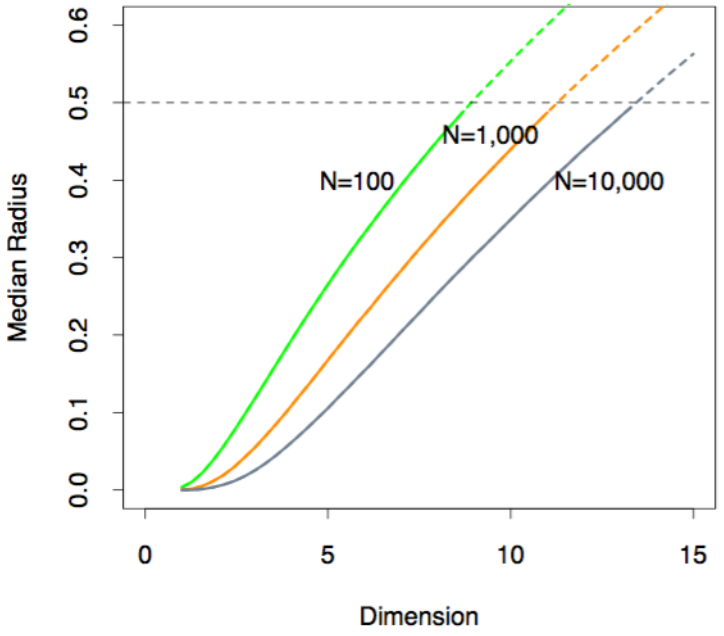
volumes and radiuses diverge very quickly?

only capturing r^d of the entire dataset.

Curse of dimensionality Ex. 2

$\{X_i\}_{i=1}^n$ are uniformly distributed over $[-.5, .5]^p$.





What is the median distance from a point at origin to its 1NN?

n datapoints spread through R^d

As dimension gets really high, nothing is local. Everything is essentially equally far away from you. Nearest point is about the same distance from farthest point? Ratio of distances goes to one.

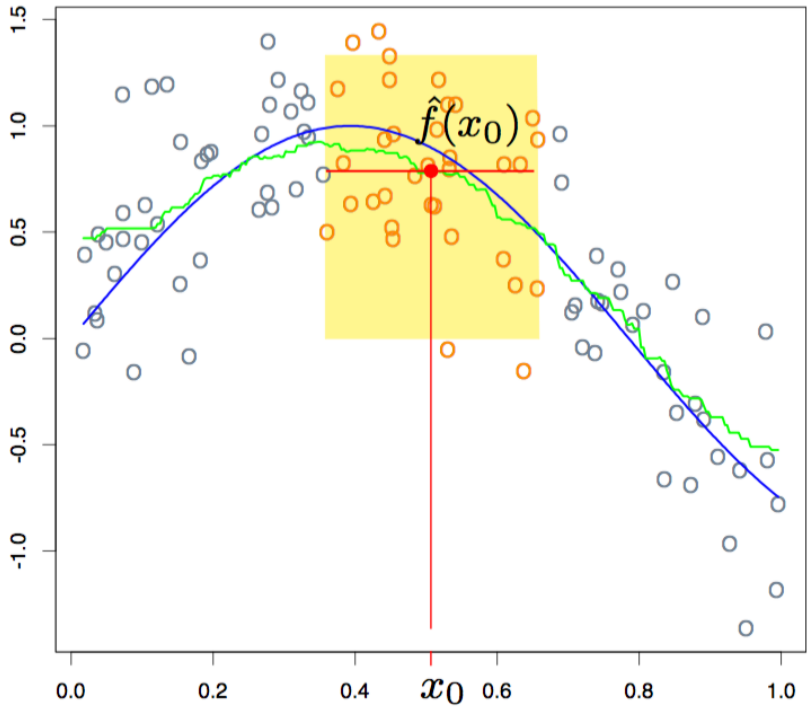
Takeaways

- Very simple to explain and implement. No training!
- You can use other forms of distance (not just Euclidean)
- With a lot of data, “local methods” have strong, simple theoretical guarantees.
- Without a lot of data, neighborhoods aren’t “local” and methods suffer.

Finding nearest neighbors can be slow to compute? If you have a large dataset it is hard to calculate the nearest neighbor? Loop through entire dataset (there are better implementations)

Nearest neighbor regression

$$\{(x_i, y_i)\})_{i=1}^{n}$$



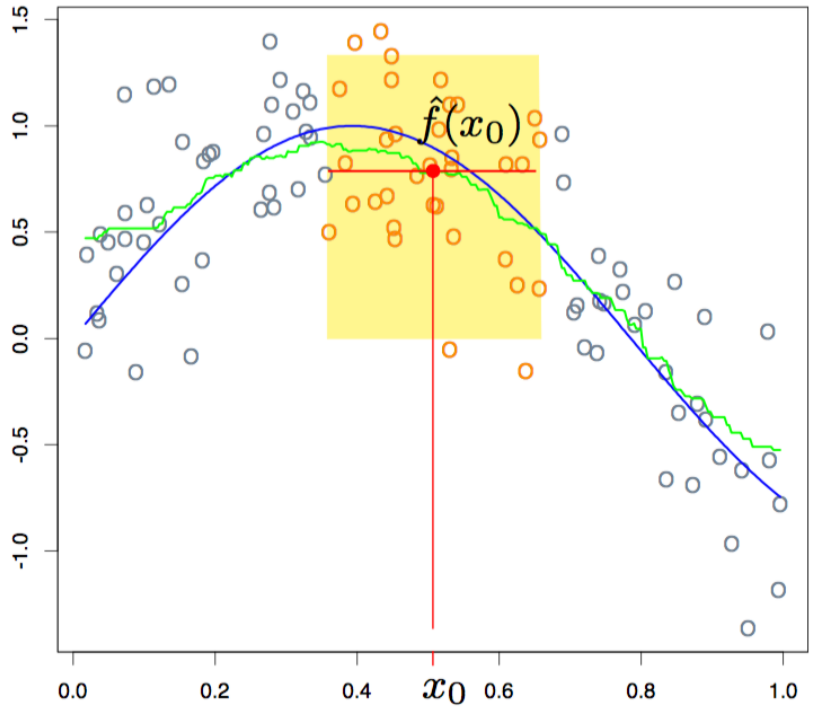
$$\mathcal{N}_k(x_0) = k\text{-nearest neighbors of } x_0$$

$$\widehat{f}(x_0) = \sum_{x_i \in \mathcal{N}_k(x_0)} \frac{1}{k}\, y_i$$

average y of nearest k neighbors

Nearest neighbor regression

$$\{(x_i, y_i)\})_{i=1}^n$$



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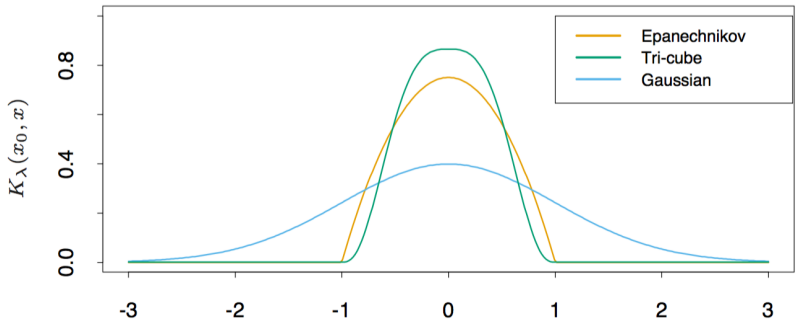
Why are far-away neighbors weighted same as close neighbors!

