CPSC 340: Machine Learning and Data Mining

More Regularization

Spring 2022 (2021W2)

Last Time: L2-Regularization

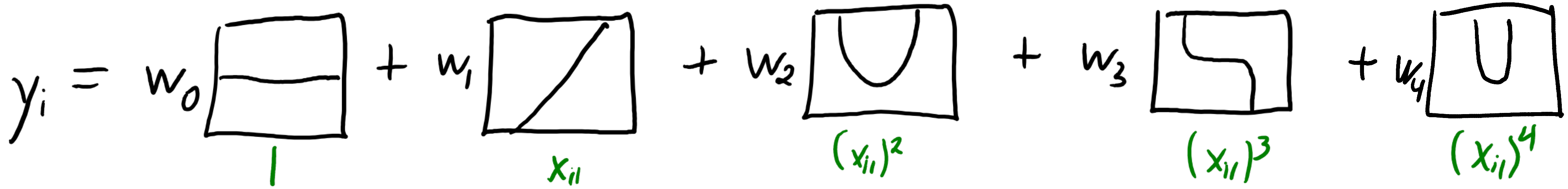
- We discussed regularization:
  - Adding a continuous penalty on the model complexity:

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

  - 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:
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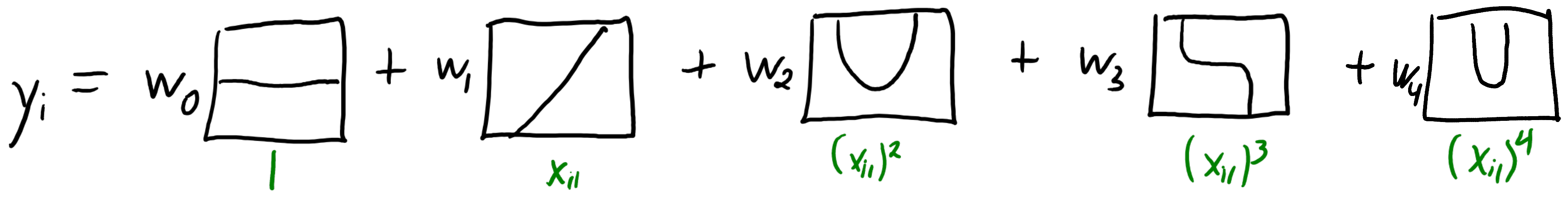

- But polynomials are not the only possible bases:
  - Exponentials, logarithms, trigonometric functions, etc.
  - The right basis will vastly improve performance.
  - If we use the wrong basis, our accuracy is limited even with lots of data.
  - But the right basis may not be obvious.

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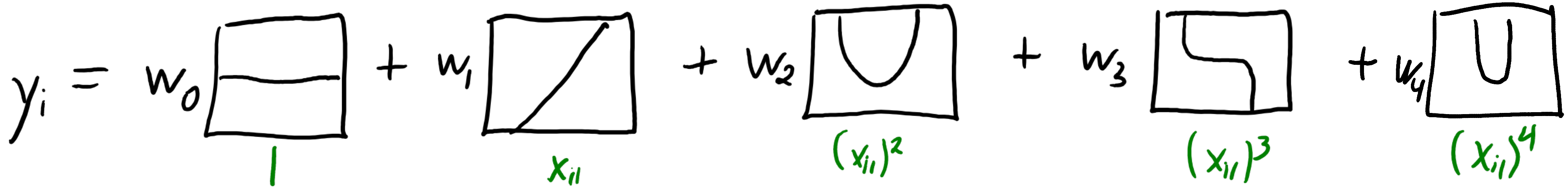

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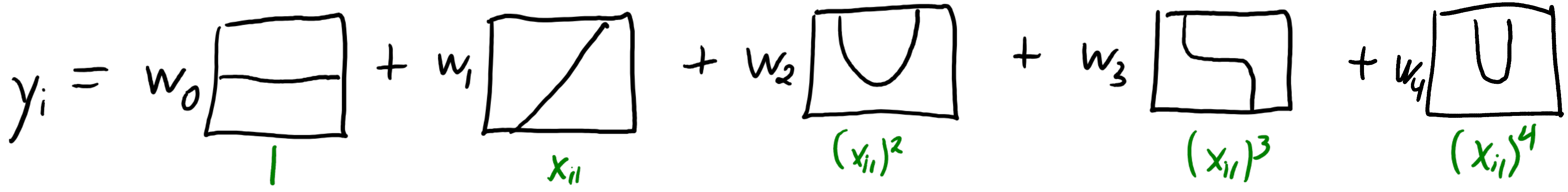
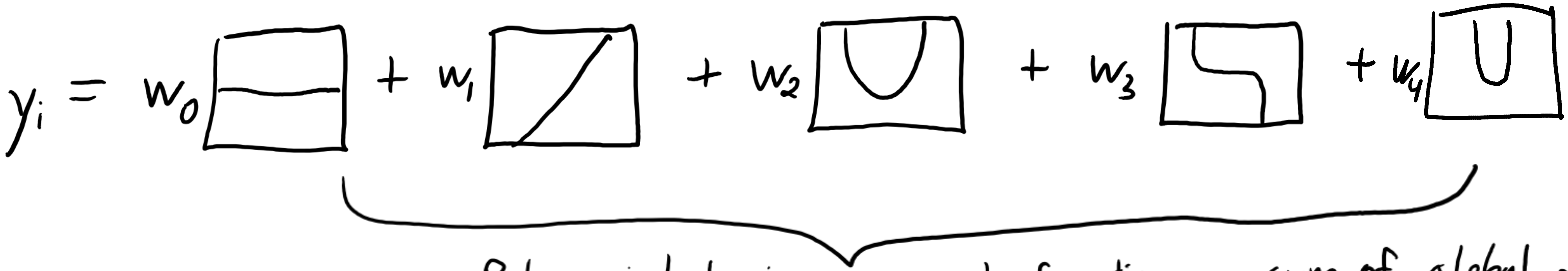


- Alternative is non-parametric bases:
  - Size of basis (number of features) grows with 'n'.
  - Model gets more complicated as you get more data.
  - Can model complicated functions where you don't know the right basis.
    - With enough data.
  - Classic example is "Gaussian RBFs" ("Gaussian" == "normal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

Gaussian RBFs: A Sum of “bumps”



Polynomial basis represents function as sum of <u>global</u> polynomials.

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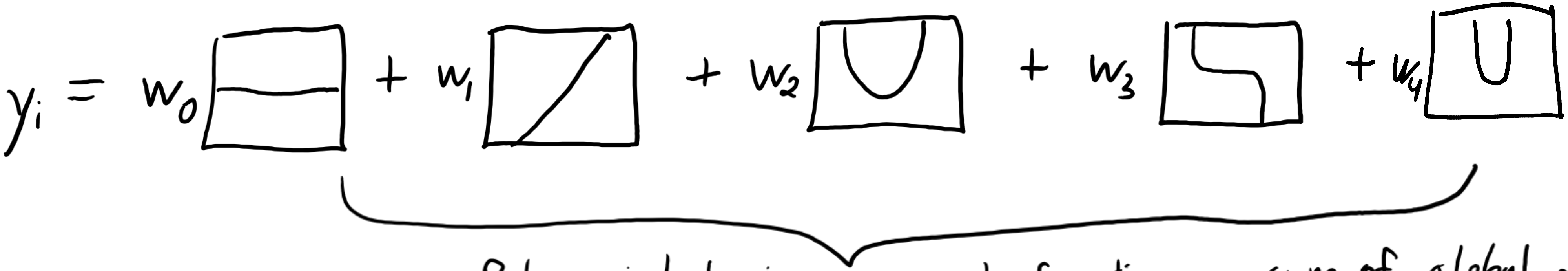

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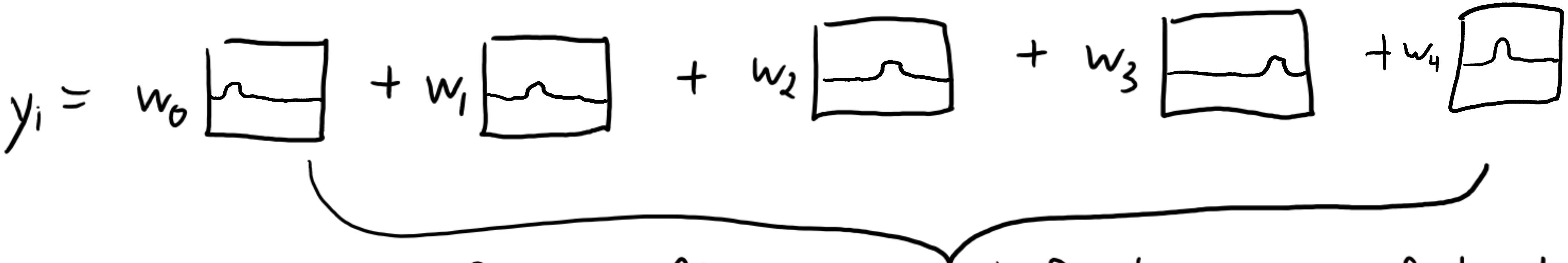

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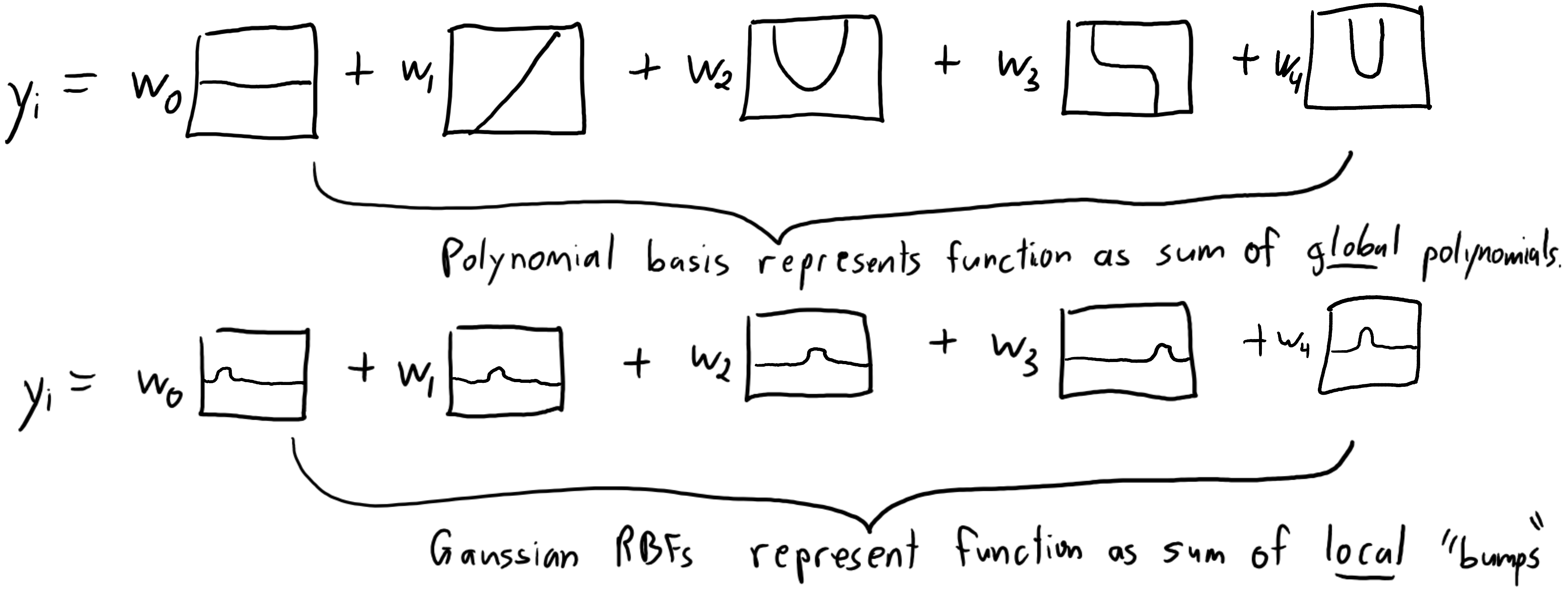

- Gaussian RBFs are universal approximators (on compact subets of $\mathbb{R}^d$)
  - Enough bumps can approximate any continuous function to arbitrary precision.
  - Achieve optimal test error as 'n' goes to infinity.

