CPSC 340:
Machine Learning and Data Mining

More Regularization

Fall 2018

Admin

- Midterm is tomorrow.
  - October 18th at 6:30pm.
  - Last names starting with A-L: BUCH A102.
  - Last names starting with M-Z: BUCH A104.
  - 80 minutes.
  - Closed-book.
  - One doubled-sided ‘cheat sheet’ for midterm.
  - Auditors do not take the midterm.
  - Mike will go over midterm questions/solutions in his lecture Friday.

- There will be two types of questions on the midterm:
  - ‘Technical’ questions requiring things like pseudo-code or derivations.
    - Similar to assignment questions, and will only be on topics related to those in assignments.
  - ‘Conceptual’ questions testing understanding of key concepts.
    - All lecture slide material except “bonus slides” is fair game here.

Last Time: L2-Regularization

- We discussed regularization:
  - Adding a continuous penalty on the model complexity:

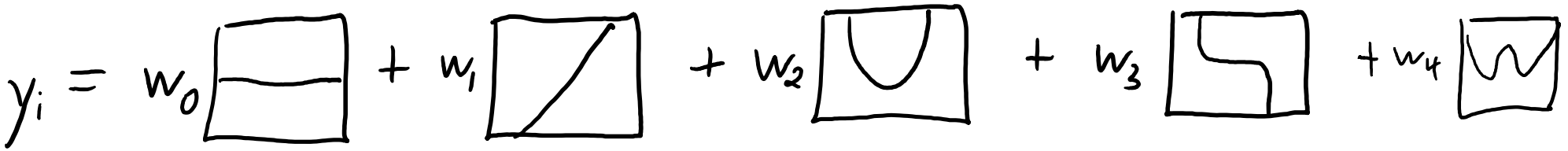
$$f(w) = \frac{1}{2}\|Xw - y\|^2 + \frac{\lambda}{2}\|w\|^2$$

  - Best parameter λ almost always leads to improved test error.
    - L2-regularized least squares is also known as "ridge regression".
    - Can be solved as a linear system like least squares.

  - Numerous other benefits:
    - Solution is unique, less sensitive to data, gradient descent converges faster.

Parametric vs. Non-Parametric Transforms

- We've been using linear models with polynomial bases:



- But polynomials are not the only possible bases:
  - Exponentials, logarithms, trigonometric functions, etc.
  - The right basis will vastly improve performance.
  - If we use the wrong basis, our accuracy is limited even with lots of data.
  - But the right basis may not be obvious.

Parametric vs. Non-Parametric Transforms

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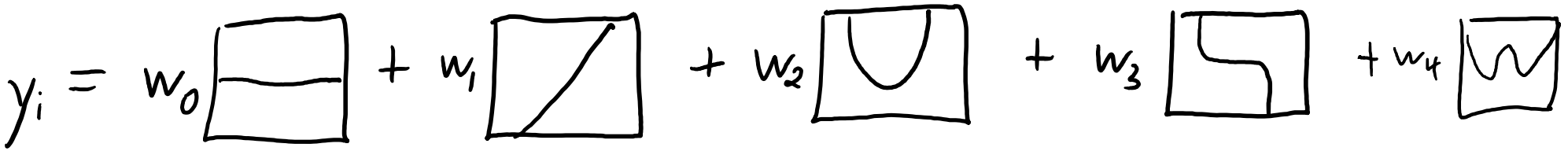
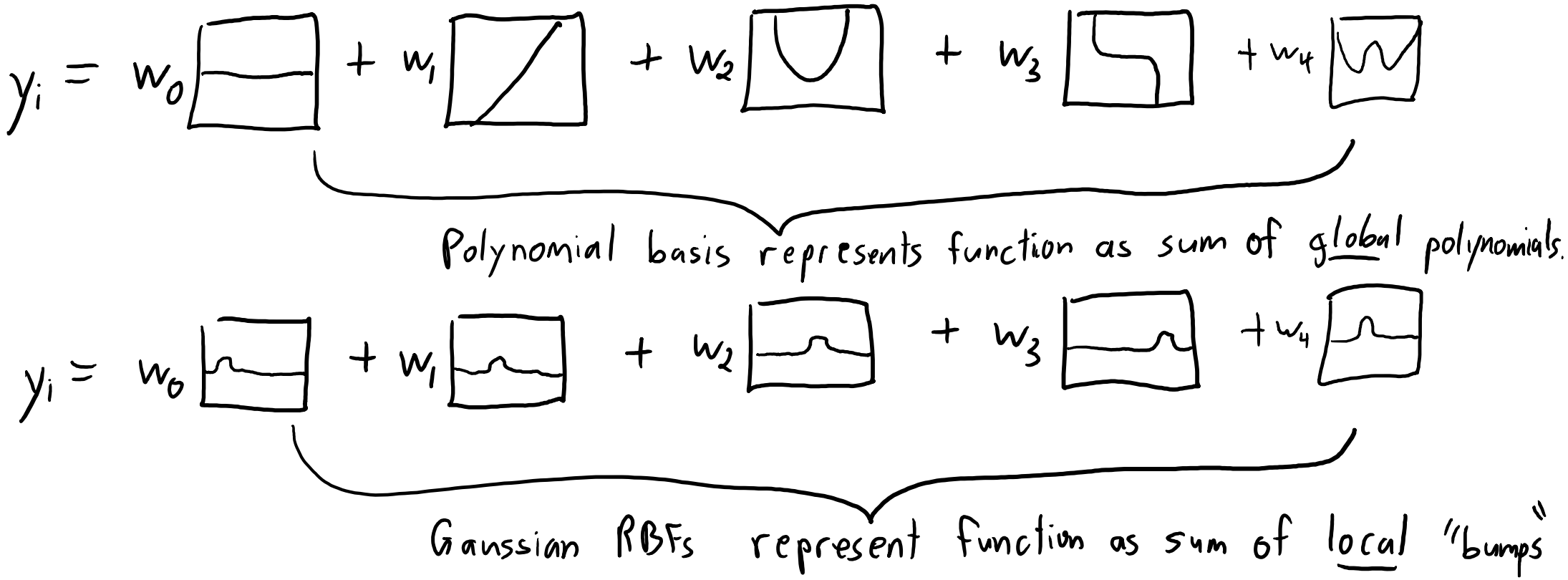


- Alternative is non-parametric bases:
  - Size of basis (number of features) grows with 'n'.
  - Model gets more complicated as you get more data.
  - Can model complicated functions where you don't know the right basis.
    - With enough data.
  - Classic example is "Gaussian RBFs".

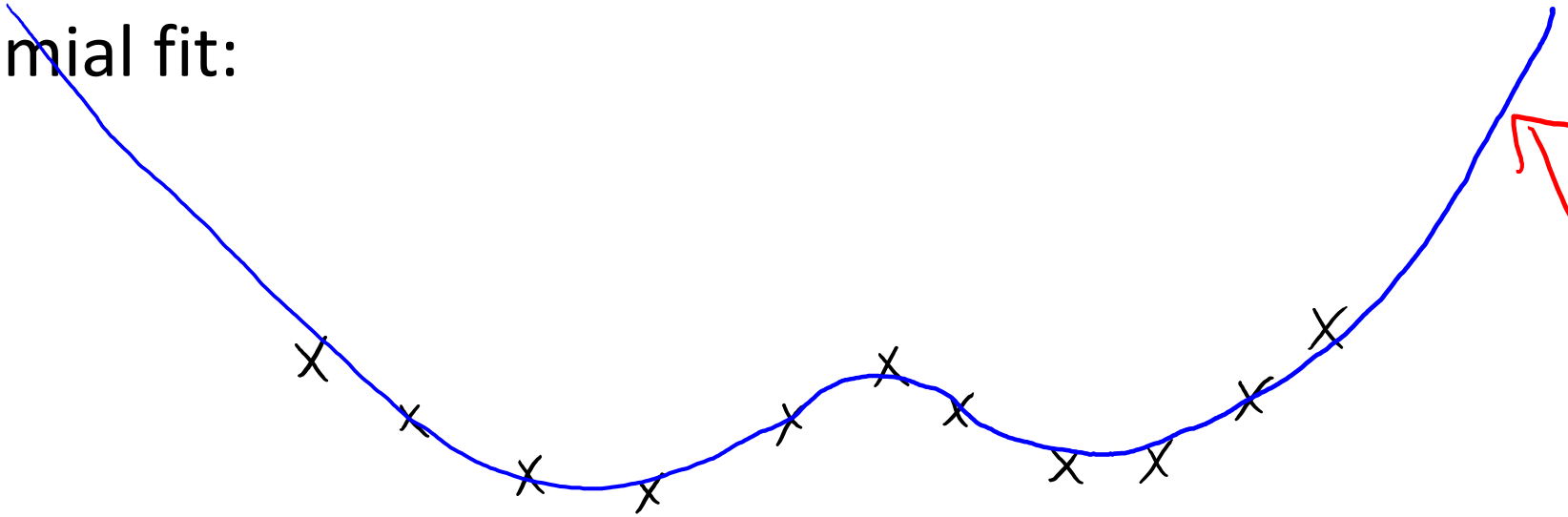
Gaussian RBFs: A Sum of "bumps"