Kernel smoothing: $K(x, y)$

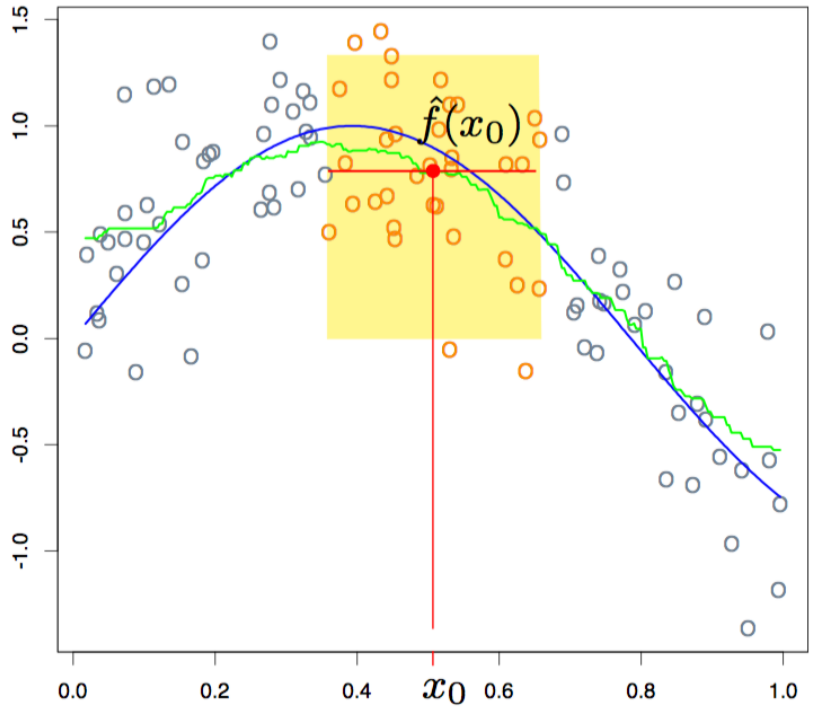


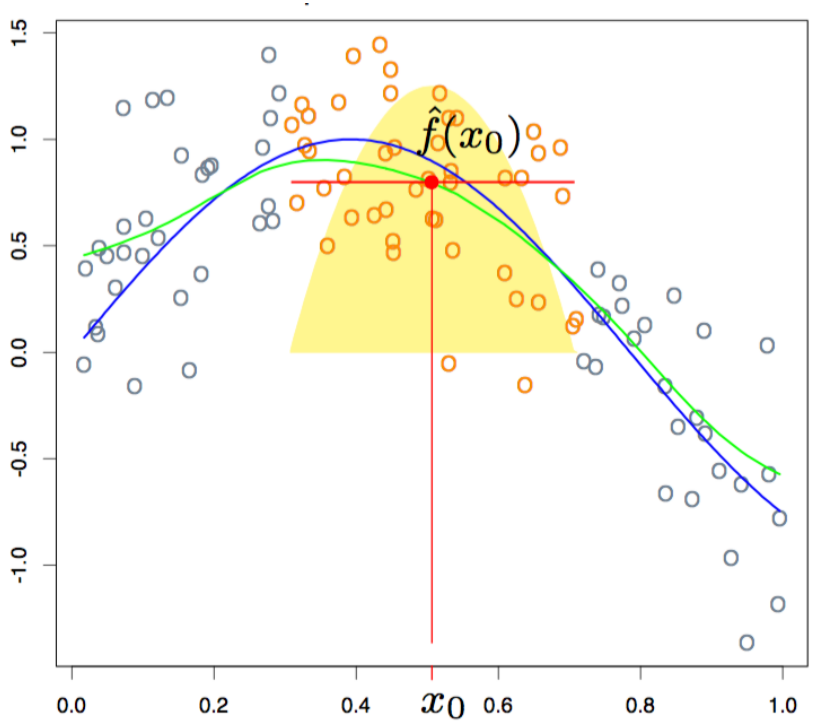
Can choose to weight nearby neighbors more than those farther away rather than a straight average of the y values.

$$\widehat{f}(x_0) = \frac{\sum_{i=1}^n K(x_0, x_i) y_i}{\sum_{i=1}^n K(x_0, x_i)}$$