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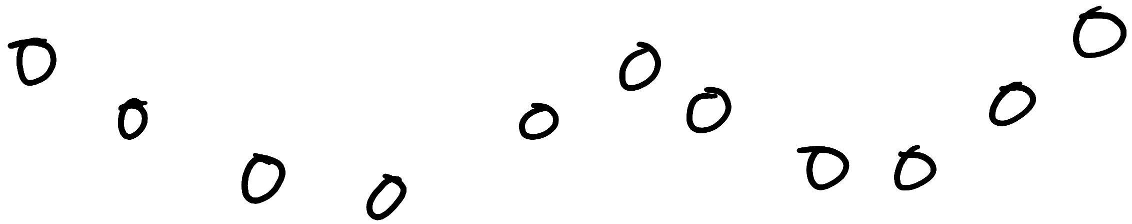

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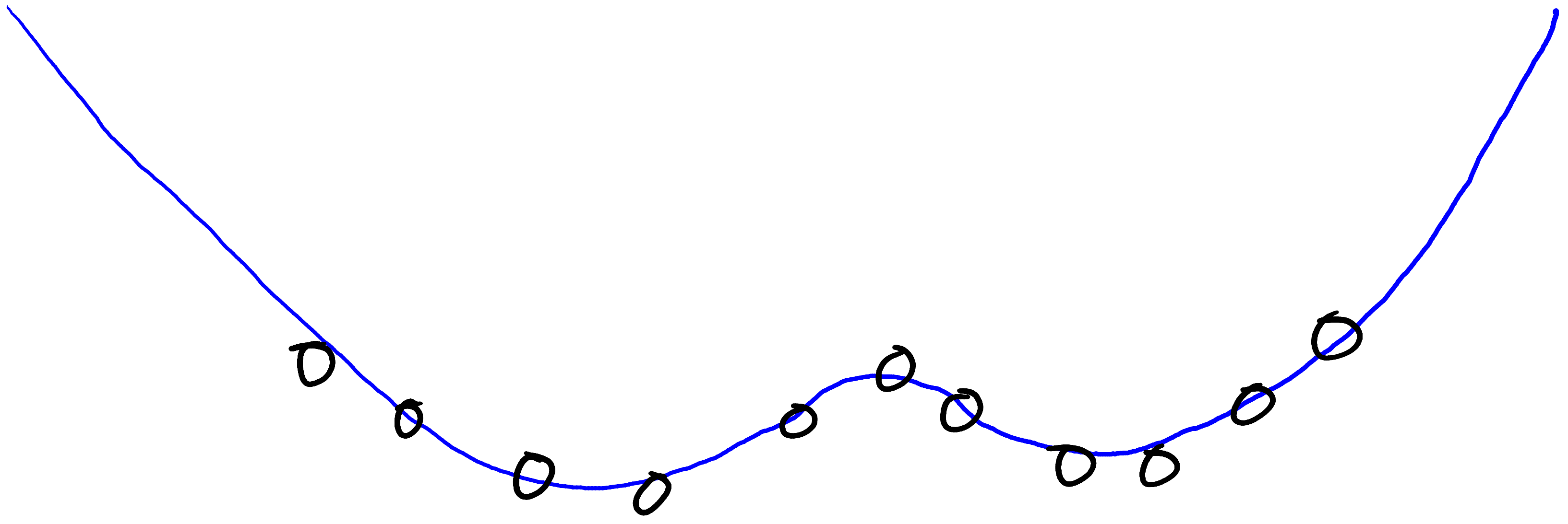

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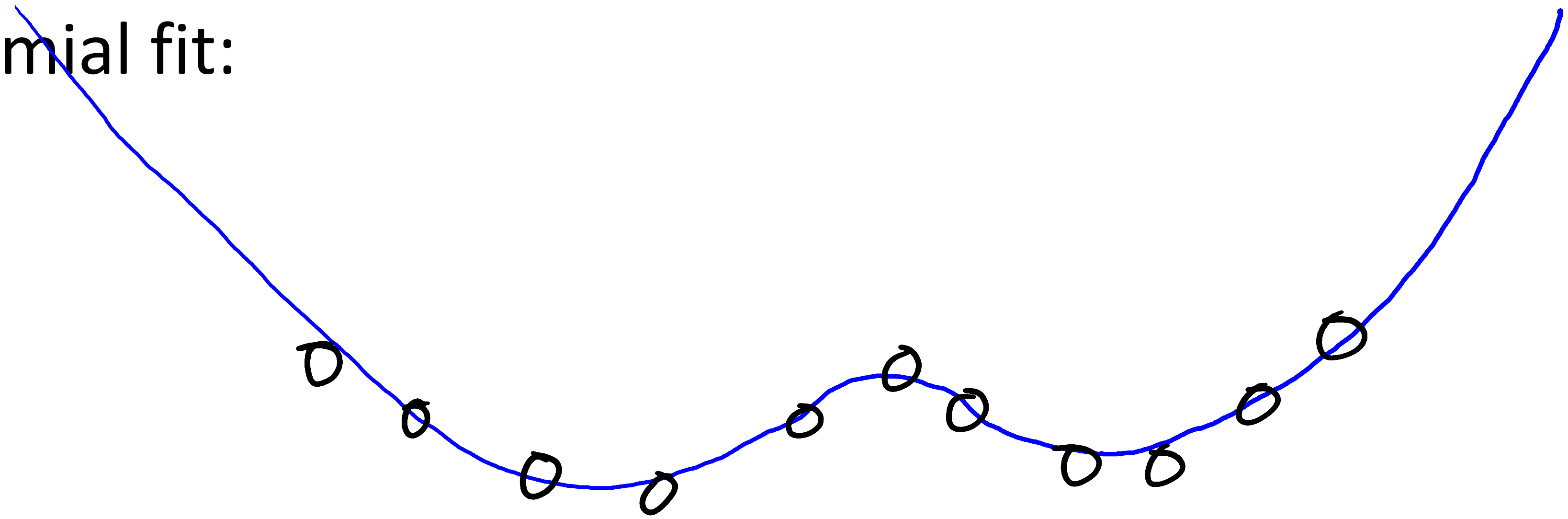
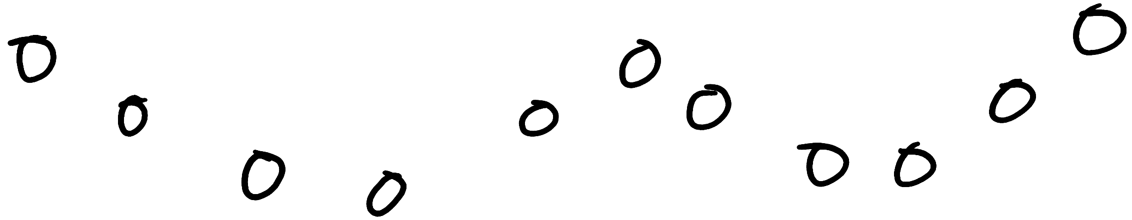


- Constructing a function from bumps ("smooth histogram"):



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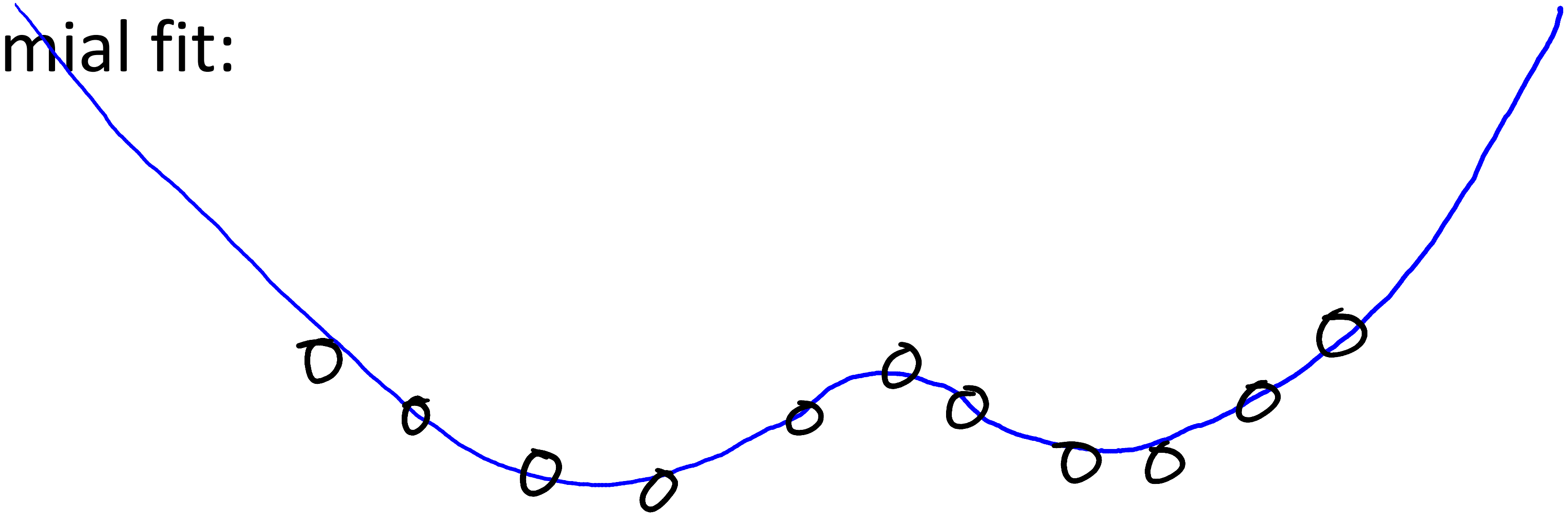

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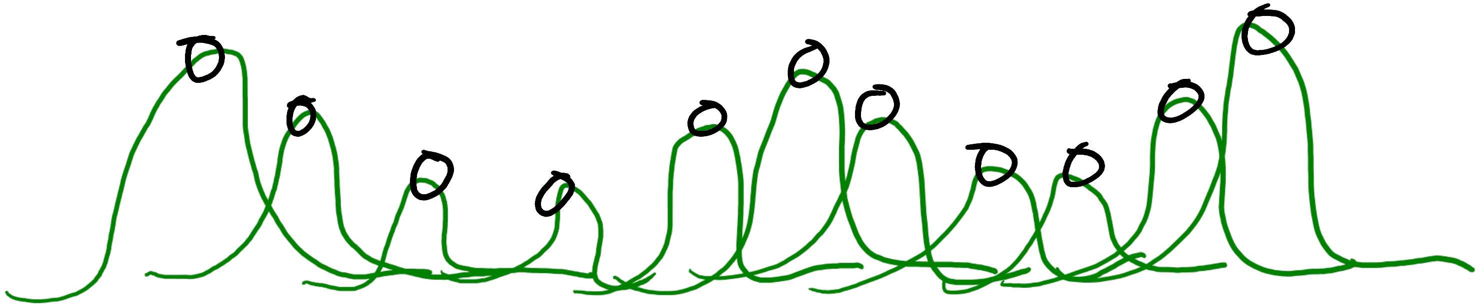