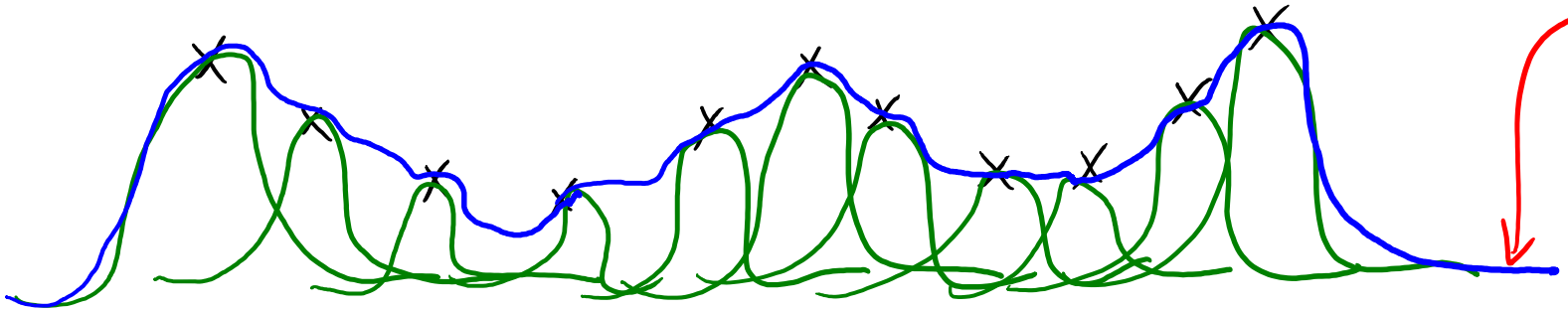
- Gaussian RBFs are universal approximators (compact subets of $\mathbb{R}^d$)
  - Enough bumps can approximate any continuous function to arbitrary precision.
  - Achieve optimal test error as 'n' goes to infinity.

Gaussian RBFs: A Sum of "Bumps"

- Polynomial fit:



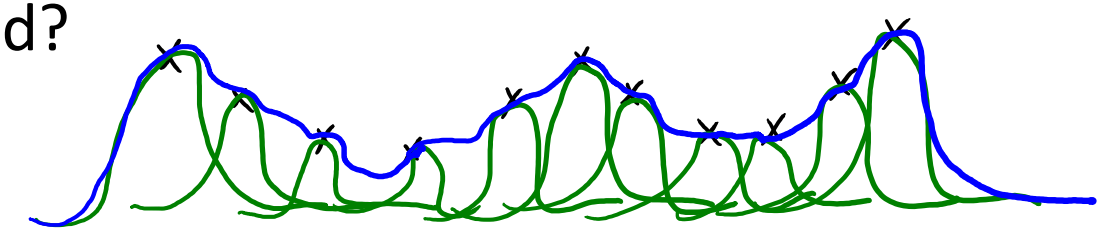
- Constructing a function from bumps ("smooth histogram"):



- Bonus slides: challenges of "far from data" (and future) predictions.

Gaussian RBF Parameters

- Some obvious questions:
  1. How many bumps should we use?
  2. Where should the bumps be centered?
  3. How high should the bumps go?
  4. How wide should the bumps be?



- The usual answers:
  1. We use ‘n’ bumps (non-parametric basis).
  2. Each bump is centered on one training example x_i.
  3. Fitting regression weights ‘w’ gives us the heights (and signs).
  4. The width is a hyper-parameter (narrow bumps == complicated model).

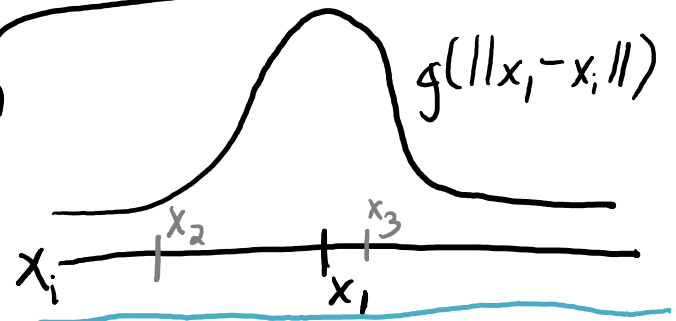
Gaussian RBFs: Formal Details

- What is a radial basis functions (RBFs)?
  - A set of non-parametric bases that depend on distances to training points.

Replace $X = \begin{bmatrix} & \\ & \end{bmatrix}$ (n rows, d columns) by $Z = \begin{bmatrix} g(\|x_1 - x_1\|) & g(\|x_1 - x_2\|) & \cdots & g(\|x_1 - x_n\|) \\ g(\|x_2 - x_1\|) & g(\|x_2 - x_2\|) & \cdots & g(\|x_2 - x_n\|) \\ \vdots & & & \\ g(\|x_n - x_1\|) & g(\|x_n - x_2\|) & \cdots & g(\|x_n - x_n\|) \end{bmatrix}$ (n rows, n columns)

  - Most common 'g' is Gaussian RBF:

$$g(\varepsilon) = \exp\left(-\frac{\varepsilon^2}{2\sigma^2}\right)$$



- Variance σ^2 is a hyper-parameter controlling "width".
  - This affects fundamental trade-off (set it using a validation set).

Do we need $\sigma\sqrt{2\pi}$?
-No because $v^T z_i = (\frac{1}{\beta} v)^T (\beta z_i)$

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To make predictions on $\tilde{X} = \begin{bmatrix} & \\ & \end{bmatrix}$ (t rows, d columns) use $\tilde{Z} = \begin{bmatrix} g(\|\tilde{x}_i - x_j\|) \end{bmatrix}$ (t rows, n columns)

Number of "features" is number of training examples.

Gaussian RBFs: Pseudo-Code

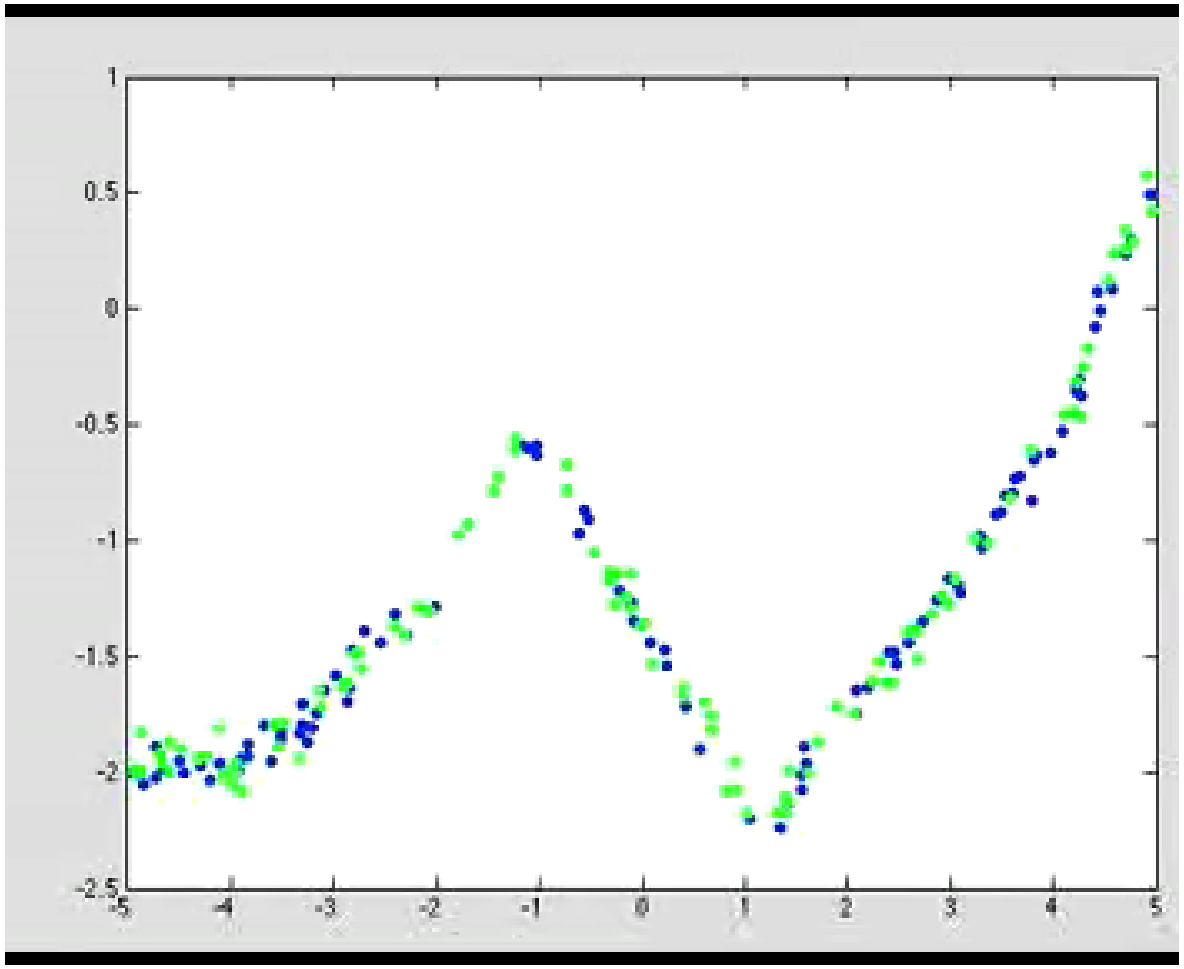
Constructing Gaussian RBFs given data 'X' and hyper-parameter σ:

```
Z = zeros(n, n)
for i1 in 1:n
    for i2 in 1:n
        Z[i1, i2] = exp(-norm(X[i1, :] - X[i2, :])^2 / 2σ^2)
```

With test data $\tilde{X}$: form $\tilde{Z}$ based on distances to training examples.