Nearest neighbor regression

$\{(x_i, y_i)\})_{i=1}^n$





$\mathcal{N}_k(x_0) = k$-nearest neighbors of x_0

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Nearest neighbor regression

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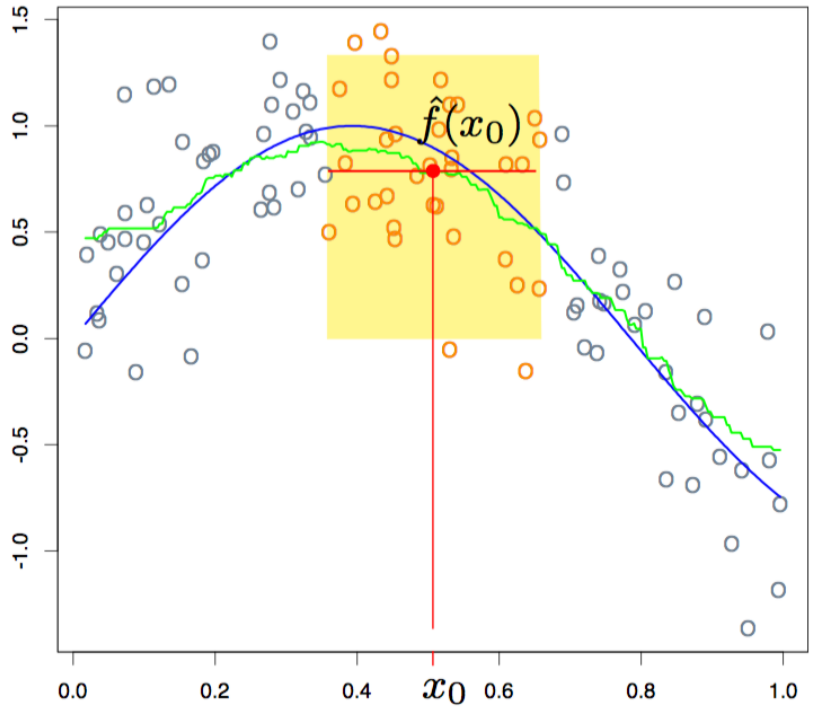
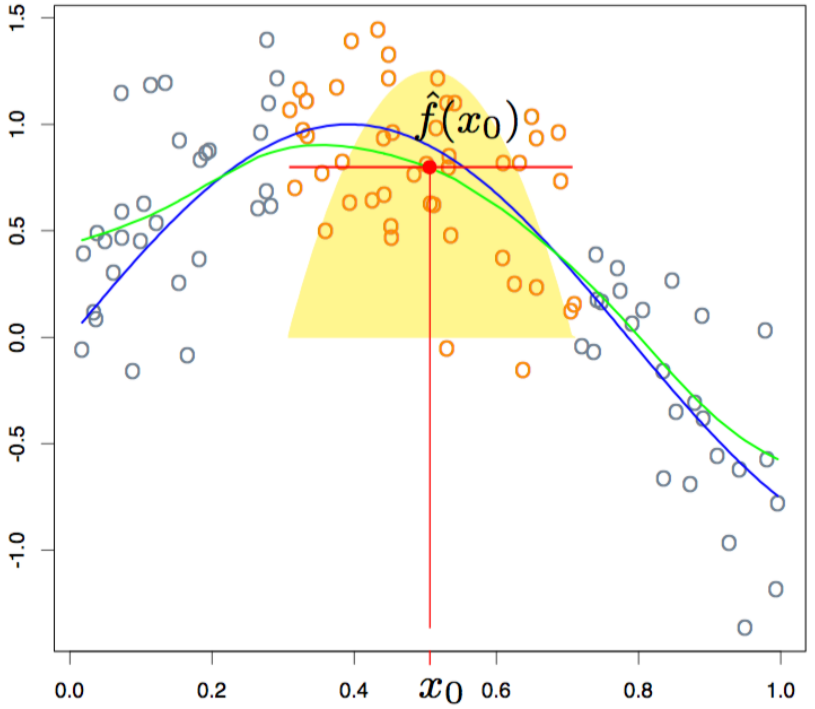




$\mathcal{N}_k(x_0) = k$-nearest neighbors of x_0

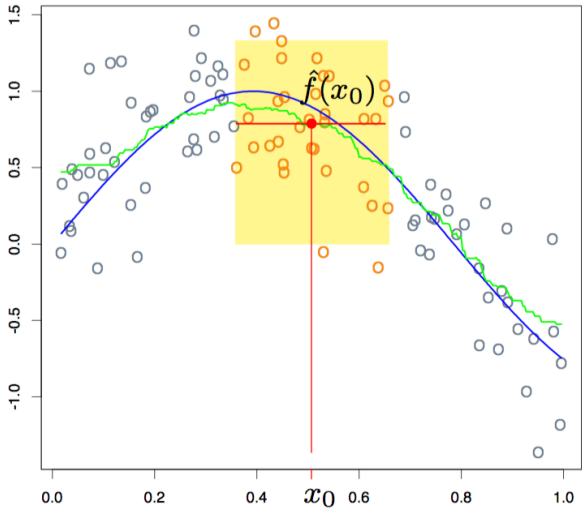
$$\widehat{f}(x_0) = \sum_{x_i \in \mathcal{N}_k(x_0)} \frac{1}{k}\, y_i$$

Why just average them?

$$\widehat{f}(x_0) = \frac{\sum_{i=1}^n K(x_0, x_i) y_i}{\sum_{i=1}^n K(x_0, x_i)}$$

Nearest neighbor regression

$$\{(x_i, y_i)\})_{i=1}^{n}$$



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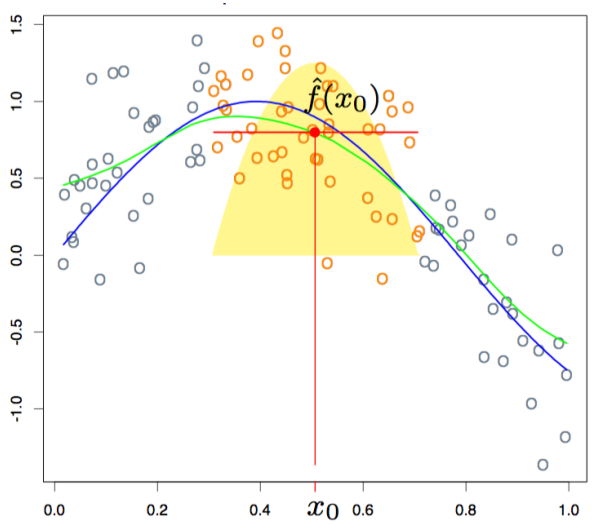

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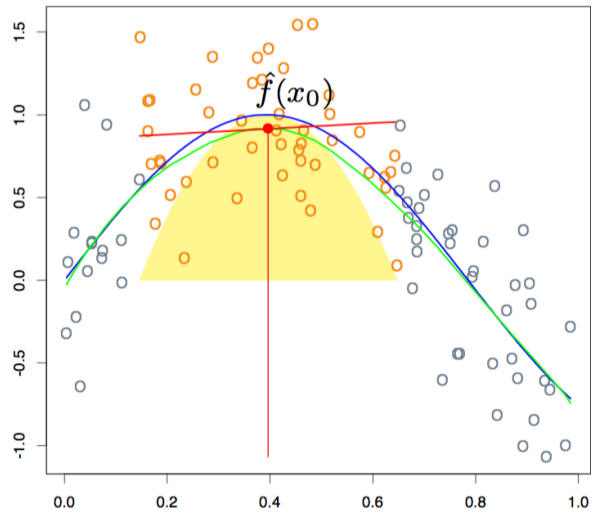


Linear regression between k nearest neighbors

$$\hat{f}(x_0) = b(x_0) + w(x_0)^T x_0$$

$$w(x_0), b(x_0) = \arg\min_{w,b} \sum_{i=1}^{n} K(x_0, x_i)(y_i - (b + w^T x_i))^2$$

Local Linear Regression

Nearest Neighbor Overview

- Very simple to explain and implement
- No training! But finding nearest neighbors in large dataset at test can be computationally demanding (kD-trees help)
- You can use other forms of distance (not just Euclidean)
- Smoothing with Kernels and local linear regression can improve performance (at the cost of higher variance)
- With a lot of data, "local methods" have strong, simple theoretical guarantees. bad GLOBAL information
- Without a lot of data, neighborhoods aren't "local" and methods suffer.