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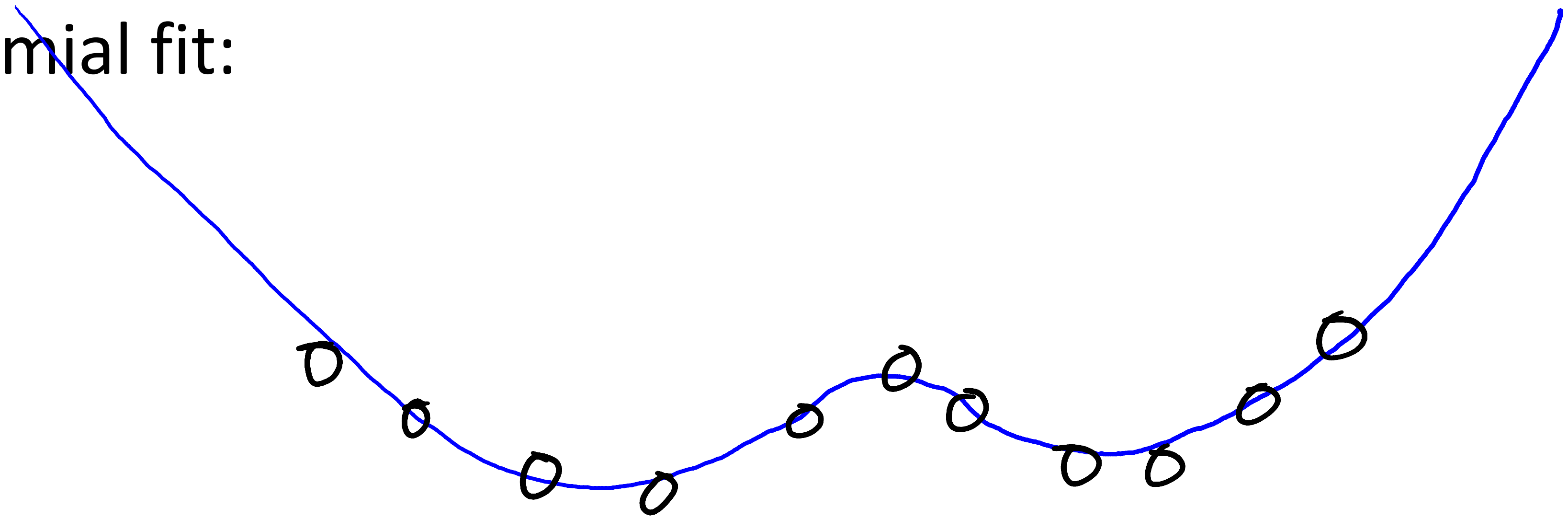

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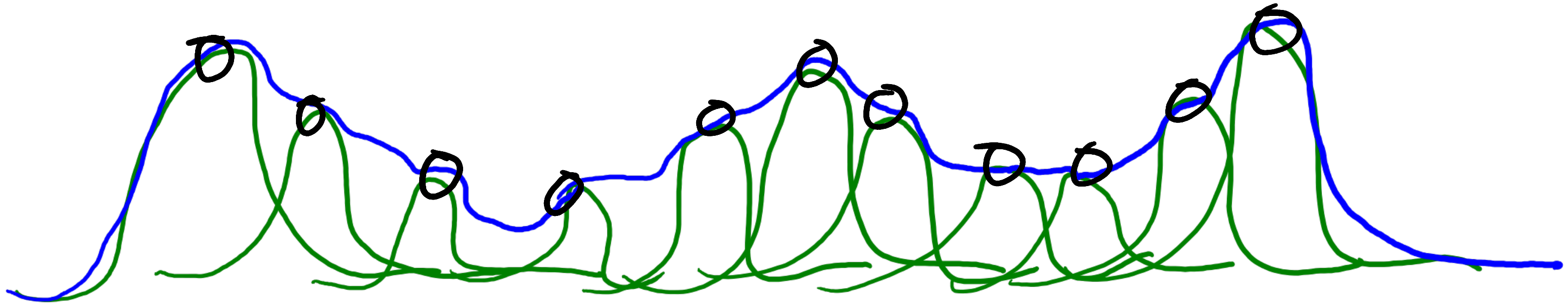

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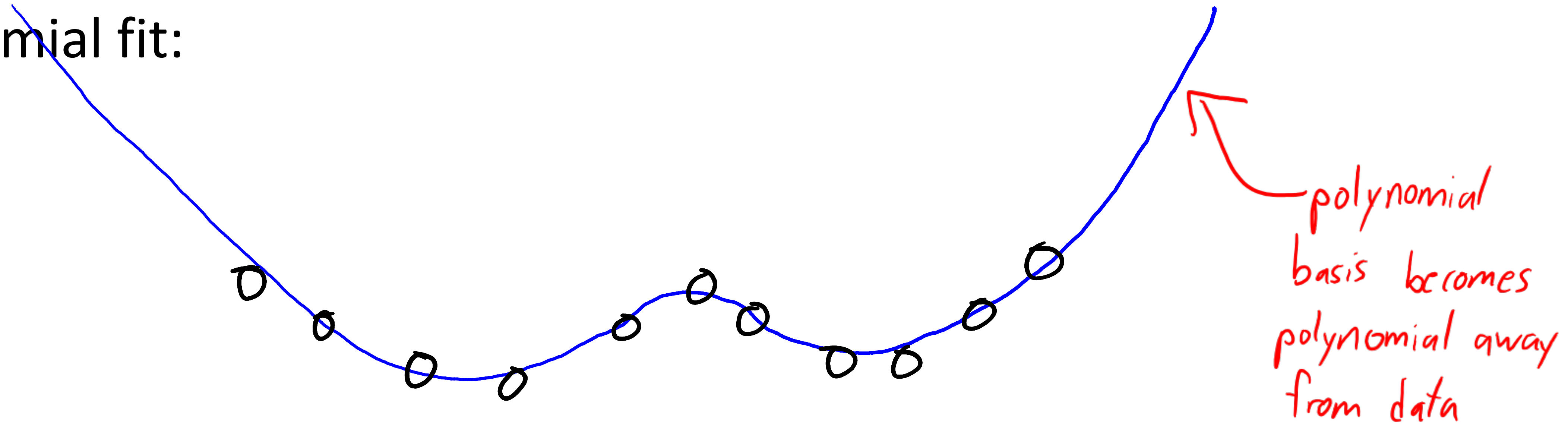

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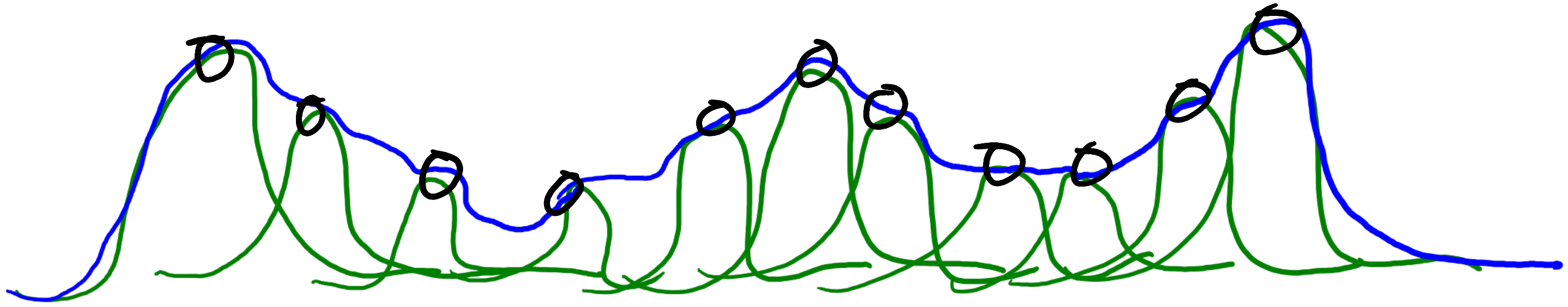

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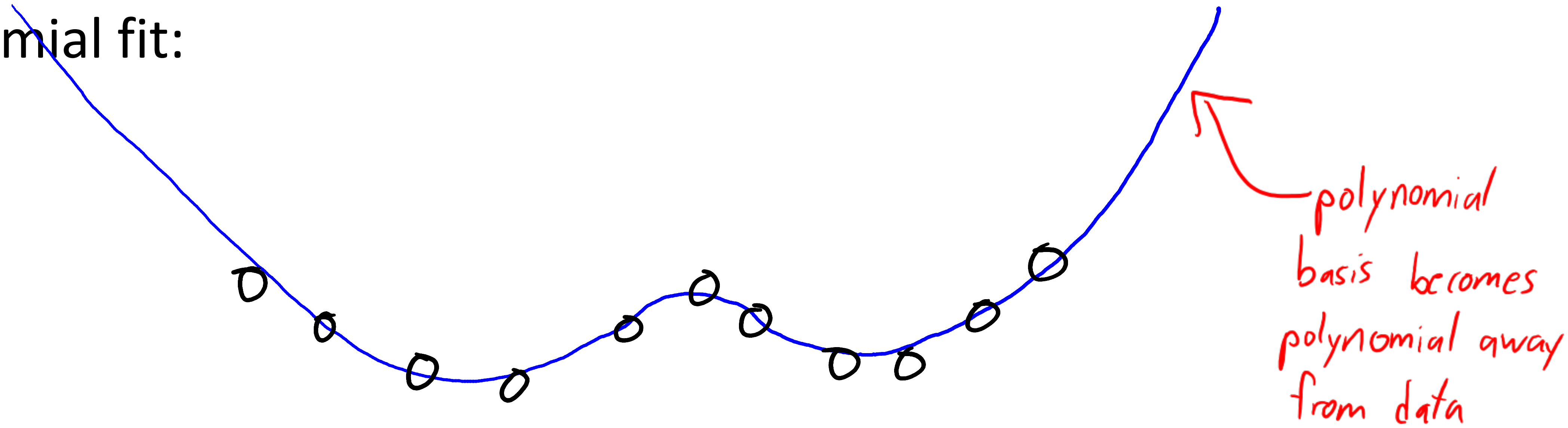

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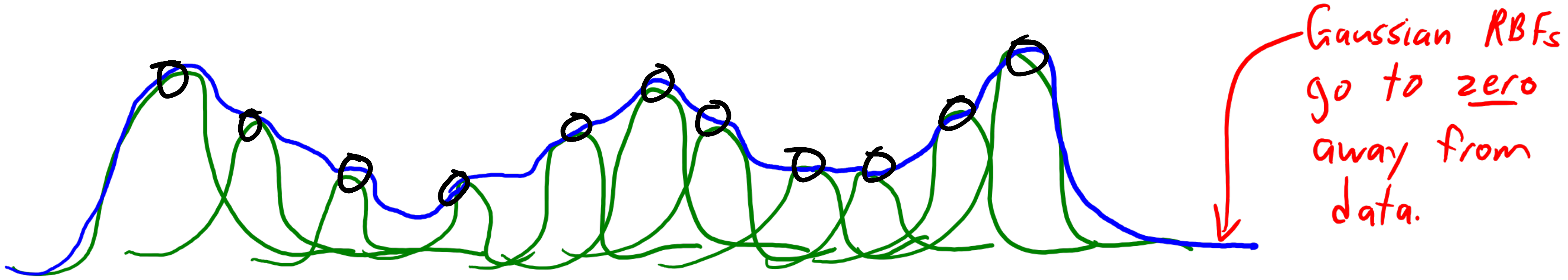