Non-Parametric Basis: RBFs

- Least squares with Gaussian RBFs for different σ values:



Could add bias and linear basis:

$$Z = \begin{bmatrix} 1 & x_1 & g(\|x_1 - x_1\|) & \cdots & g(\|x_1 - x_n\|) \\ 1 & x_2 & & & \\ 1 & x_3 & & & \\ \vdots & \vdots & & & \\ 1 & x_n & g(\|x_1 - x_n\|) & \cdots & g(\|x_n - x_n\|) \end{bmatrix}$$

1 d n

This reverts to linear regression instead of 0 away from data.

RBFs and Regularization

- Gaussian Radial basis functions (RBFs) predictions:

$$\hat{y}_i = w_1 \exp\left(-\frac{\|x_i - x_1\|^2}{2\sigma^2}\right) + w_2 \exp\left(-\frac{\|x_i - x_2\|^2}{2\sigma^2}\right) + \cdots + w_n \exp\left(-\frac{\|x_i - x_n\|^2}{2\sigma^2}\right)$$

$$= \sum_{j=1}^{n} w_j \exp\left(-\frac{\|x_i - x_j\|^2}{2\sigma^2}\right)$$

  - Flexible bases that can model any continuous function.
  - But with 'n' data points RBFs have 'n' basis functions.

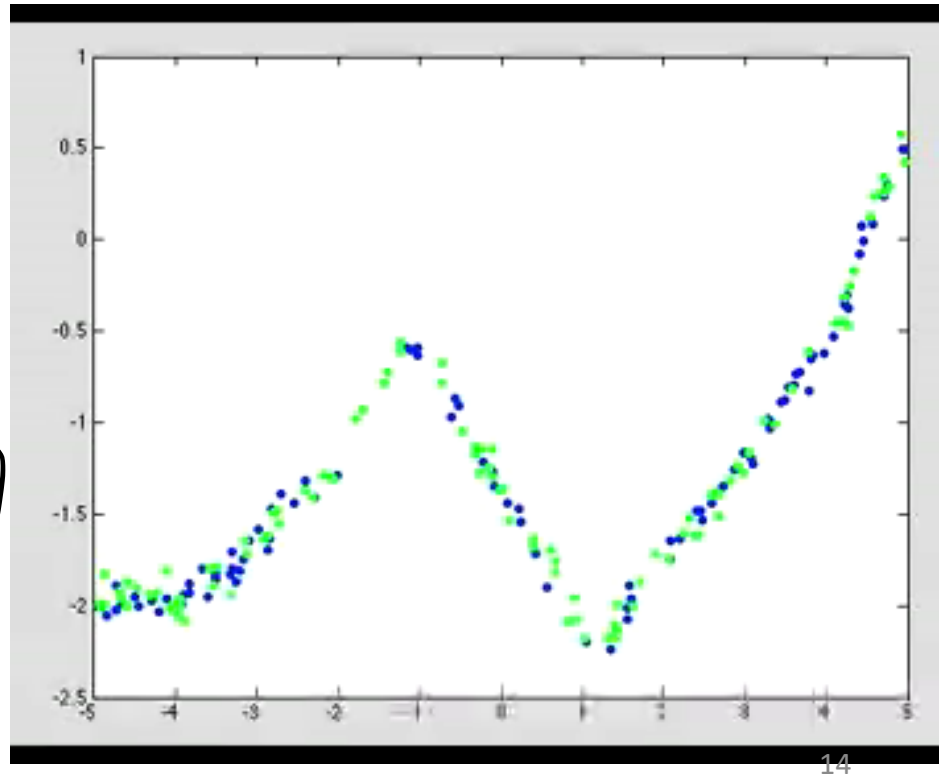
- How do we avoid overfitting with this huge number of features?
  - We regularize 'w' and use validation error to choose σ and λ.

RBFs, Regularization, and Validation

- A model that is hard to beat:
  - RBF basis with L2-regularization and cross-validation to choose σ and λ.
  - Flexible non-parametric basis, magic of regularization, and tuning for test error.

for each value of λ and σ:

- Compute Z on training data (and σ)
- Compute best v: $v = (Z^T Z + \lambda I)^{-1} Z^T y$
- Compute $\tilde{Z}$ on validation data (using train data distances)
- Make predictions $\hat{y} = \underset{t \times n}{\tilde{Z}} \underset{n \times 1}{v}$
- Compute validation error $\|\hat{y} - \tilde{y}\|^2$



RBFs, Regularization, and Validation

- A model that is hard to beat:
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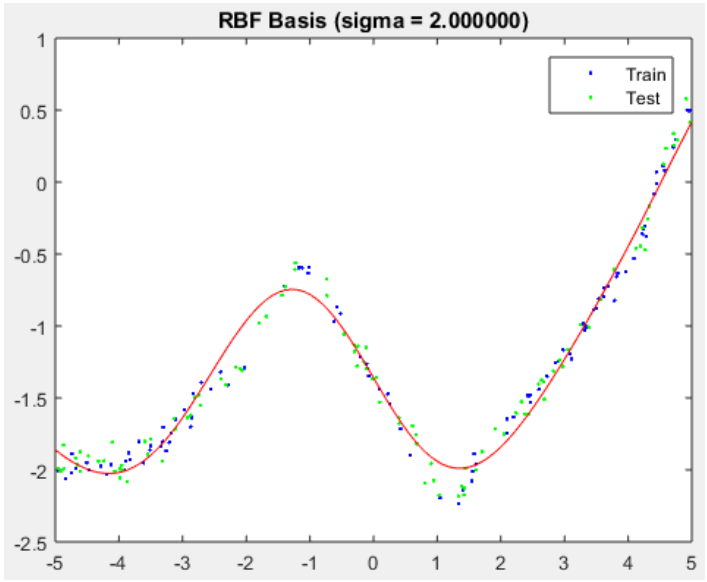
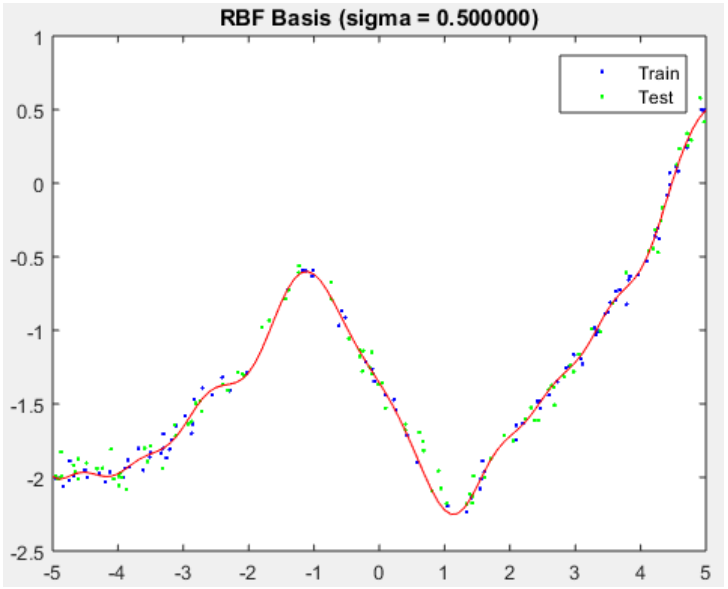
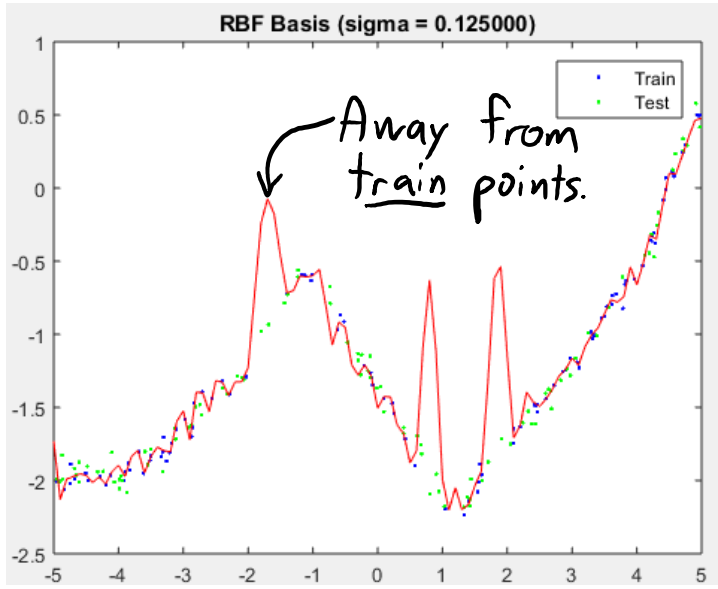






  - Expensive at test time: needs distance to all training examples.

Hyper-Parameter Optimization

- In this setting we have 2 hyper-parameters (σ and λ).
- More complicated models have even more hyper-parameters.
  - This makes searching all values expensive (increases over-fitting risk).