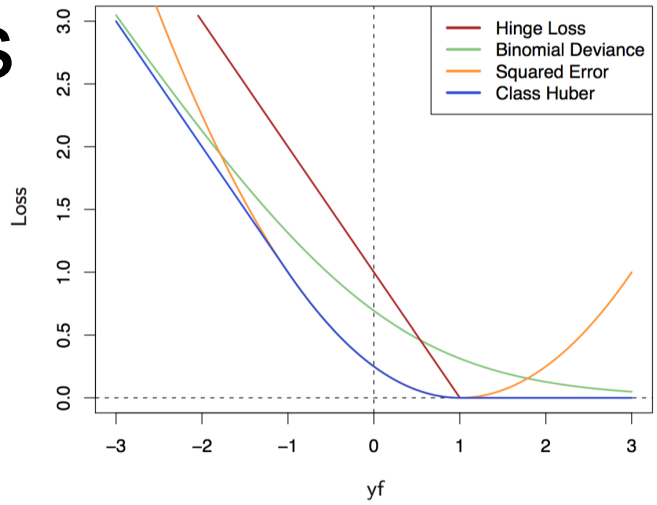
Kernels

Machine Learning – CSE446

Kevin Jamieson
University of Washington

May 6, 2019

Machine Learning Problems



- Have a bunch of iid data of the form:

$$\{(x_i, y_i)\}_{i=1}^{n} \qquad x_i \in \mathbb{R}^d \qquad y_i \in \mathbb{R}$$

- Learning a model's parameters:

$$\text{Each } \ell_i(w) \text{ is convex.} \qquad \sum_{i=1}^{n} \ell_i(w)$$

$$\text{Hinge Loss: } \ell_i(w) = \max\{0, 1 - y_i x_i^T w\}$$

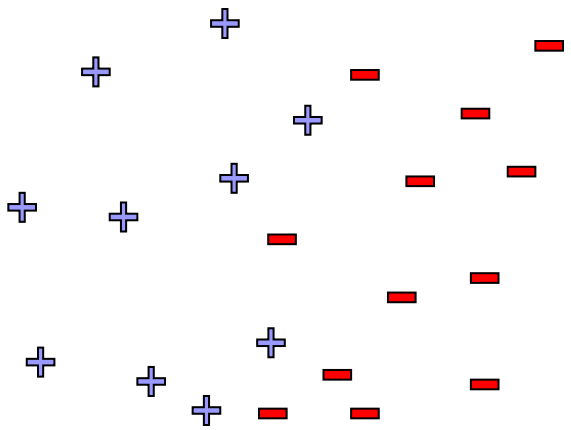
$$\text{Logistic Loss: } \ell_i(w) = \log(1 + \exp(-y_i\, x_i^T w))$$

$$\text{Squared error Loss: } \ell_i(w) = (y_i - x_i^T w)^2$$

w is always interacting through an inner product.

All in terms of inner products! Even nearest neighbor can use inner products!

What if the data is not linearly separable?



Use features of features of features of features….

$$\phi(x) : \mathbb{R}^d \rightarrow \mathbb{R}^p$$

where typically p >> d

Feature space can get really large really quickly!

Dot-product of polynomials

$\Phi(\mathbf{u}) \cdot \Phi(\mathbf{v}) =$ polynomials of degree exactly d

$$d = 1 : \phi(u) = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \quad \langle \phi(u), \phi(v) \rangle = u_1 v_1 + u_2 v_2$$

$$d = 2 : \phi(u) = \begin{bmatrix} u_1^2 \\ u_2^2 \\ u_1 u_2 \\ u_2 u_1 \end{bmatrix} \quad \langle \phi(u), \phi(v) \rangle = u_1^2 v_1^2 + u_2^2 v_2^2 + 2 u_1 u_2 v_1 v_2$$

General d :

Dimension of $\phi(u)$ is roughly p^d if $u \in \mathbb{R}^p$

Kernel Trick

$$\widehat{w} = \arg\min_{w} \sum_{i=1}^{n} (y_i - x_i^T w)^2 + \lambda ||w||_2^2$$

$$\text{There exists an } \alpha \in \mathbb{R}^n \text{: } \widehat{w} = \sum_{i=1}^{n} \alpha_i x_i$$

hat{w} is living in the span of all the x_i. Suppose not then hat{w} = sum(a_ix_i) + W_perp. Note that W_perp x_i = 0 by definition, so it does not change the sum(y_i - x_iw)^2 term. So it would only increase the norm of w. Since hat{w} minimizes this, it will have a W_perp = 0

$$\widehat{\alpha} = \arg\min_{\alpha} \sum_{i=1}^{n} (y_i - \sum_{j=1}^{n} \alpha_j \langle x_j, x_i \rangle)^2 + \lambda \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j \langle x_i, x_j \rangle$$

$$= \arg\min_{\alpha} \sum_{i=1}^{n} (y_i - \sum_{j=1}^{n} \alpha_j K(x_i, x_j))^2 + \lambda \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j K(x_i, x_j)$$

inner product in some space

$$= \arg\min_{\alpha} ||\mathbf{y} - \mathbf{K}\alpha||_2^2 + \lambda \alpha^T \mathbf{K} \alpha$$

$$K(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle$$

END LECTURE MON MAY 6

Why regularization?

Typically, $\mathbf{K} \succ 0$. What if $\lambda = 0$?

$$\widehat{\alpha} = \arg\min_{\alpha} ||\mathbf{y} - \mathbf{K}\alpha||_2^2 + \lambda \alpha^T \mathbf{K} \alpha$$

Why regularization?

Typically, $\mathbf{K} \succ 0$. What if $\lambda = 0$?

$$\widehat{\alpha} = \arg\min_{\alpha} ||\mathbf{y} - \mathbf{K}\alpha||_2^2 + \lambda \alpha^T \mathbf{K} \alpha$$

Unregularized kernel least squares can (over) fit **any data**!

$$\widehat{\alpha} = \mathbf{K}^{-1}\mathbf{y}$$

Common kernels

- Polynomials of degree exactly d

$$K(\mathbf{u}, \mathbf{v}) = (\mathbf{u} \cdot \mathbf{v})^d$$

- Polynomials of degree up to d

$$K(\mathbf{u}, \mathbf{v}) = (\mathbf{u} \cdot \mathbf{v} + 1)^d$$

- Gaussian (squared exponential) kernel

$$K(\mathbf{u}, \mathbf{v}) = \exp\left(-\frac{||\mathbf{u} - \mathbf{v}||_2^2}{2\sigma^2}\right)$$

- Sigmoid

$$K(\mathbf{u}, \mathbf{v}) = \tanh(\eta \mathbf{u} \cdot \mathbf{v} + \nu)$$

Mercer's Theorem

- When do we have a valid Kernel K(x,x')?
- Sufficient:

  $K(x, x')$ is a valid kernel if there exists $\phi(x)$ such that $K(x, x') = \phi(x)^T \phi(x')$