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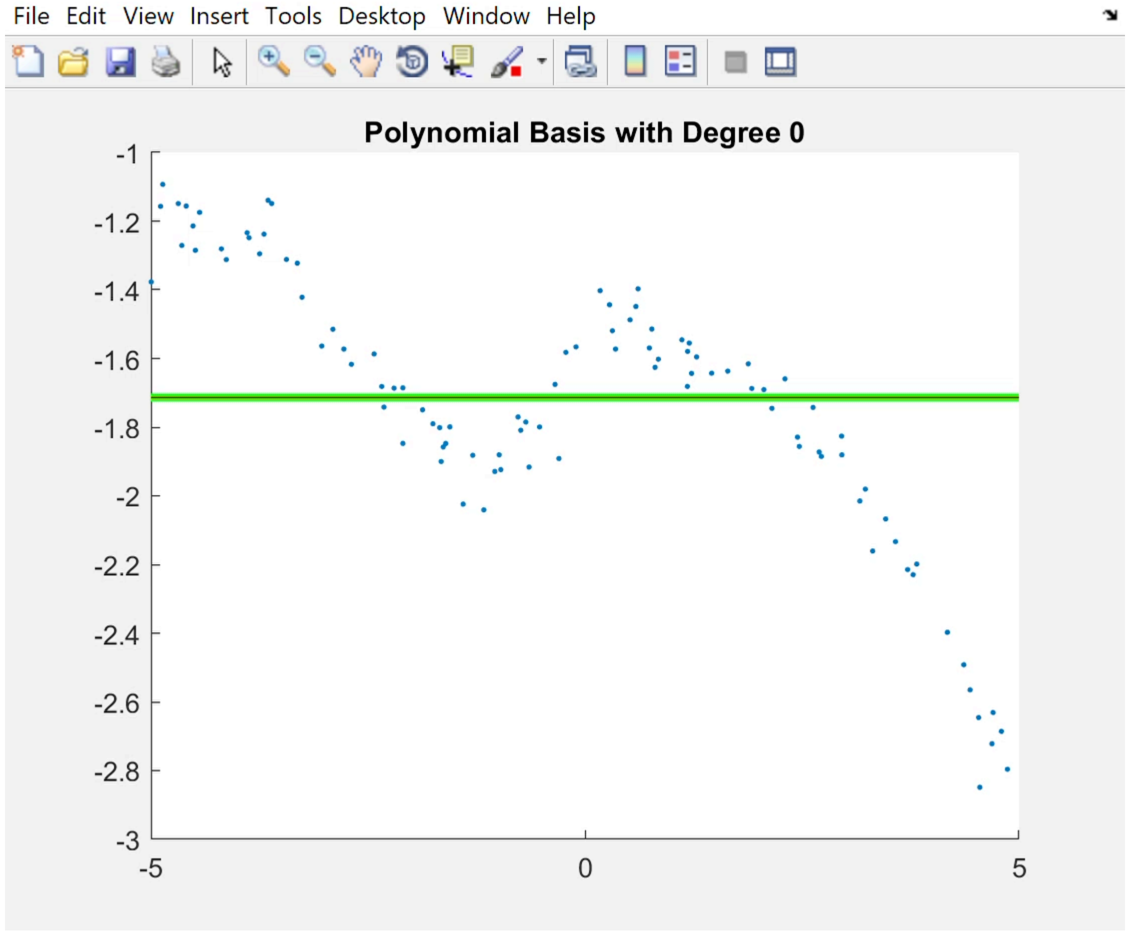

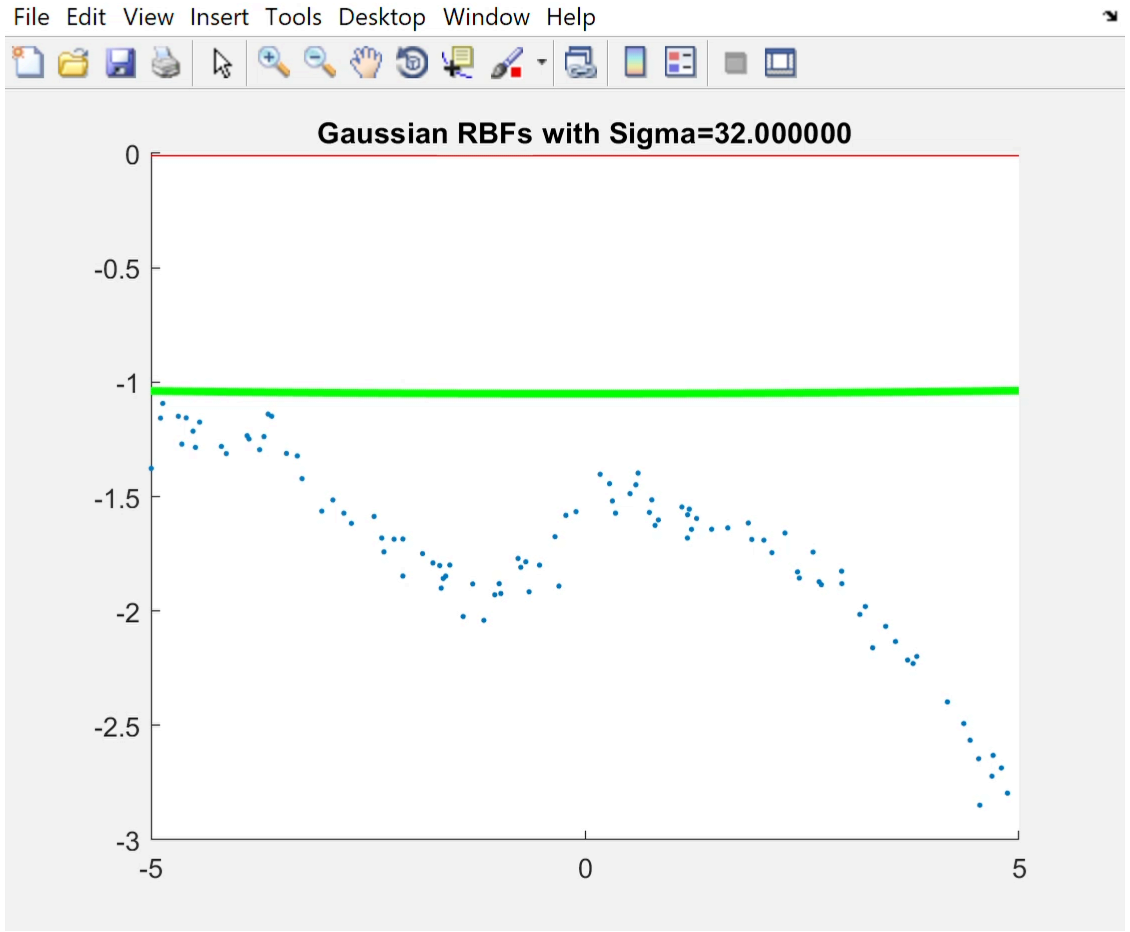

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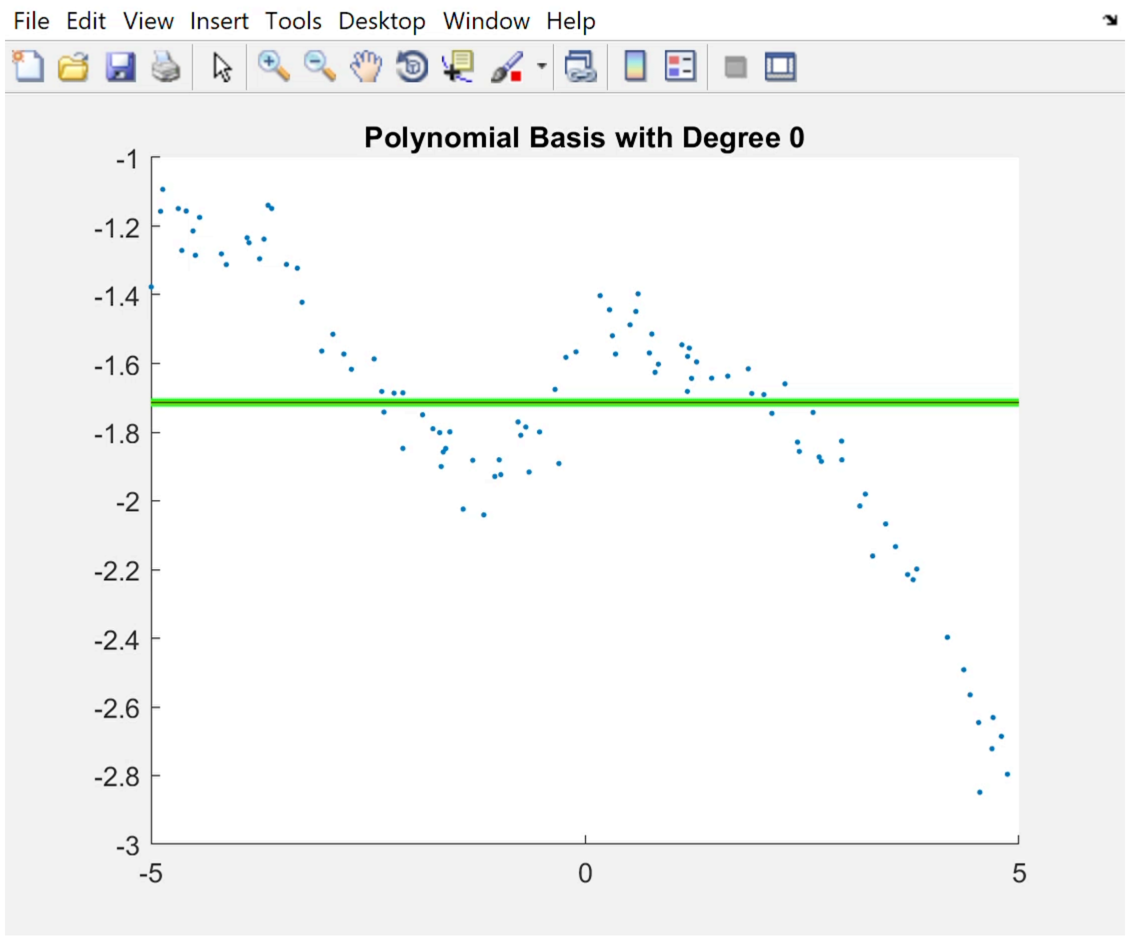