- Leads to the problem of hyper-parameter optimization.
  - Try to efficiently find "best" hyper-parameters.

- Simplest approaches:
  - Exhaustive search: try all combinations among a fixed set of σ and λ values.
  - Random search: try random values.

Hyper-Parameter Optimization

- Other common hyper-parameter optimization methods:
  - Exhaustive search with pruning:
    - If it "looks" like test error is getting worse as you decrease λ, stop decreasing it.
  - Coordinate search:
    - Optimize one hyper-parameter at a time, keeping the others fixed.
    - Repeatedly go through the hyper-parameters
  - Stochastic local search:
    - Generic global optimization methods (simulated annealing, genetic algorithms, etc.).
  - Bayesian optimization (Mike's PhD research topic):
    - Use RBF regression to build model of how hyper-parameters affect validation error.
    - Try the best guess based on the model.

(pause)

Previously: Search and Score

- We talked about search and score for feature selection:
  - Define a "score" and "search" for features with the best score.
- Usual scores count the number of non-zeroes ("L0-norm"):

$$f(w) = \frac{1}{2}\|Xw - y\|^2 + \lambda \|w\|_0$$

number of non-zeroes in 'w'

- But it's hard to find the 'w' minimizing this objective.
- We discussed forward selection, but requires fitting $O(d^2)$ models.
  - For robust regression, need to run gradient descent $O(d^2)$ times.
  - With regularization, need to search for lambda $O(d^2)$ times.

L1-Regularization

- Consider regularizing by the L1-norm:

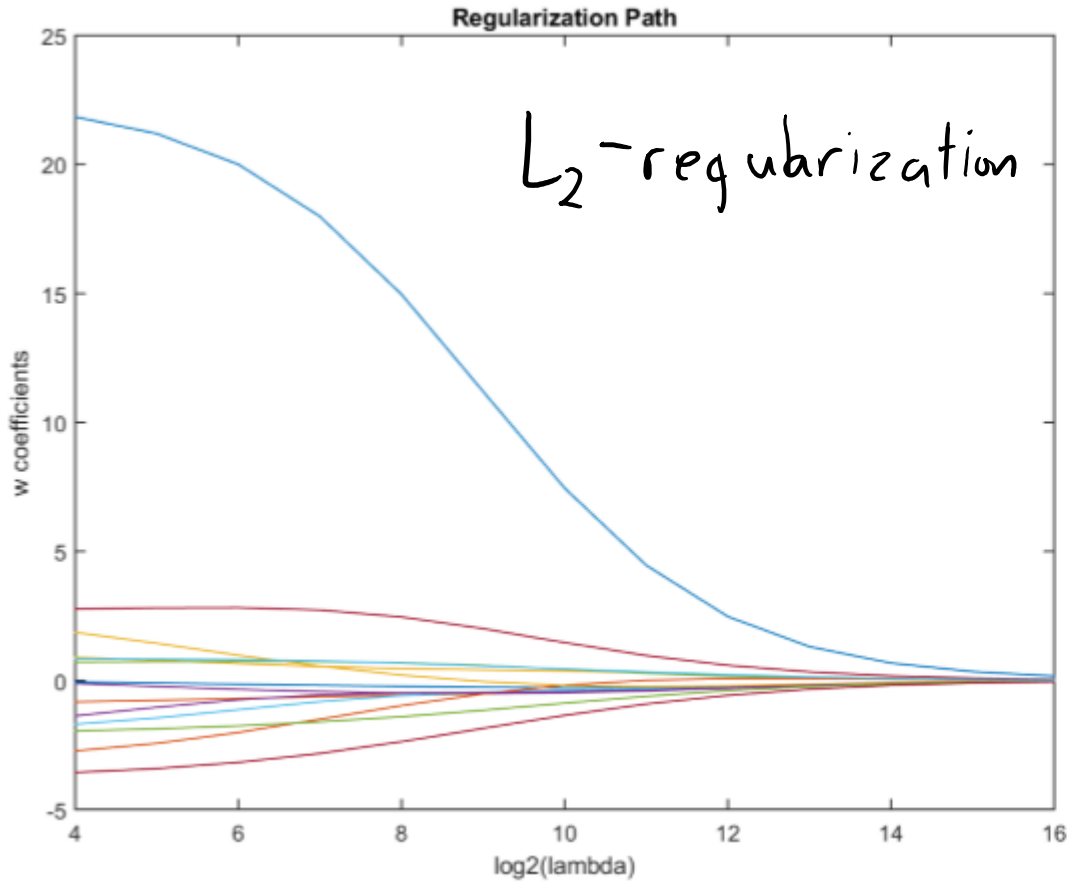
$$f(w) = \frac{1}{2}\|Xw - y\|^2 + \lambda\|w\|_1$$

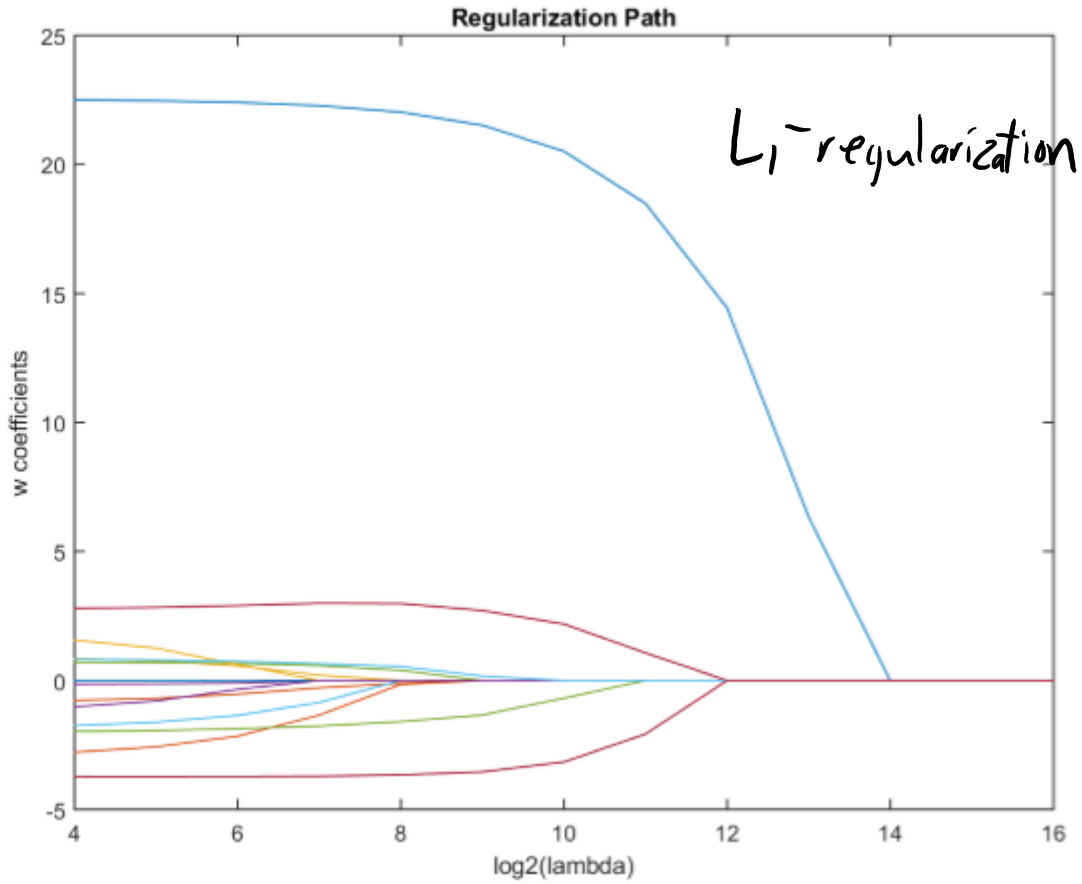
- Like L2-norm, it's convex and improves our test error.
- Like L0-norm, it encourages elements of 'w' to be exactly zero.

- L1-regularization simultaneously regularizes and selects features.
  - Very fast alternative to search and score.
  - Sometimes called "LASSO" regularization.

L2-Regularization vs. L1-Regularization

- Regularization path of w_i values as 'λ' varies:





Regularizers and Sparsity

- L1-regularization give sparsity but L2-regularization doesn't.
  - But don't they both shrink variables to zero?
- Consider problem where 3 vectors can get minimum training error:

$$w^1 = \begin{bmatrix} 100 \\ 0.02 \end{bmatrix} \qquad w^2 = \begin{bmatrix} 100 \\ 0 \end{bmatrix} \qquad w^3 = \begin{bmatrix} 99.99 \\ 0.02 \end{bmatrix}$$

- Without regularization, we could choose any of these 3.
  - They all have same error, so regularization will "break tie".
- With L0-regularization, we would choose w^2:

$$\|w^1\|_0 = 2 \qquad \|w^2\|_0 = 1 \qquad \|w^3\|_0 = 2$$

Regularizers and Sparsity

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- With L2-regularization, we would choose w^3:

$$\|w^1\|^2 = 100^2 + 0.02^2 = 10000.0004 \qquad \|w^2\|^2 = 100^2 + 0^2 = 10000 \qquad \|w^3\|^2 = 99.99^2 + 0.02^2 = 9998.0005$$

- L2-regularization focuses on decreasing largest (makes w_j similar).