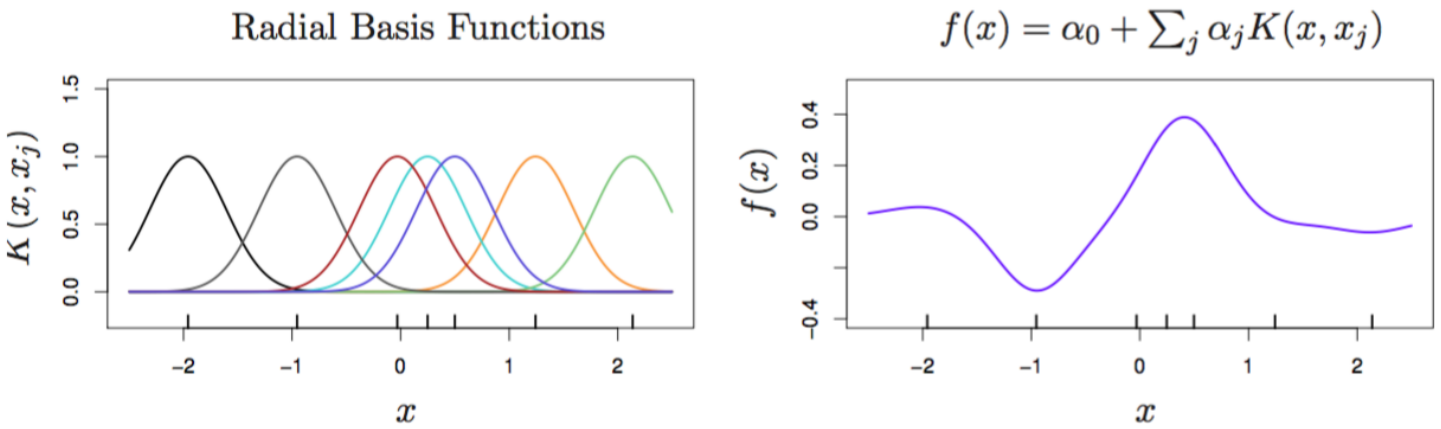
- Mercer's Theorem:

  $K(x, x')$ is a valid kernel if and only if $\mathbf{K}$ is symmetric and positive semi-definite for any pointset $(x_1, \ldots, x_n)$ where $\mathbf{K}_{i,j} = K(x_i, x_j)$.

RBF Kernel

$$K(\mathbf{u}, \mathbf{v}) = \exp\left(-\frac{||\mathbf{u} - \mathbf{v}||_2^2}{2\sigma^2}\right)$$

- Note that this is like weighting "bumps" on each point like kernel smoothing but now we **learn** the weights

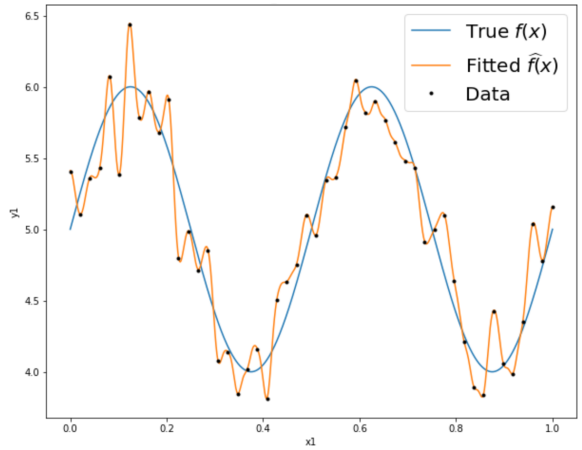


RBF Kernel

$$K(\mathbf{u}, \mathbf{v}) = \exp\left(-\frac{||\mathbf{u} - \mathbf{v}||_2^2}{2\sigma^2}\right)$$

The bandwidth sigma has an enormous effect on fit:

$\sigma = 10^{-2}$ $\lambda = 10^{-4}$



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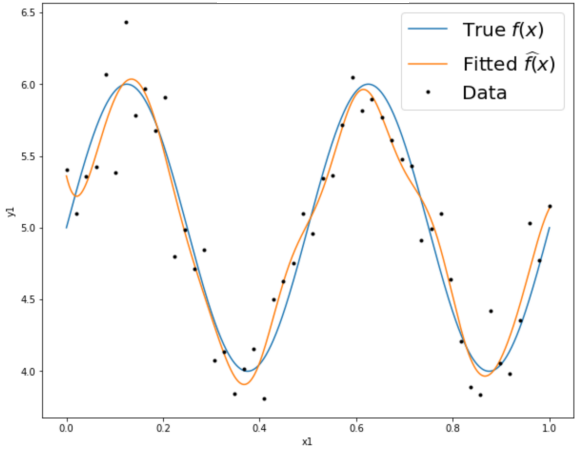

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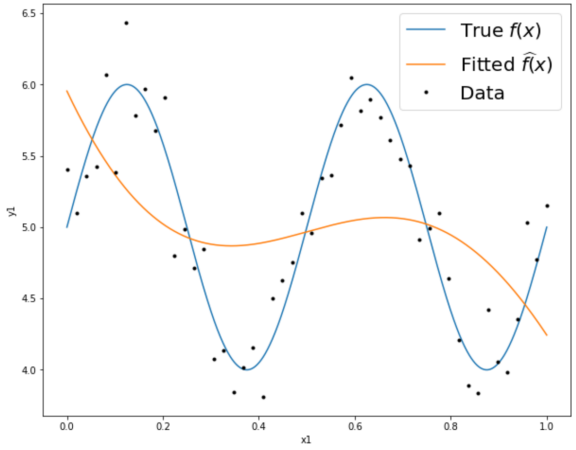

$$\widehat{f}(x) = \sum_{i=1}^{n} \widehat{\alpha}_i K(x_i, x)$$

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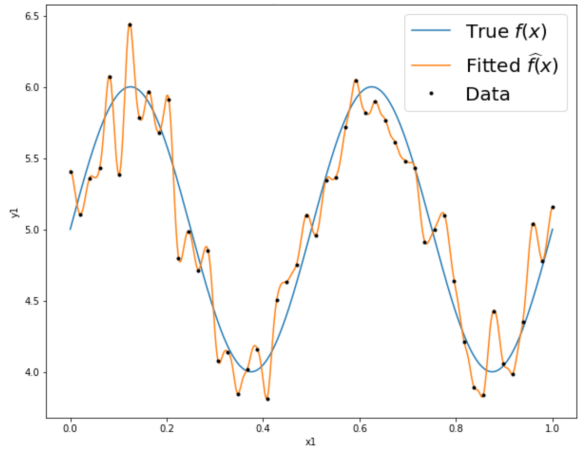