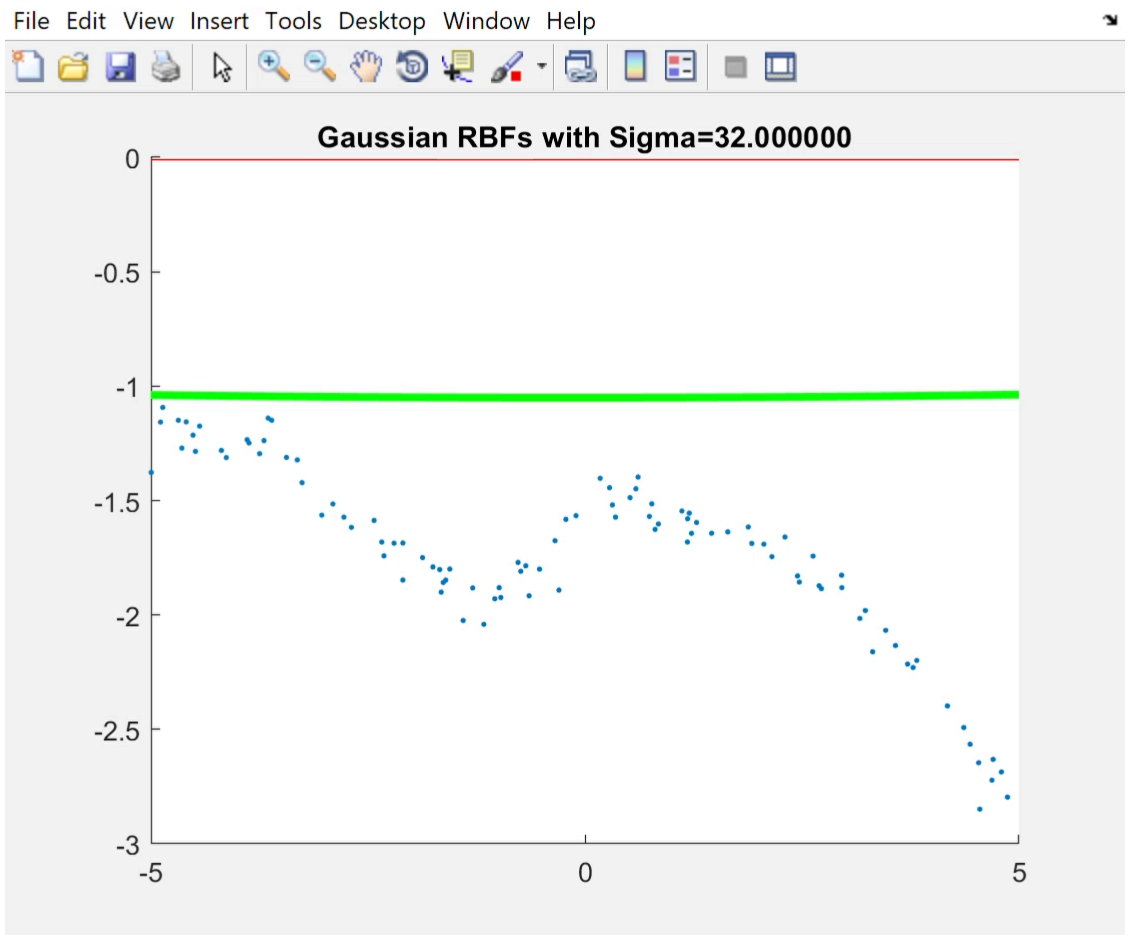

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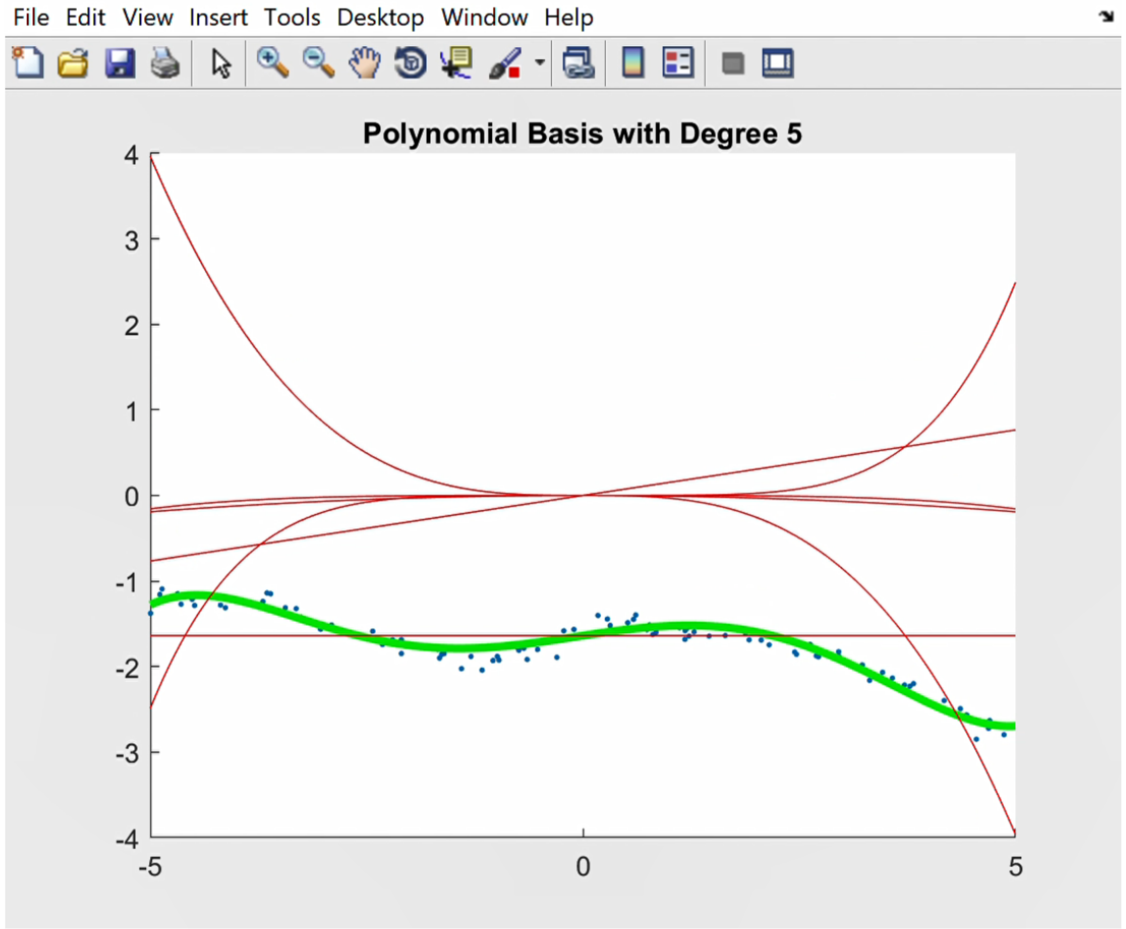

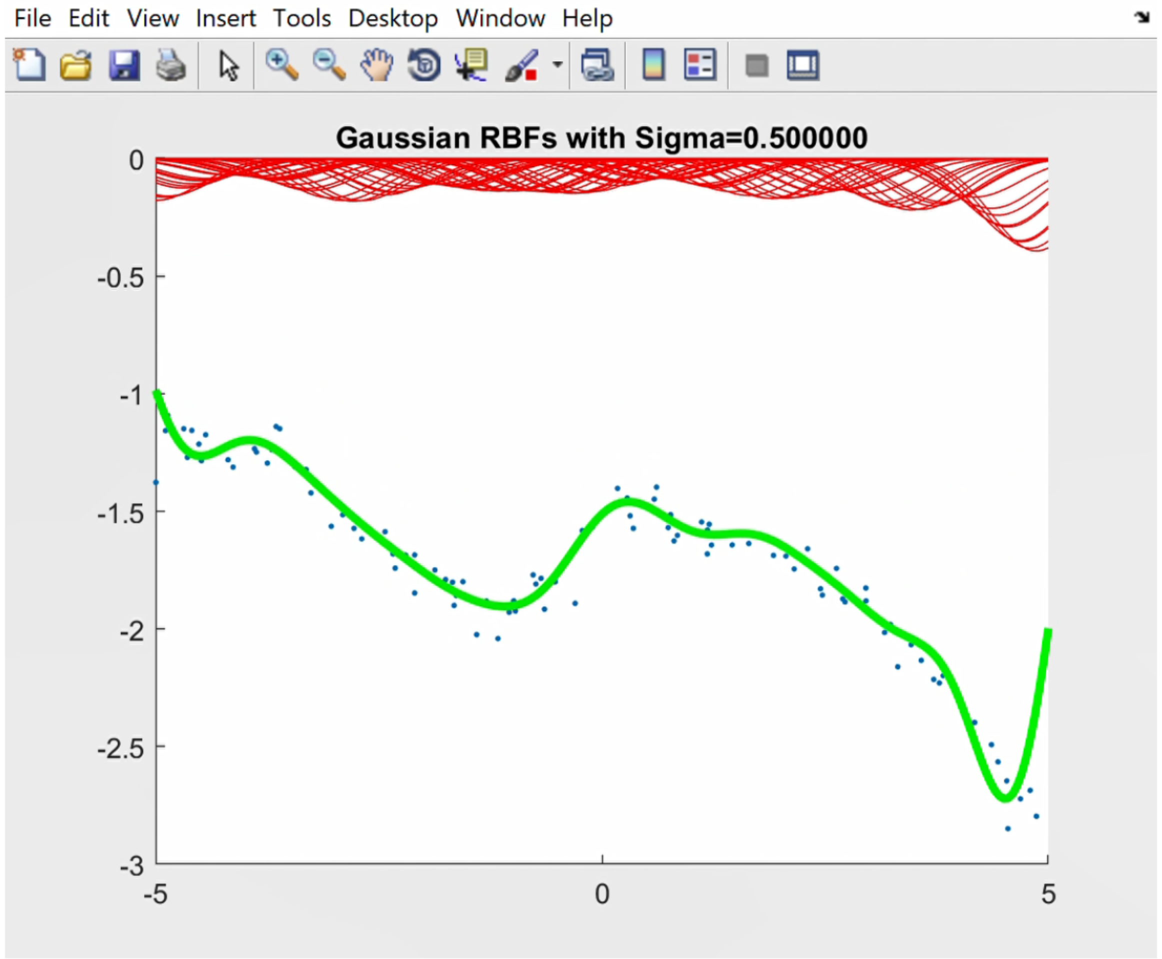

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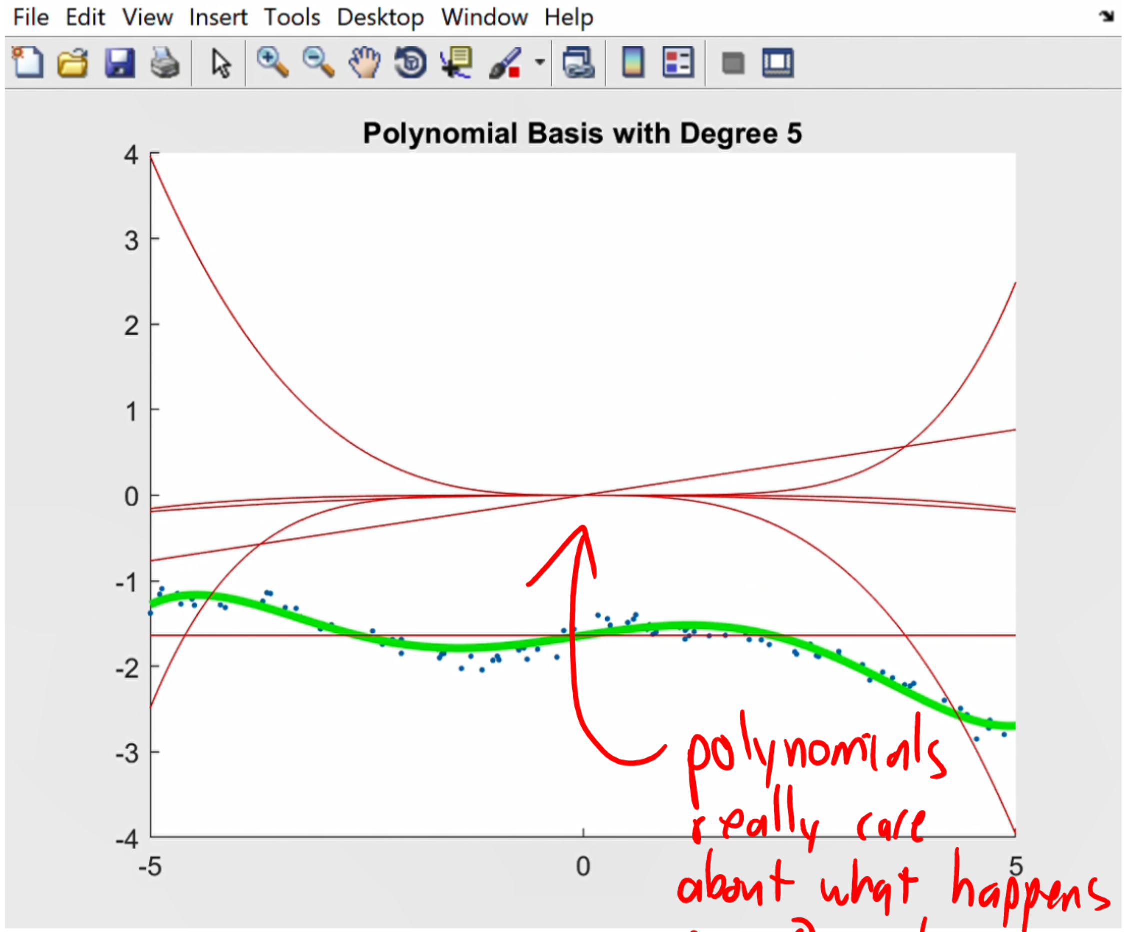