Regularizers and Sparsity

- L1-regularization give sparsity but L2-regularization doesn't.
  - But don't they both shrink variables to zero?
- Consider problem where 3 vectors can get minimum training error:

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- With L1-regularization, we would choose w^2:

$$\|w^1\|_1 = 100 + 0.02 = 100.02 \qquad \|w^2\|_1 = 100 + 0 = 100 \qquad \|w^3\|_1 = 99.99 + 0.02 = 100.01$$

- L1-regularization focuses on decreasing all w_j until they are 0.

Why doesn't L2-Regularization set variables to 0?

- Consider an L2-regularized least squares problem with 1 feature:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(wx_i - y_i)^2 + \frac{\lambda}{2}w^2$$

- Let's solve for the optimal 'w':

$$f'(w) = \sum_{i=1}^{n} x_i(wx_i - y_i) + \lambda w$$

Set equal to 0:

$$\sum_{i=1}^{n} x_i^2 w - \sum_{i=1}^{n} x_i y_i + \lambda w = 0$$

re-arrange

$$w\left(\underbrace{\sum_{i=1}^{n} x_i^2}_{\|x\|^2} + \lambda\right) = \underbrace{\sum_{i=1}^{n} x_i y_i}_{y^T x}$$

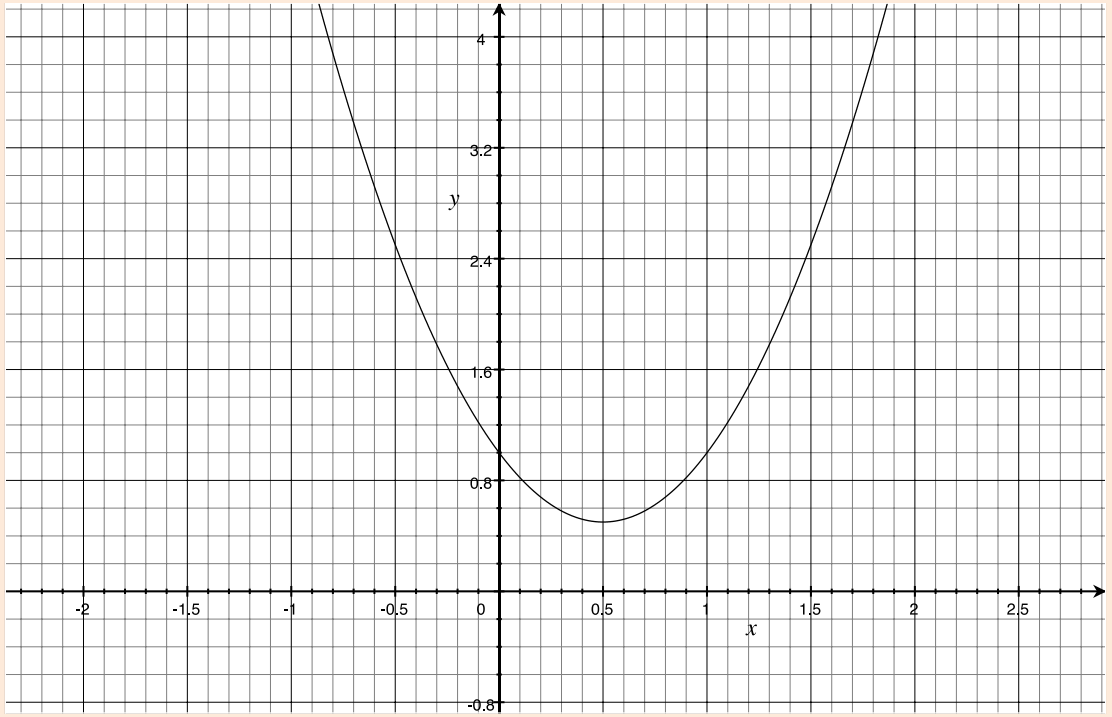
or

$$w = \frac{y^T x}{\|x\|^2 + \lambda}$$

- So as λ gets bigger, 'w' converges to 0.
- However, for all finite λ 'w' will be non-zero unless $y^T x = 0$ exactly.
  - But it's very unlikely that $y^T x$ will be exactly zero.

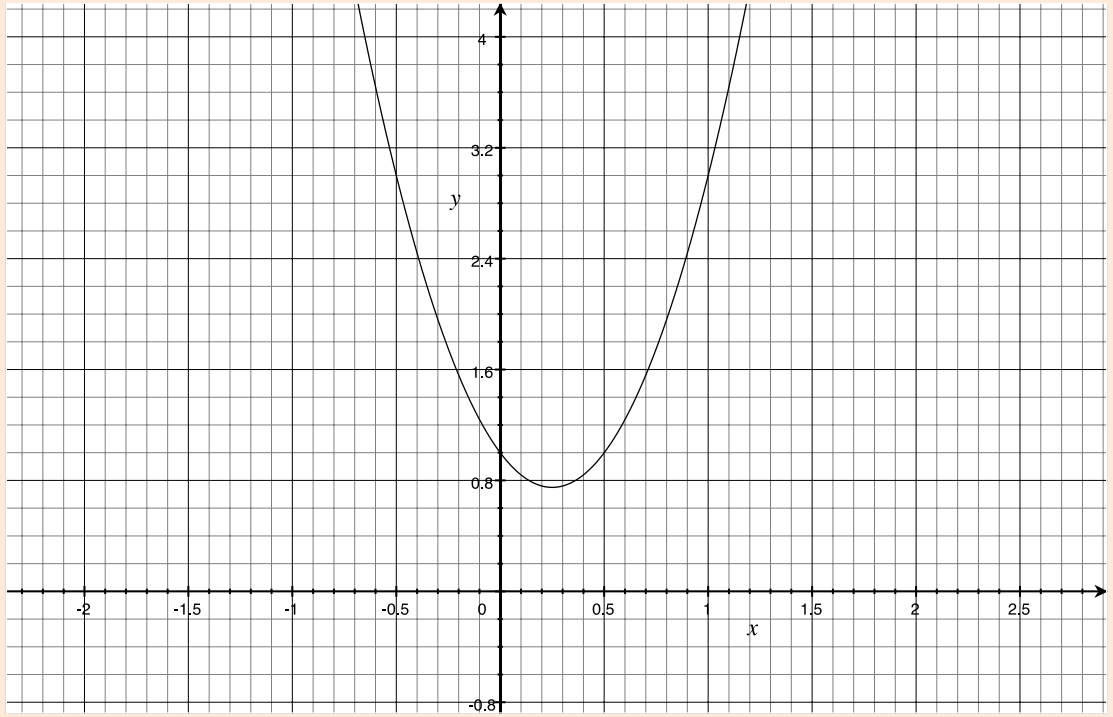
Why doesn't L2-Regularization set variables to 0?

- Small λ



- Solution further from zero

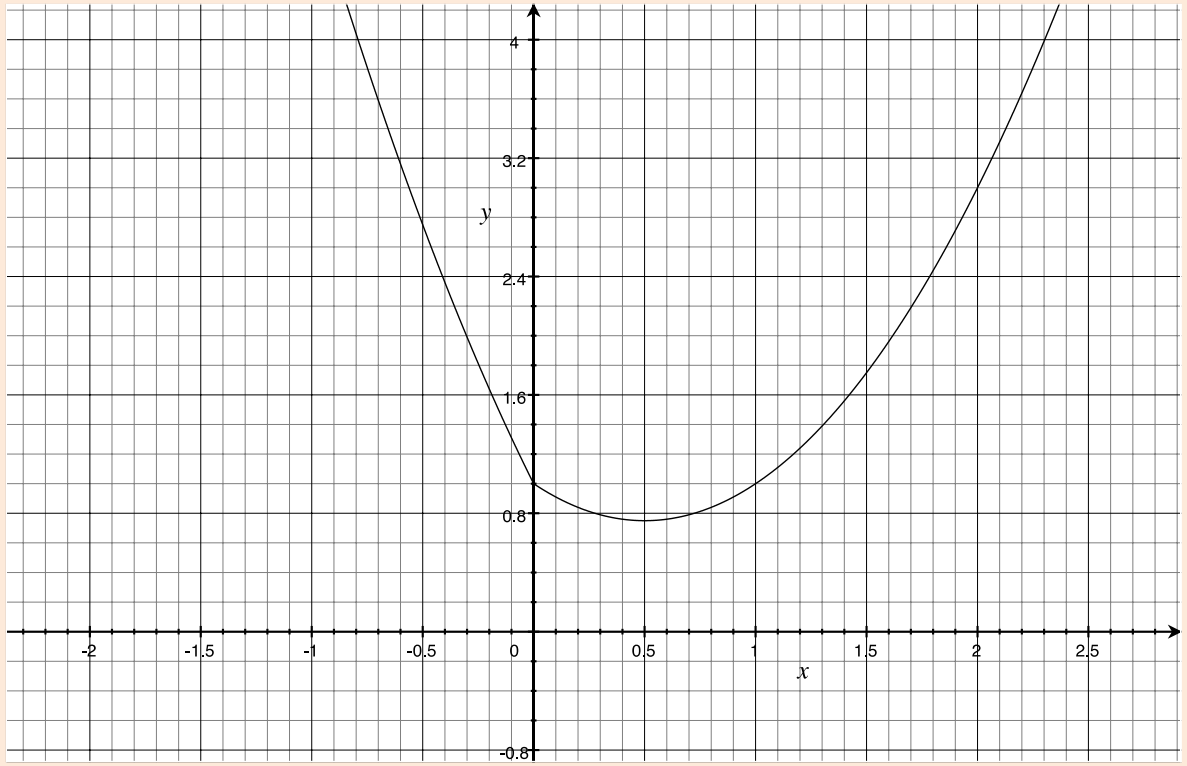
Big λ



Solution closer to zero
(but not exactly 0)

Why does L1-Regularization set things to 0?