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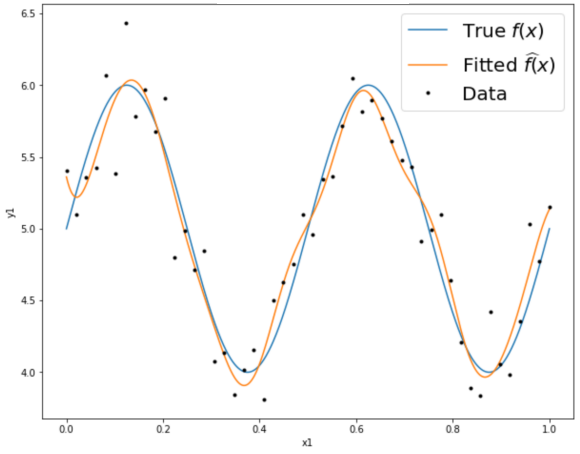
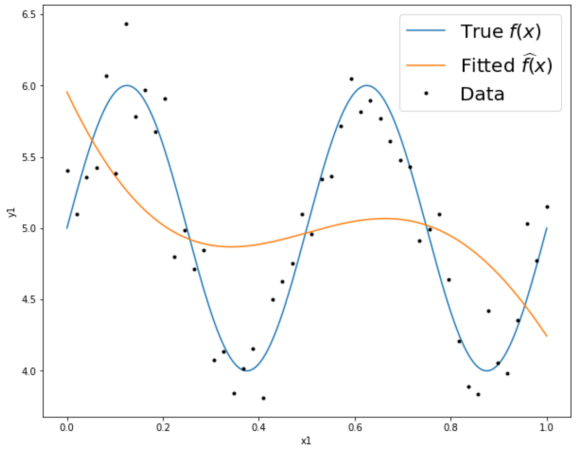
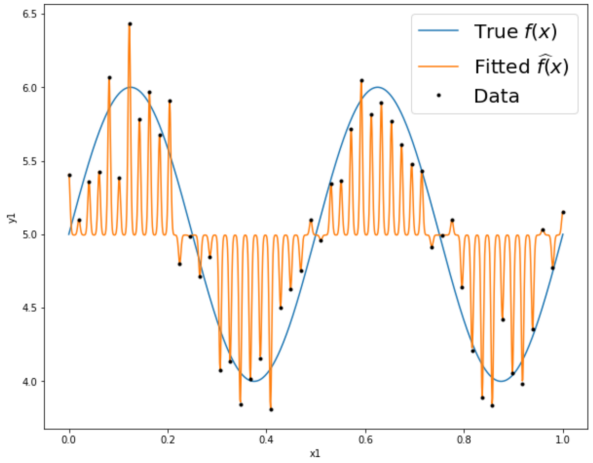


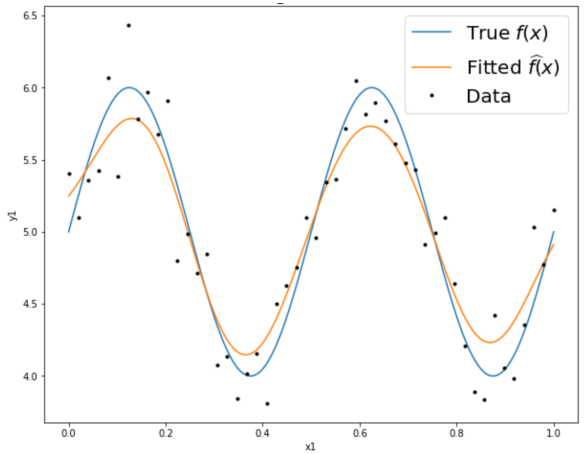
$\sigma = 10^{-0}$ $\lambda = 10^{-4}$



$\sigma = 10^{-3}$ $\lambda = 10^{-4}$



$\sigma = 10^{-1}$ $\lambda = 10^{-0}$



$$\widehat{f}(x) = \sum_{i=1}^{n} \widehat{\alpha}_i K(x_i, x)$$

RBF Kernel

$$K(\mathbf{u}, \mathbf{v}) = \exp\left(-\frac{||\mathbf{u} - \mathbf{v}||_2^2}{2\sigma^2}\right)$$

Basis representation in 1d?

$$[\phi(x)]_i = \frac{1}{\sqrt{i!}} e^{-\frac{x^2}{2}} x^i \quad \text{for } i = 0, 1, \ldots$$

$$\begin{aligned}
\phi(x)^T \phi(x') &= \sum_{i=0}^{\infty} \left(\frac{1}{\sqrt{i!}} e^{-\frac{x^2}{2}} x^i\right)\left(\frac{1}{\sqrt{i!}} e^{-\frac{(x')^2}{2}} (x')^i\right) \\
&= e^{-\frac{x^2+(x')^2}{2}} \sum_{i=0}^{\infty} \frac{1}{i!} (xx')^i \\
&= e^{-|x-x'|^2/2}
\end{aligned}$$

If n is very large, allocating an n-by-n matrix is tough. Can we truncate the above sum to approximate the kernel?

RBF kernel and random features

$$2\cos(\alpha)\cos(\beta) = \cos(\alpha+\beta) + \cos(\alpha-\beta)$$

$$e^{jz} = \cos(z) + j\sin(z)$$

Recall HW1 where we used the feature map:

$$\phi(x) = \begin{bmatrix} \sqrt{2}\cos(w_1^T x + b_1) \\ \vdots \\ \sqrt{2}\cos(w_p^T x + b_p) \end{bmatrix} \qquad \begin{aligned} w_k &\sim \mathcal{N}(0, 2\gamma\, I) \\ b_k &\sim \text{uniform}(0, \pi) \end{aligned}$$

$$\begin{aligned} \mathbb{E}[\frac{1}{p}\phi(x)^T\phi(y)] &= \frac{1}{p}\sum_{k=1}^{p}\mathbb{E}[2\cos(w_k^T x + b_k)\cos(w_k^T y + b_k)] \\ &= \mathbb{E}_{w,b}[2\cos(w^T x + b)\cos(w^T y + b)] \end{aligned}$$