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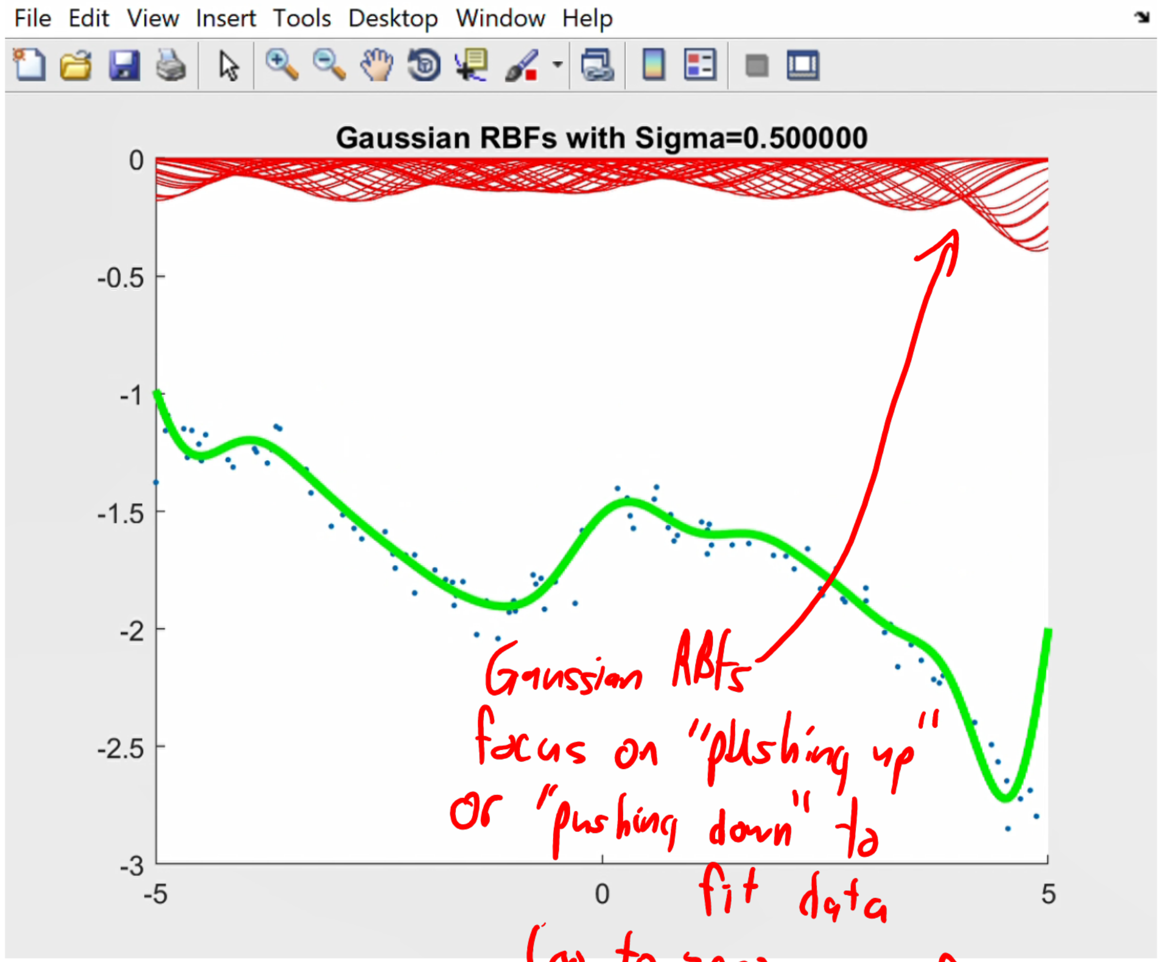

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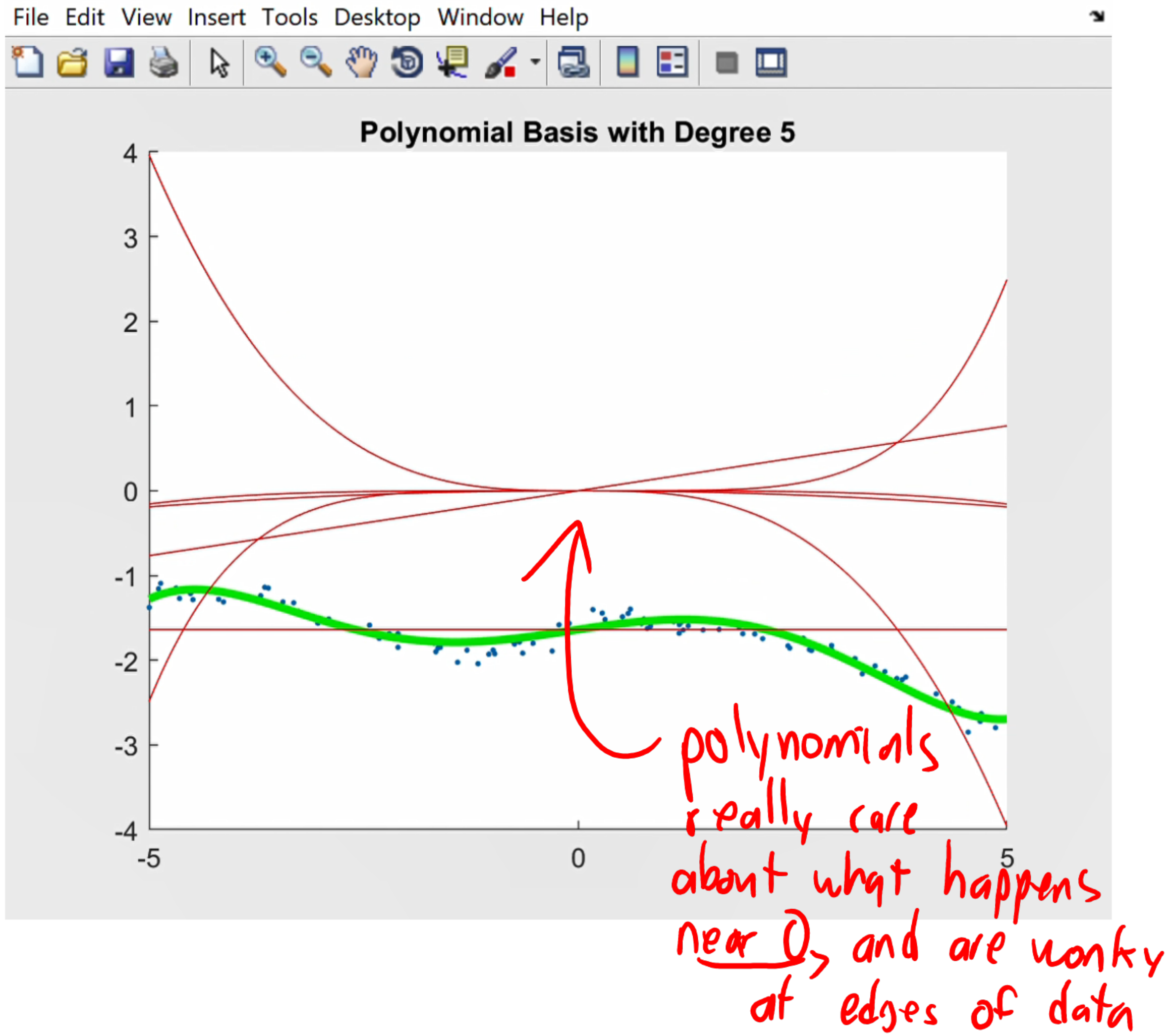