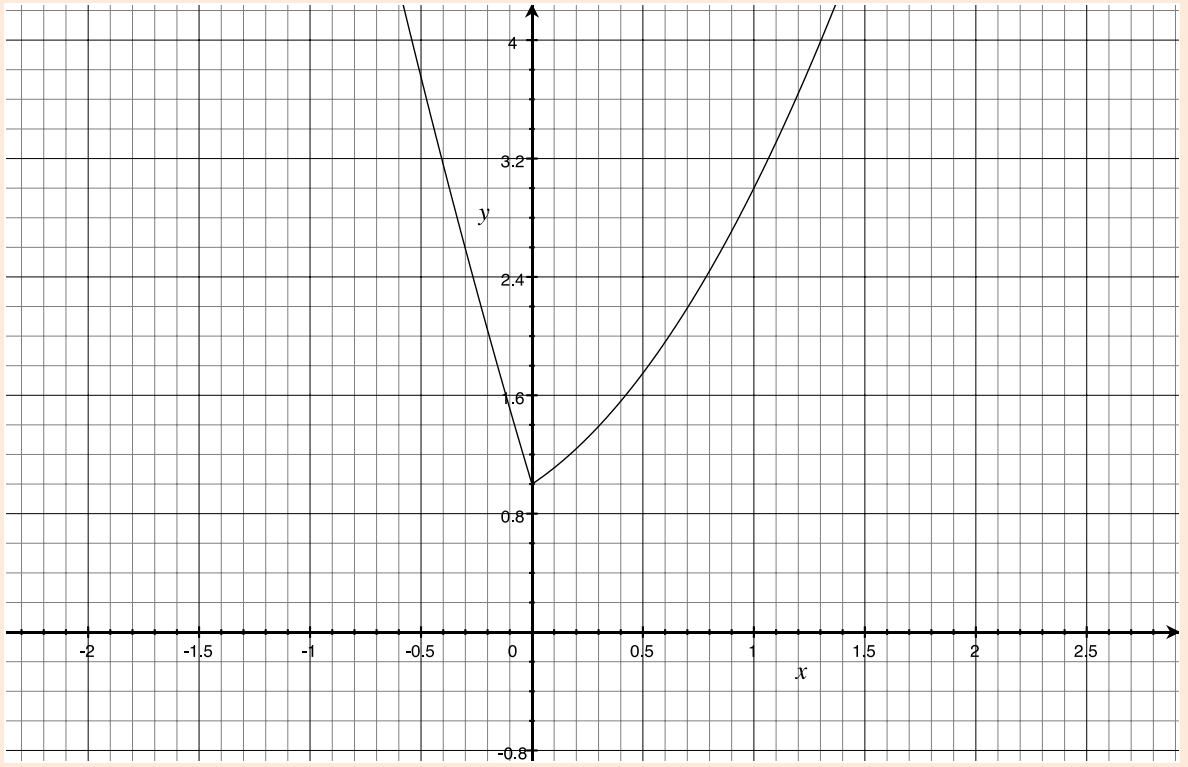
- Small λ



- Solution nonzero

(minimum of left parabola is past origin, but right parabola is not)

Big λ



Solution exactly zero

(minimum of both parabola are past the origin)

Why does L1-Regularization set things to 0?

- Consider an L1-regularized least squares problem with 1 feature:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(wx_i - y_i)^2 + \lambda|w|$$

- If (w = 0), then "left" limit and "right" limit are given by:

$$f^-(0) = \sum_{i=1}^{n} x_i(0x_i - y_i) - \lambda = \sum_{i=1}^{n} x_i y_i - \lambda$$

$$f^+(0) = \sum_{i=1}^{n} x_i(0x_i - y_i) + \lambda = \sum_{i=1}^{n} x_i y_i + \lambda$$

- So which direction should "gradient descent" go in?

— $f^-(0) = -y^Tx + \lambda$ } If these are positive $(-y^Tx > \lambda)$,
— $f^+(0) = -y^Tx - \lambda$ } we can improve by increasing 'w'.

If these are negative $(y^Tx > \lambda)$, we can improve by decreasing 'w'.

} But if left and right "gradient descent" directions point in opposite directions $(|y^Tx| \leq \lambda)$, minimum is 0.

L2-regularization vs. L1-regularization

- So with 1 feature:
  - L2-regularization only sets ‘w’ to 0 if $y^Tx = 0$.
    - There is a only a single possible y^Tx value where the variable gets set to zero.
    - And λ has nothing to do with the sparsity.
  - L1-regularization sets ‘w’ to 0 if $|y^Tx| \leq \lambda$.
    - There is a range of possible y^Tx values where the variable gets set to zero.
    - And increasing λ increases the sparsity since the range of y^Tx grows.
- Note that it’s important that the function is non-differentiable:
  - Differentiable regularizers penalizing size would need $y^Tx = 0$ for sparsity.

L2-Regularization vs. L1-Regularization

- L2-Regularization:
  - Insensitive to changes in data.
  - Decreased variance:
    - Lower test error.
  - Closed-form solution.
  - Solution is unique.
  - All ‘w’ tend to be non-zero.
  - Can learn with *linear* number of irrelevant features.
    - E.g., only O(d) relevant features.

- L1-Regularization:
  - Insensitive to changes in data.
  - Decreased variance:
    - Lower test error.
  - Requires iterative solver.
  - Solution is not unique.
  - Many ‘w’ tend to be zero.
  - Can learn with **exponential** number of irrelevant features.
    - E.g., only O(log(d)) relevant features.

    Paper on this result by Andrew Ng

L1-loss vs. L1-regularization

- Don't confuse the L1 loss with L1-regularization!
  - L1-loss is robust to outlier data points.
    - You can use this instead of removing outliers.
  - L1-regularization is robust to irrelevant features.
    - You can use this instead of removing features.
- And note that you can be robust to outliers and select features:

$$f(w) = \underbrace{\|Xw - y\|_1}_{L_1\text{-loss}} + \underbrace{\lambda \|w\|_1}_{L_1\text{-regularizer}}$$

- Why aren't we smoothing and using "Huber regularization"?
  - Huber regularizer is still robust to irrelevant features.
  - But it's the non-smoothness that sets weights to exactly 0.

Summary

- Radial basis functions:
  - Non-parametric bases that can model any function.
- L1-regularization:
  - Simultaneous regularization and feature selection.
  - Robust to having lots of irrelevant features.

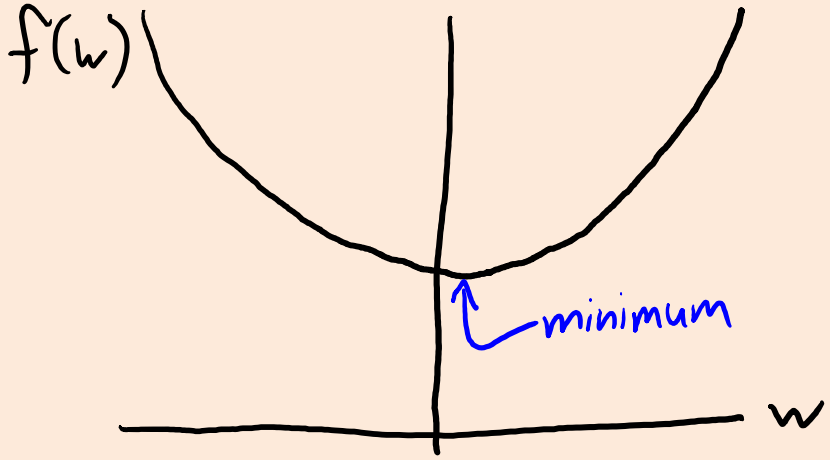
- Next time: are we really going to use regression for classification?

Sparsity and Least Squares

- Consider 1D least squares objective:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w x_i - y_i)^2$$

- This is a convex 1D quadratic function of 'w' (i.e., a parabola):



- This variable does not look relevant (minimum is close to 0).
  - But for finite 'n' the minimum is unlikely to be exactly zero.