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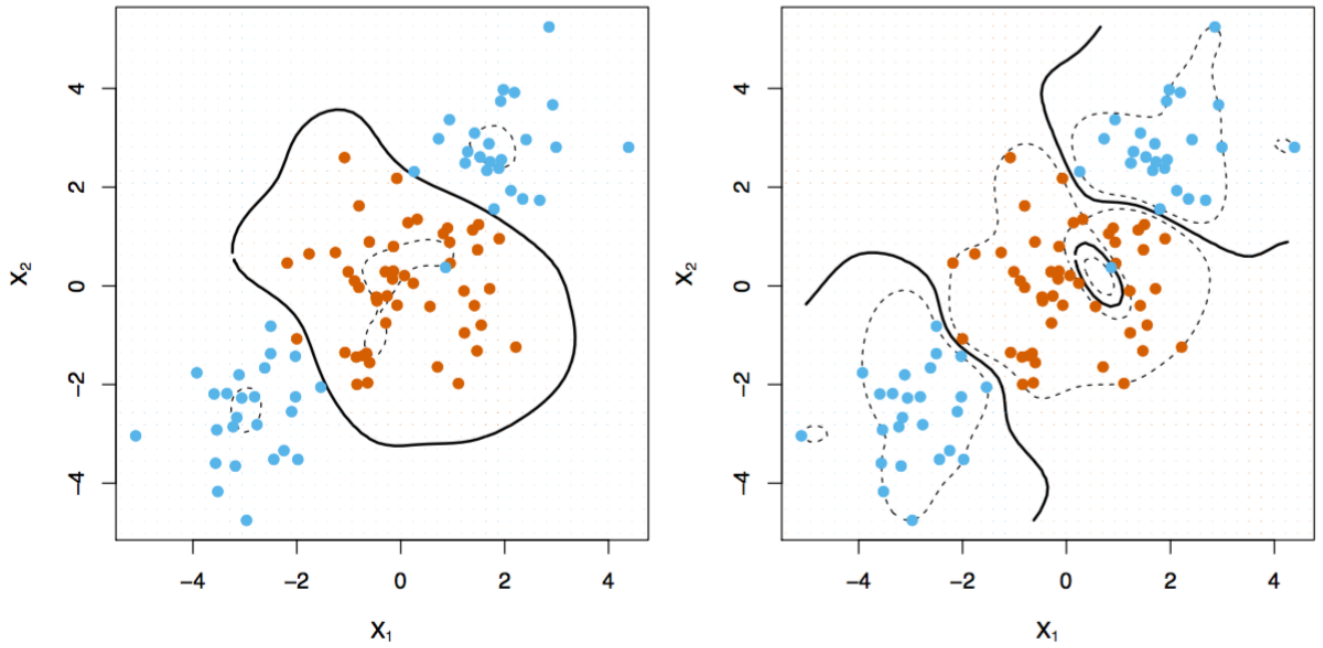
[Rahimi, Recht NIPS 2007]
"NIPS Test of Time Award, 2018"

RBF Classification

$$\widehat{w} = \sum_{i=1}^{n} \max\{0, 1 - y_i(b + x_i^T w)\} + \lambda ||w||_2^2$$

$$\min_{\alpha,b} \sum_{i=1}^{n} \max\{0, 1 - y_i(b + \sum_{j=1}^{n} \alpha_j \langle x_i, x_j \rangle)\} + \lambda \sum_{i,j=1}^{n} \alpha_i \alpha_j \langle x_i, x_j \rangle$$



Wait, infinite dimensions?

- Isn’t everything separable there? How are we not overfitting?

- Regularization! Fat shattering (R/margin)^2

String Kernels

Example from Efron and Hastie, 2016

Amino acid sequences of different lengths:

x1

IPTSALVKETLALLSTHRTLLIANETLRIPVPVHKNHQLCTEEIFQGIGTLESQTVQGGTV
ERLFKNLSLIKKYIDGQKKKCGEERRRVNQFLDY**LQE**FLGVMNTEWI

x2

PHRRDLCSRSIWLARKIRSDLTALTESYVKHQGLWSELTEAER**LQE**NLQAYRTFHVLLA
RLLEDQQVHFTPTEGDFHQAIHTLLLQVAAFAYQIEELMILLEYKIPRNEADGMLFEKK
LWGLKV**LQE**LSQWTVRSIHDLRFISSHQTGIP

All subsequences of length 3 (of possible 20 amino acids) $20^3 = 8{,}000$

$$h^3_{\text{LQE}}(x_1) = 1 \text{ and } h^3_{\text{LQE}}(x_2) = 2.$$

Bootstrap

Machine Learning – CSE446

Kevin Jamieson
University of Washington

May 6, 2019

Limitations of CV

- An 80/20 split throws out a relatively large amount of data if only have, say, 20 examples.
- Test error is informative, but how accurate is this number? (e.g., 3/5 heads vs. 30/50)
- How do I get confidence intervals on statistics like the median or variance of a distribution?
- Instead of the error for the entire dataset, what if I want to study the error for a *particular example* x?

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The Bootstrap: Developed by Efron in 1979.

Bootstrap: basic idea

Given dataset drawn iid samples with CDF F_Z:

$$\mathcal{D} = \{z_1, \ldots, z_n\} \overset{i.i.d.}{\sim} F_Z$$

We compute a *statistic* of the data to get: $\widehat{\theta} = t(\mathcal{D})$

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For b=1,…,B define the *b*th ***bootstrapped*** dataset as drawing *n* samples **with replacement** from *D*

$$\mathcal{D}^{*b} = \{z_1^{*b}, \ldots, z_n^{*b}\} \overset{i.i.d.}{\sim} \widehat{F}_{Z,n}$$

and the *b*th bootstrapped statistic as: $\theta^{*b} = t(\mathcal{D}^{*b})$

Bootstrap: basic idea

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$$\mathcal{D} = \{z_1, \ldots, z_n\} \overset{i.i.d.}{\sim} F_Z \qquad \widehat{\theta} = t(\mathcal{D})$$

For b=1,…,B, samples sampled **with replacement** from *D*

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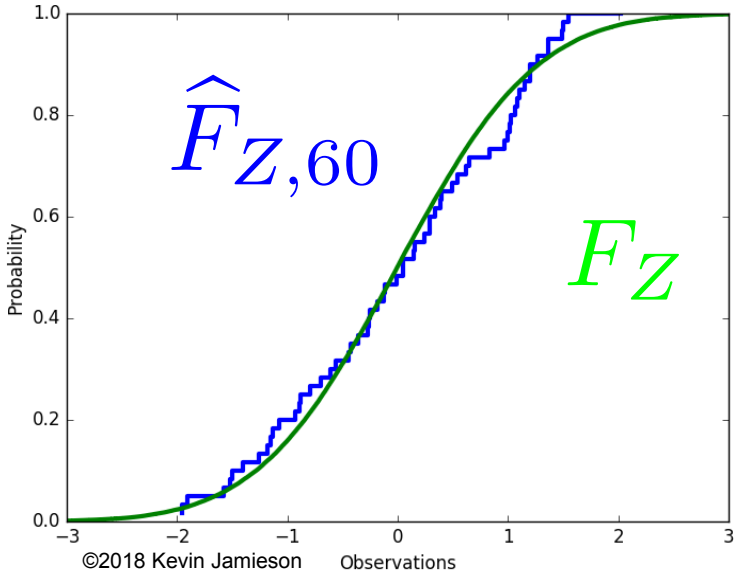