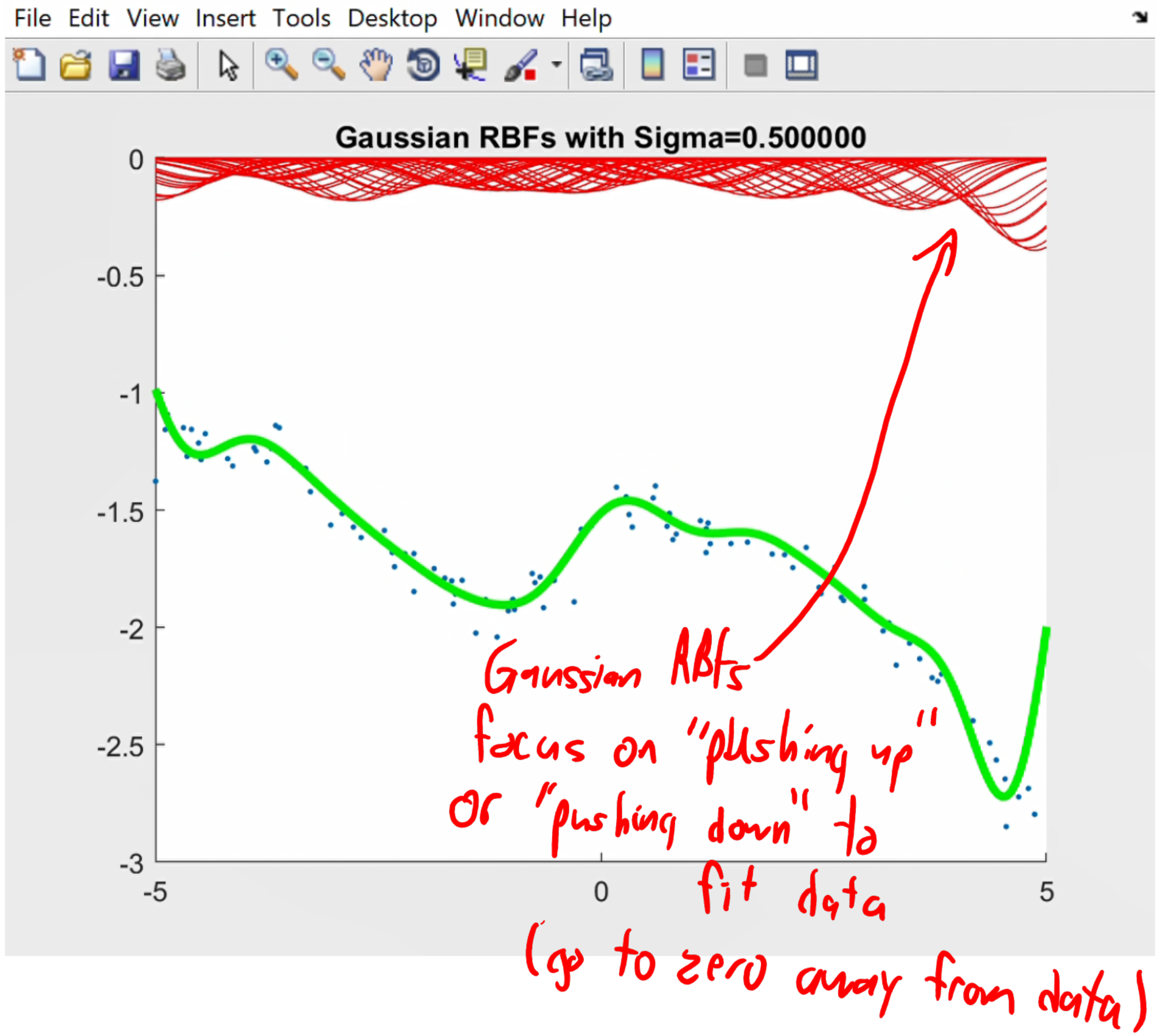

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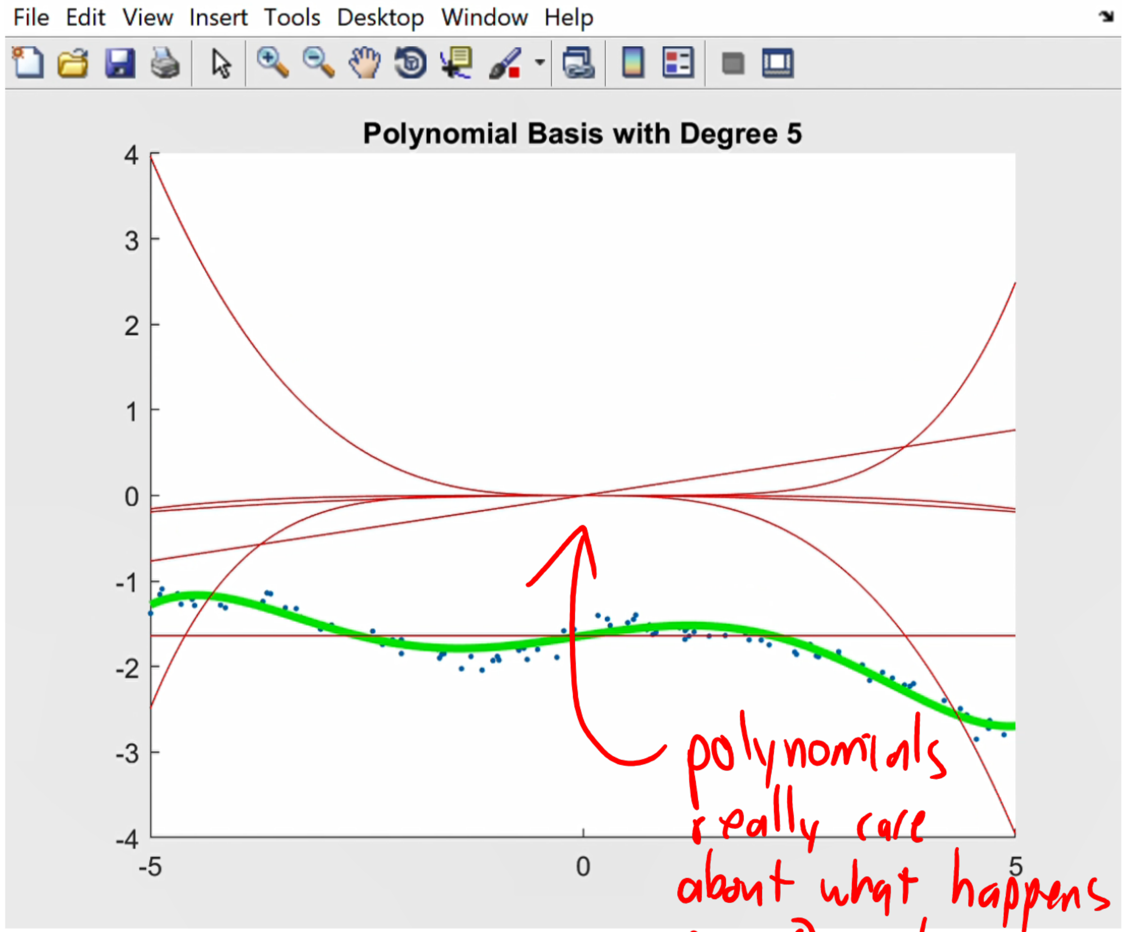

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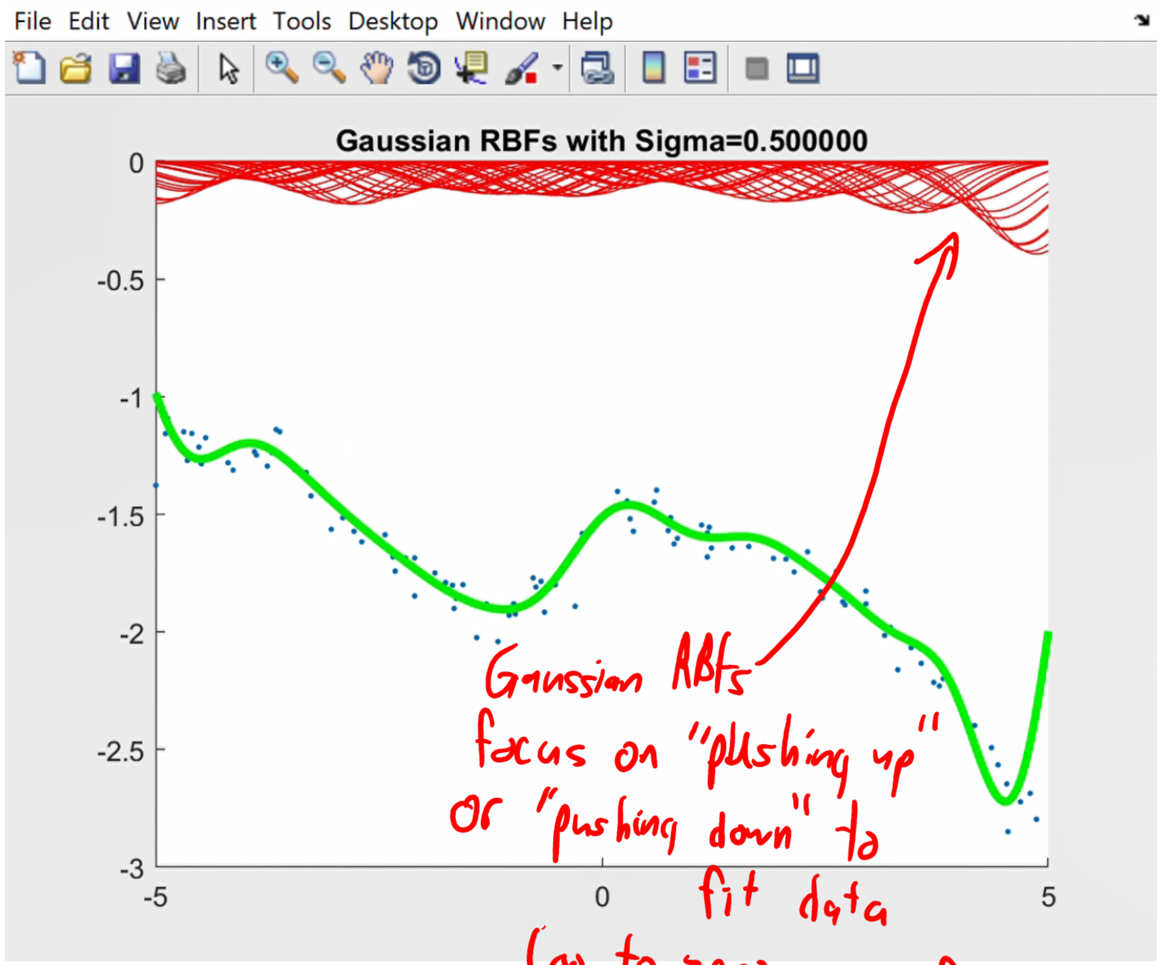

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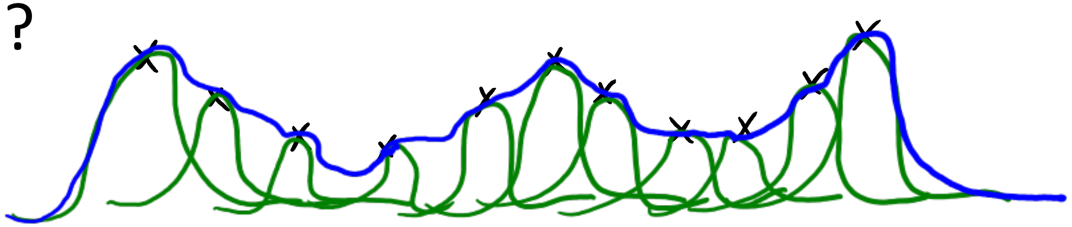

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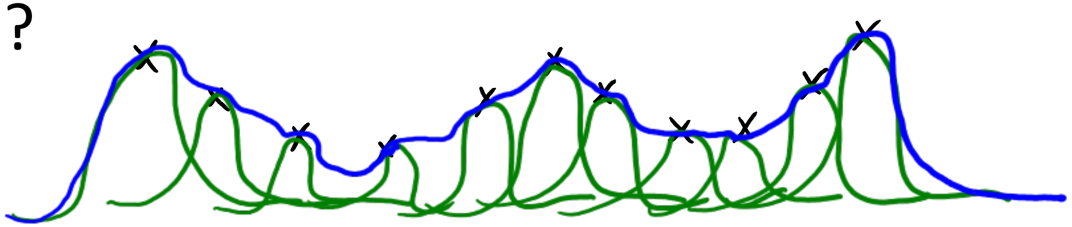

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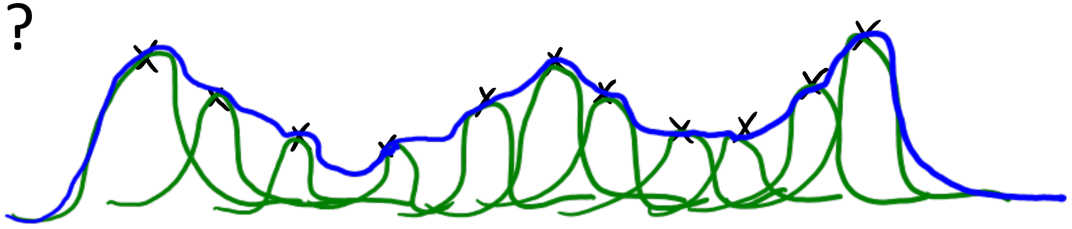

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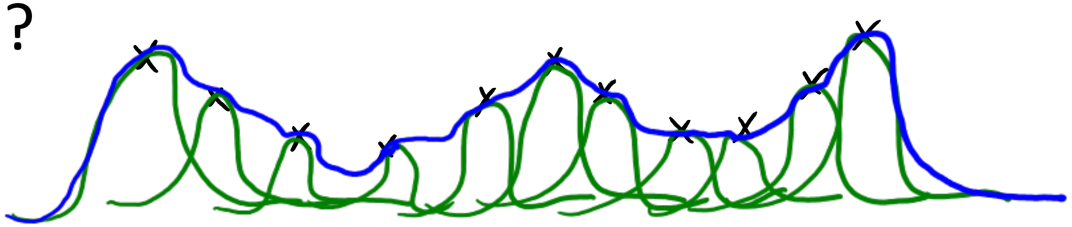

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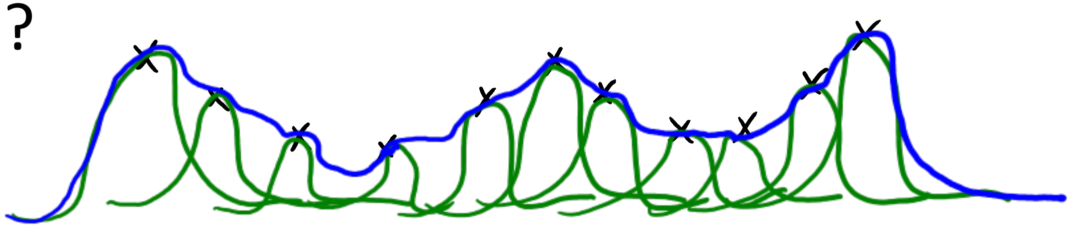

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- What is a radial basis functions (RBFs)?
  - A set of non-parametric bases that depend on distances to training points.