$f'(0) = 0$ only happens if $\sum_{i=1} y_i x_i = 0$. (bonus)

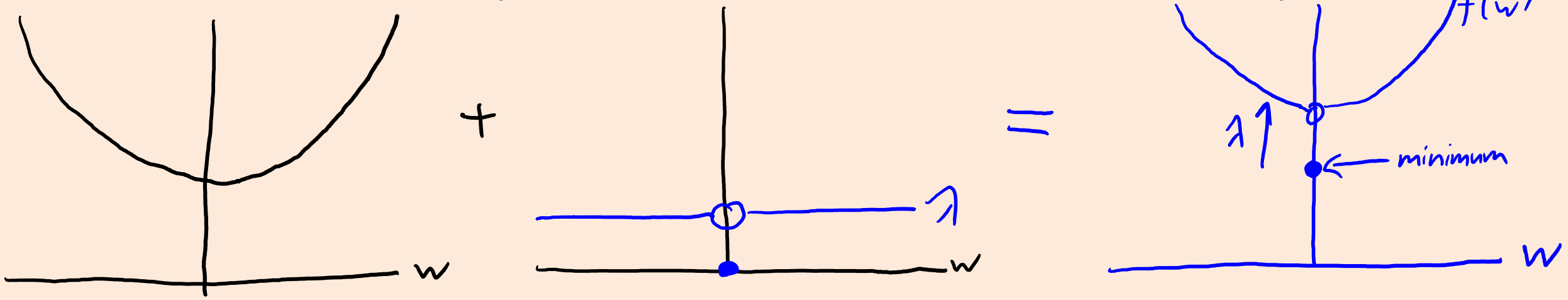
Sparsity and L0-Regularization

- Consider 1D L0-regularized least squares objective:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w x_i - y_i)^2 + \lambda \|w\|_0$$

λ if $w \neq 0$
0 if $w = 0$

- This is a convex 1D quadratic function but with a discontinuity at 0:



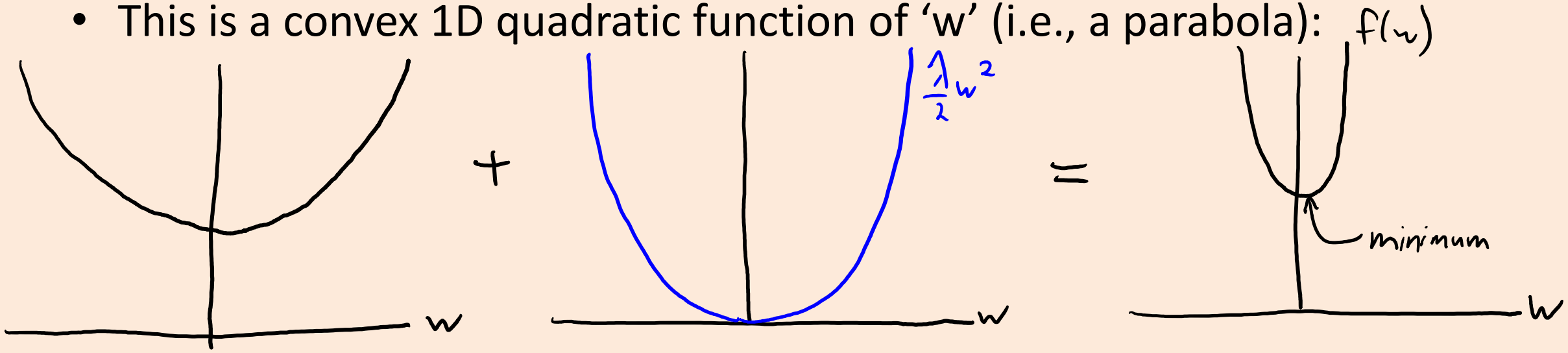
- L0-regularized minimum is often exactly at the 'discontinuity' at 0:
  - Sets the feature to exactly 0 (does feature selection), but is non-convex.

Sparsity and L2-Regularization

- Consider 1D L2-regularized least squares objective:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w x_i - y_i)^2 + \frac{\lambda}{2}w^2$$

- This is a convex 1D quadratic function of 'w' (i.e., a parabola):



- L2-regularization moves it closer to zero, but not all the way to zero.
  - It doesn't do feature selection ("penalty goes to 0 as slope goes to 0").

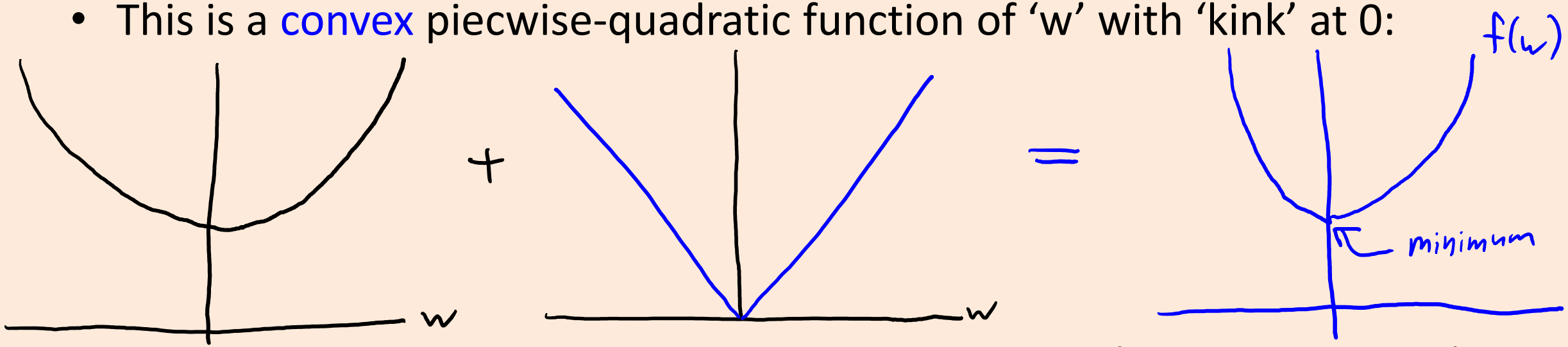
$f'(0) = 0$ only if $\sum_{i=1}^{n} y_i x_i = 0$

Sparsity and L1-Regularization

- Consider 1D L1-regularized least squares objective:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w x_i - y_i)^2 + \lambda|w|$$

- This is a convex piecewise-quadratic function of 'w' with 'kink' at 0:



- L1-regularization tends to set variables to exactly 0 (feature selection).
  - Penalty on slope is λ even if you are close to zero.
  - Big λ selects few features, small λ allows many features.

→ Happens when $|\sum_{i=1}^{n} x_i y_i| \leq \lambda$ (bonus)

L1-Loss vs. Huber Loss

- The same reasoning tells us the difference between the L1 *loss* and the Huber loss. They are very similar in that they both grow linearly far away from 0. So both are both robust but…
  - With the L1 loss the model often passes exactly through some points.
  - With Huber the model doesn't necessarily pass through any points.

- Why? With L1-regularization we were causing the elements of 'w' to be exactly 0. Analogously, with the L1-loss we cause the elements of 'r' (the residual) to be exactly zero. But zero residual for an example means you pass through that example exactly.

Non-Uniqueness of L1-Regularized Solution

- How can L1-regularized least squares solution not be unique?
  - Isn't it convex?
- Convexity implies that minimum value of f(w) is unique (if exists), but there may be multiple 'w' values that achieve the minimum.

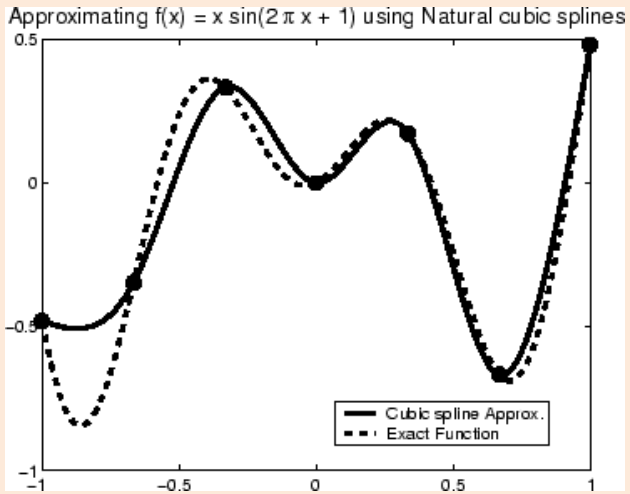
- Consider L1-regularized least squares with d=2, where feature 2 is a copy of a feature 1. For a solution (w_1,w_2) we have:

$$\hat{y}_i = w_1 x_{i1} + w_2 x_{i2} = w_1 x_{i1} + w_2 x_{i1} = (w_1 + w_2) x_{i1}$$

- So we can get the same squared error with different w_1 and w_2 values that have the same sum. Further, if neither w_1 or w_2 changes sign, then $|w_1| + |w_2|$ will be the same so the new w_1 and w_2 will be a solution.

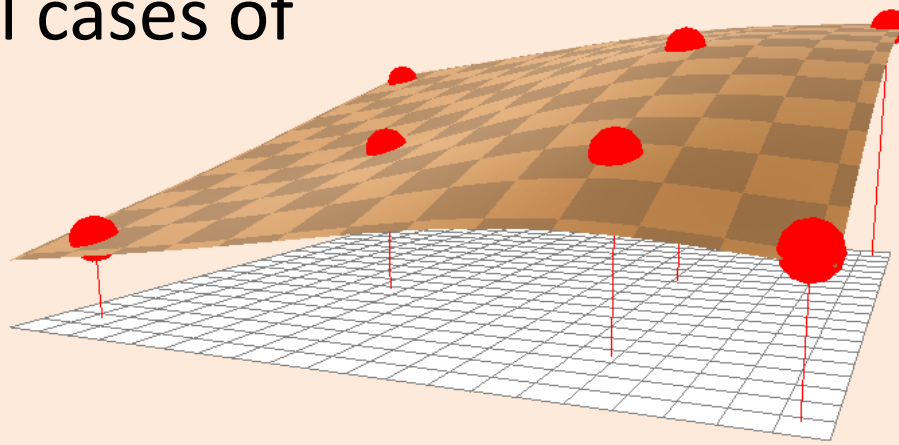
Splines in 1D

- For 1D interpolation, alternative to polynomials/RBFs are splines:
  - Use a polynomial in the region between each data point.
  - Constrain some derivatives of the polynomials to yield a unique solution.
- Most common example is cubic spline:
  - Use a degree-3 polynomial between each pair of points.
  - Enforce that f'(x) and f''(x) of polynomials agree at all point.
  - "Natural" spline also enforces f''(x) = 0 for smallest and largest x.
- Non-trivial fact: natural cubic splines are sum of:
  - Y-intercept.
  - Linear basis.
  - RBFs with $g(\varepsilon) = \varepsilon^3$.
    - Different than Gaussian RBF because it *increases with distance*.