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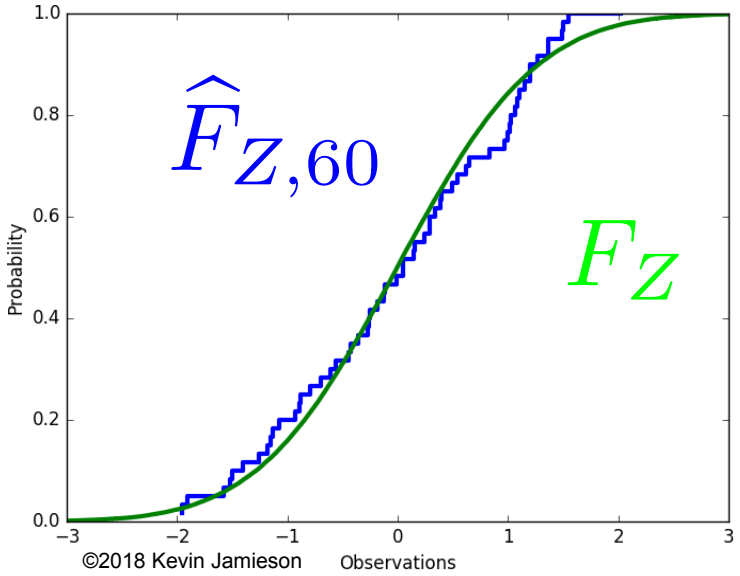
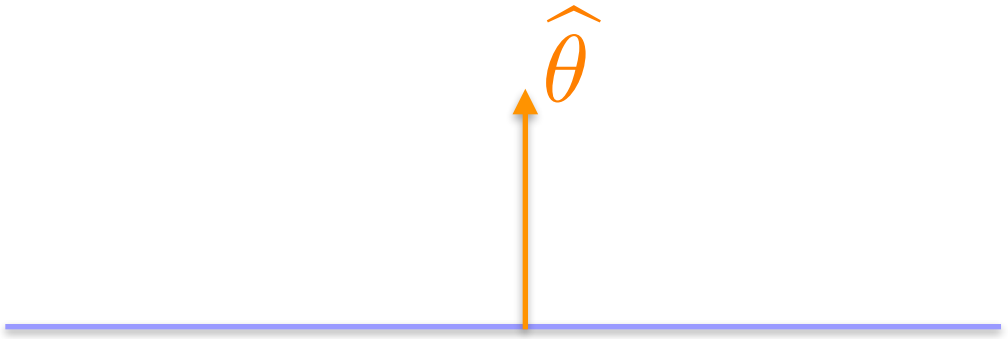


$$\sup_x |\widehat{F}_n(x) - F(x)| \to 0 \quad \text{as } n \to \infty$$

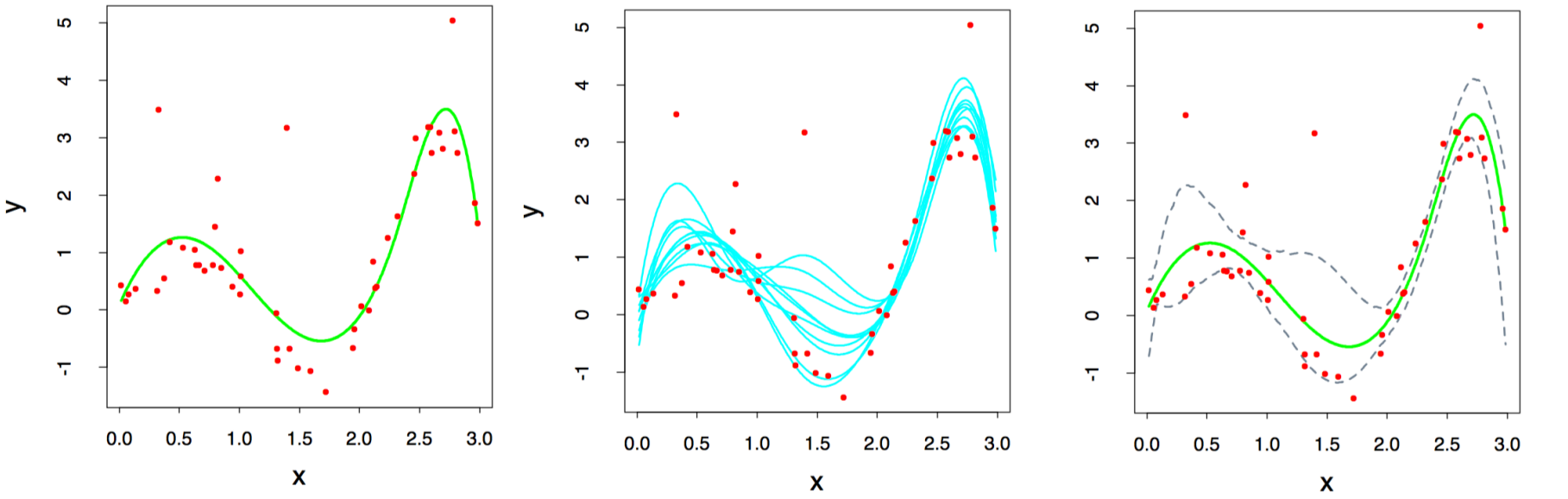


Applications

Common applications of the bootstrap:

- Estimate parameters that escape simple analysis like the variance or median of an estimate
- Confidence intervals
- Estimates of error for a particular example:

$\mathcal{D}$ $\widehat{\theta}$ θ^{*b} for $b = 1, \ldots, 10$ 95% confidence interval



Figures from Hastie et al

Takeaways

Advantages:

- Bootstrap is **very** generally applicable. Build a confidence interval around ***anything***
- **Very** simple to use
- Appears to give meaningful results even when the amount of data is very small
- Very strong **asymptotic theory** (as num. examples goes to infinity)

Takeaways

Advantages:

- Bootstrap is **very** generally applicable. Build a confidence interval around ***anything***
- **Very** simple to use
- Appears to give meaningful results even when the amount of data is very small
- Very strong **asymptotic theory** (as num. examples goes to infinity)

Disadvantages

- Very few meaningful finite-sample guarantees
- Potentially **computationally intensive**
- Reliability relies on test statistic and rate of convergence of empirical CDF to true CDF, which is unknown
- Poor performance on “extreme statistics” (e.g., the max)

Not perfect, but better than nothing.

Warm up: risk prediction with logistic regression

- Boss gives you a bunch of data on loans defaulting or not:

$$\{(x_i, y_i)\}_{i=1}^n \quad x_i \in \mathbb{R}^d, \quad y_i \in \{-1, 1\}$$

- You model the data as: $P(Y = y|x, w) = \dfrac{1}{1 + \exp(-y\, w^T x)}$
- And compute the maximum likelihood estimator:

$$\widehat{w}_{MLE} = \arg\max_w \prod_{i=1}^n P(y_i|x_i, w)$$

For a new loan application x, boss recommends to give loan if your model says they will repay it with probability at least .95 (i.e. low risk):

Give loan to x if $\dfrac{1}{1 + \exp(-\widehat{w}_{MLE}^T x)} \geq .95$

- One year later only half of loans are paid back and the bank folds. What might have happened?

How would you use the bootstrap to do this differently?