Splines in Higher Dimensions

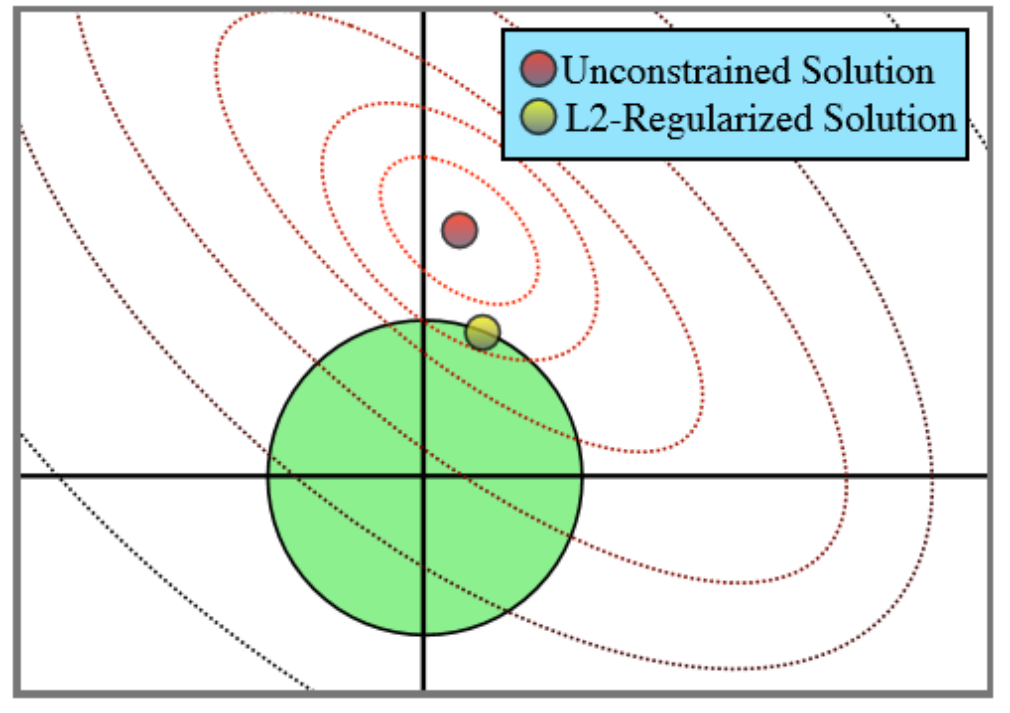
- Splines generalize to higher dimensions if data lies on a grid.
  - Many methods exist for grid-structured data (linear, cubic, splines, etc.).
  - For more general ("scattered") data, there isn't a natural generalization.
- Common 2D "scattered" data interpolation is thin-plate splines:
  - Based on curve made when bending sheets of metal.
  - Corresponds to RBFs with $g(\varepsilon) = \varepsilon^2 \log(\varepsilon)$.
- Natural splines and thin-plate splines: special cases of "polyharmonic" splines:
  - Less sensitive to parameters than Gaussian RBF.



http://step.polymtl.ca/~rv101/thinplates/

L2-Regularization vs. L1-Regularization

- L2-regularization conceptually restricts 'w' to a ball.



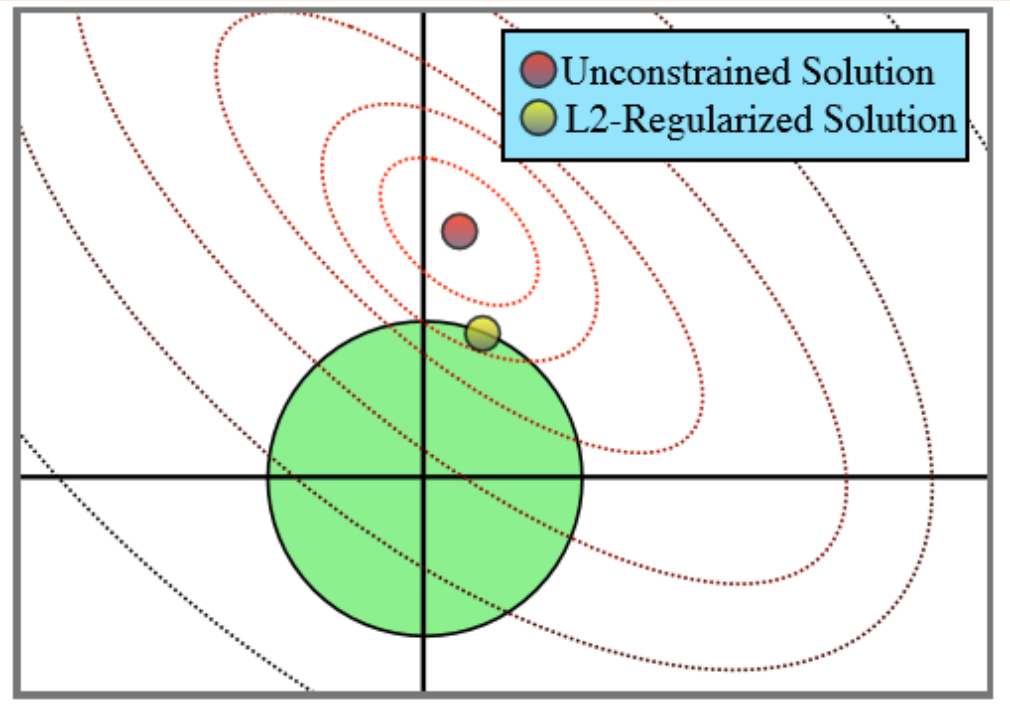
Minimizing $\frac{1}{2}\|Xw-y\|^2 + \frac{\lambda}{2}\|w\|^2$

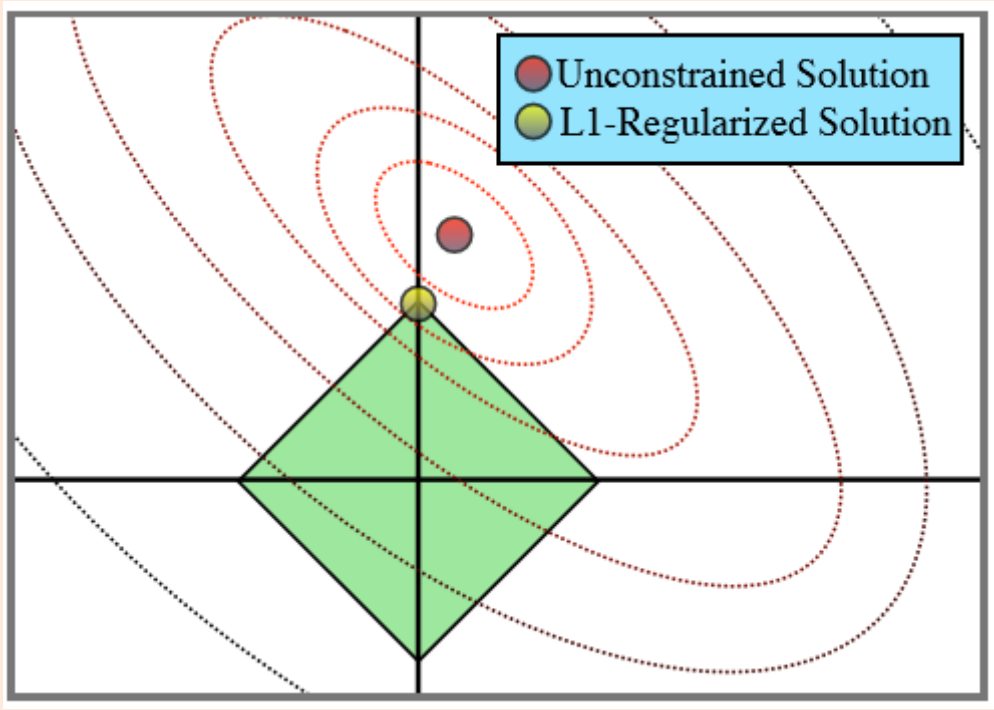
is equivalent to minimizing

$\frac{1}{2}\|Xw-y\|^2$ subject to the constraint that $\|w\| \leq \tau$ for some value 'τ'

L2-Regularization vs. L1-Regularization

- L2-regularization conceptually restricts ‘w’ to a ball.





- L1-regularization restricts to the L1 “ball”:
  - Solutions tend to be at corners where w_j are zero.

Related Infinite Series video