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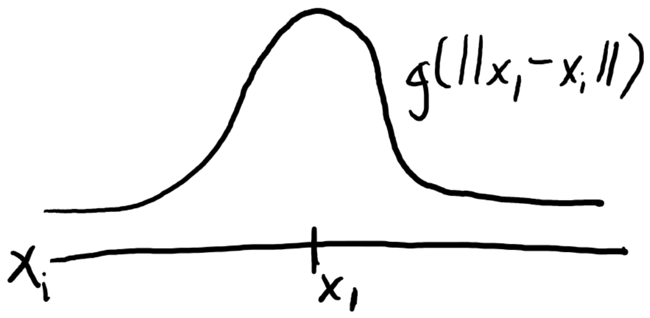

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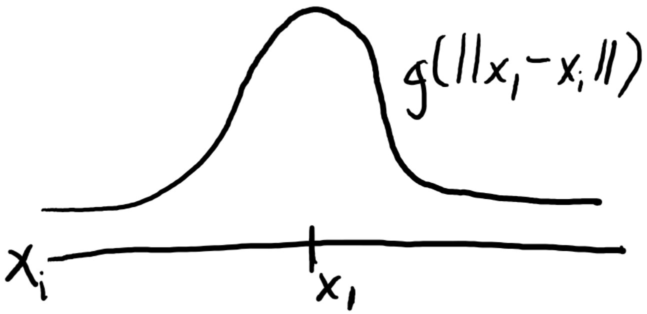

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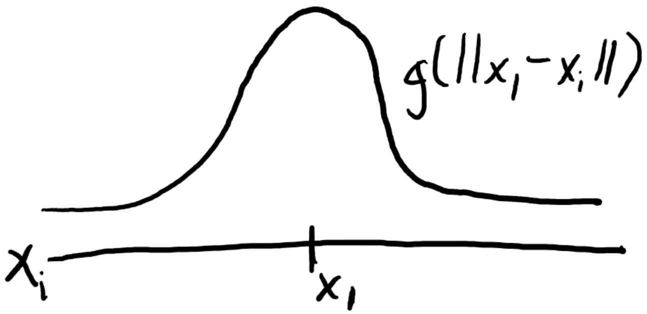

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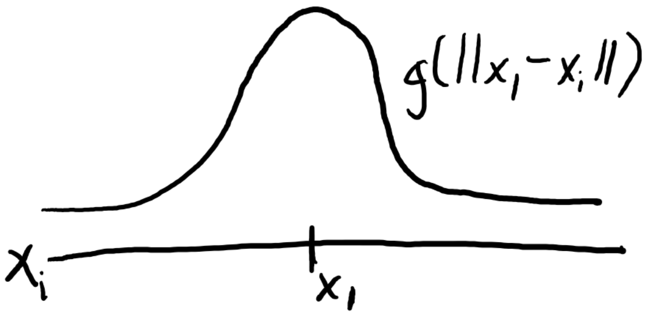

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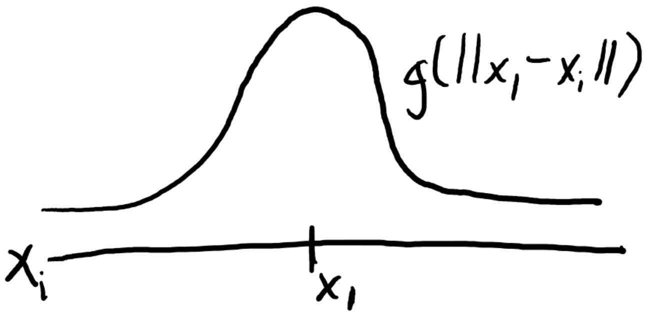

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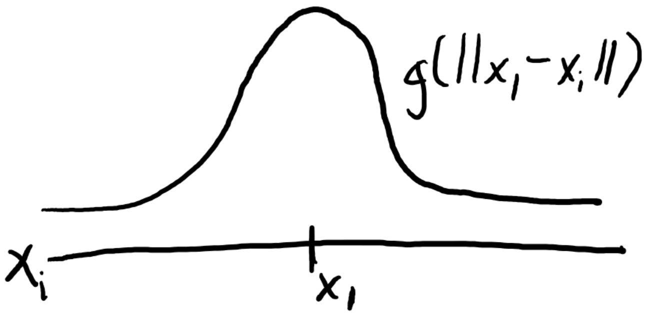

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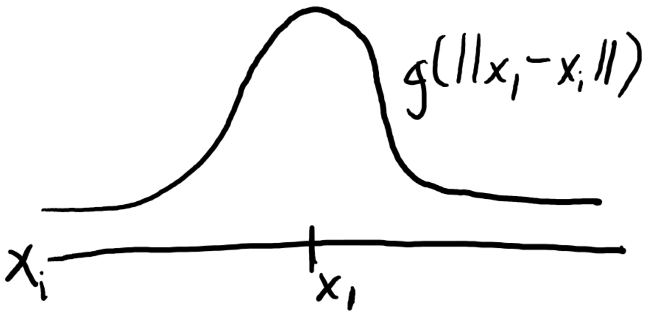

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  - If you regularize it "sort of" matters:
    - It changes the effect of a fixed λ.
    - But the regularization path is the same, so if you search for the best λ you get same predictions.

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To make predictions on $\tilde{X} = \underbrace{\left.\begin{bmatrix} \\ \\ \\ \end{bmatrix}\right\}t}_{d}$ use $\tilde{Z} = \underbrace{\left.\begin{bmatrix} \\ g(\|\tilde{x}_i - x_j\|) \\ \\ \end{bmatrix}\right\}t}_{n}$

Number of "features" is number of training examples.

Gaussian RBFs: Pseudo-Code

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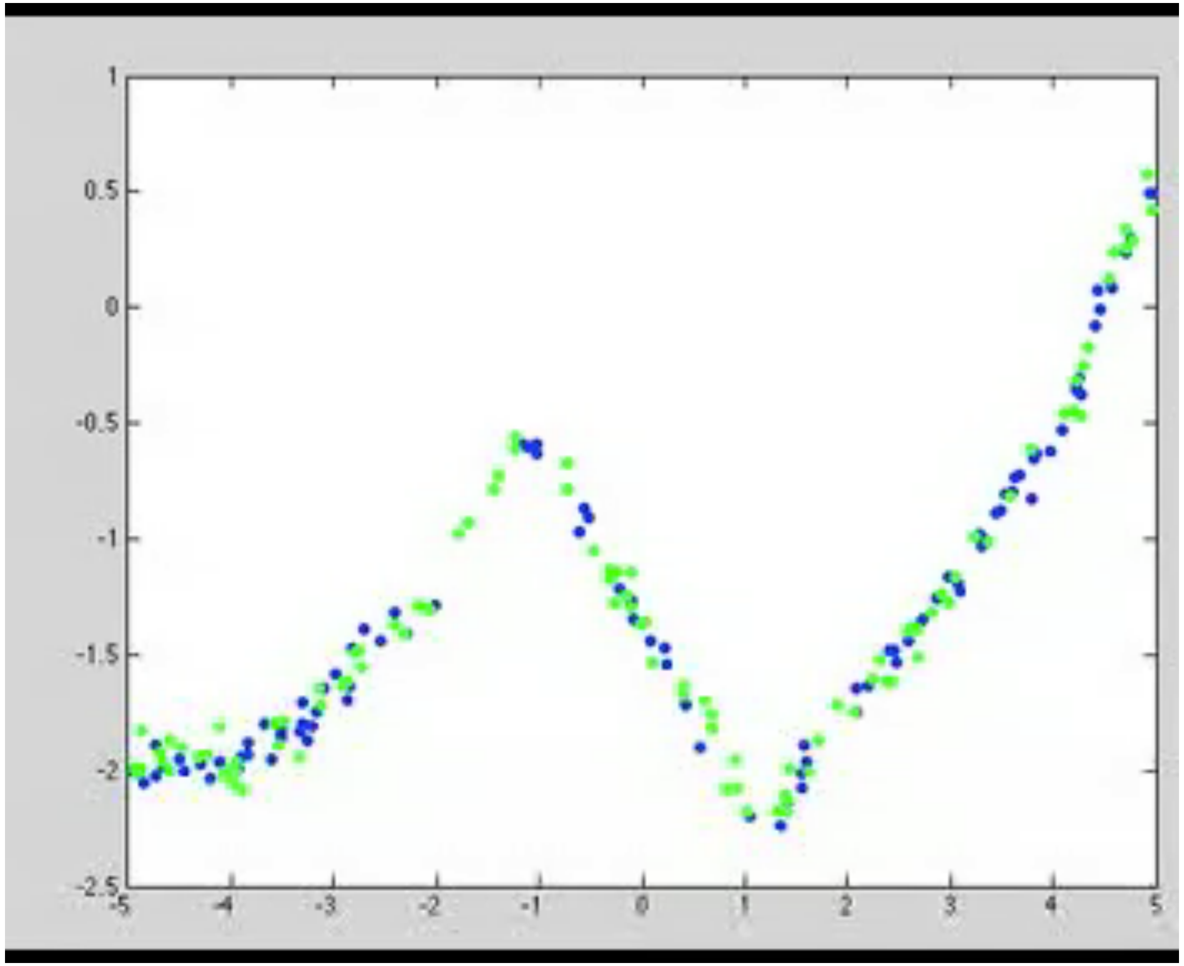
With test data $\tilde{X}$: form $\tilde{Z}$ based on distances to training examples.

Non-Parametric Basis: RBFs

- Least squares with Gaussian RBFs for different σ values:



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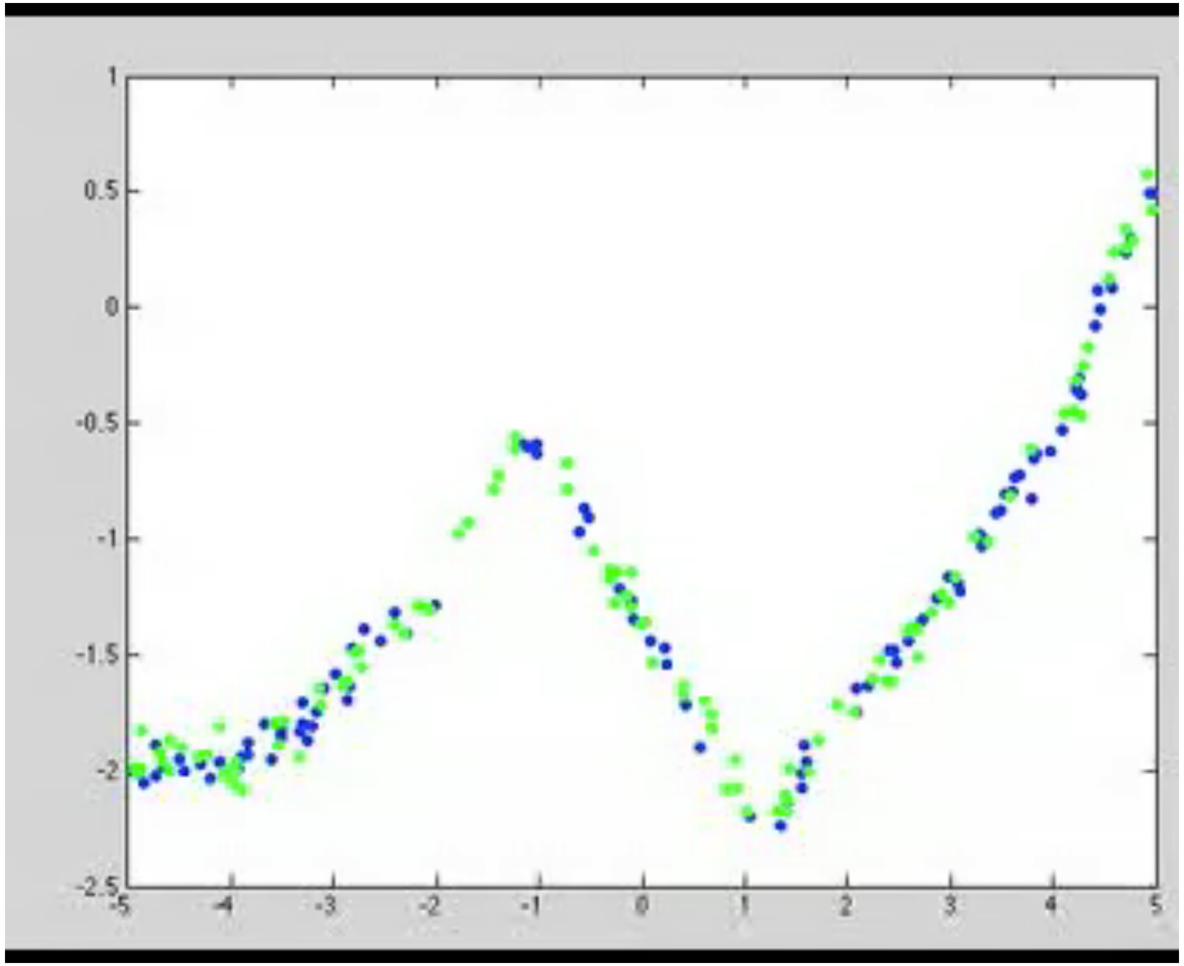

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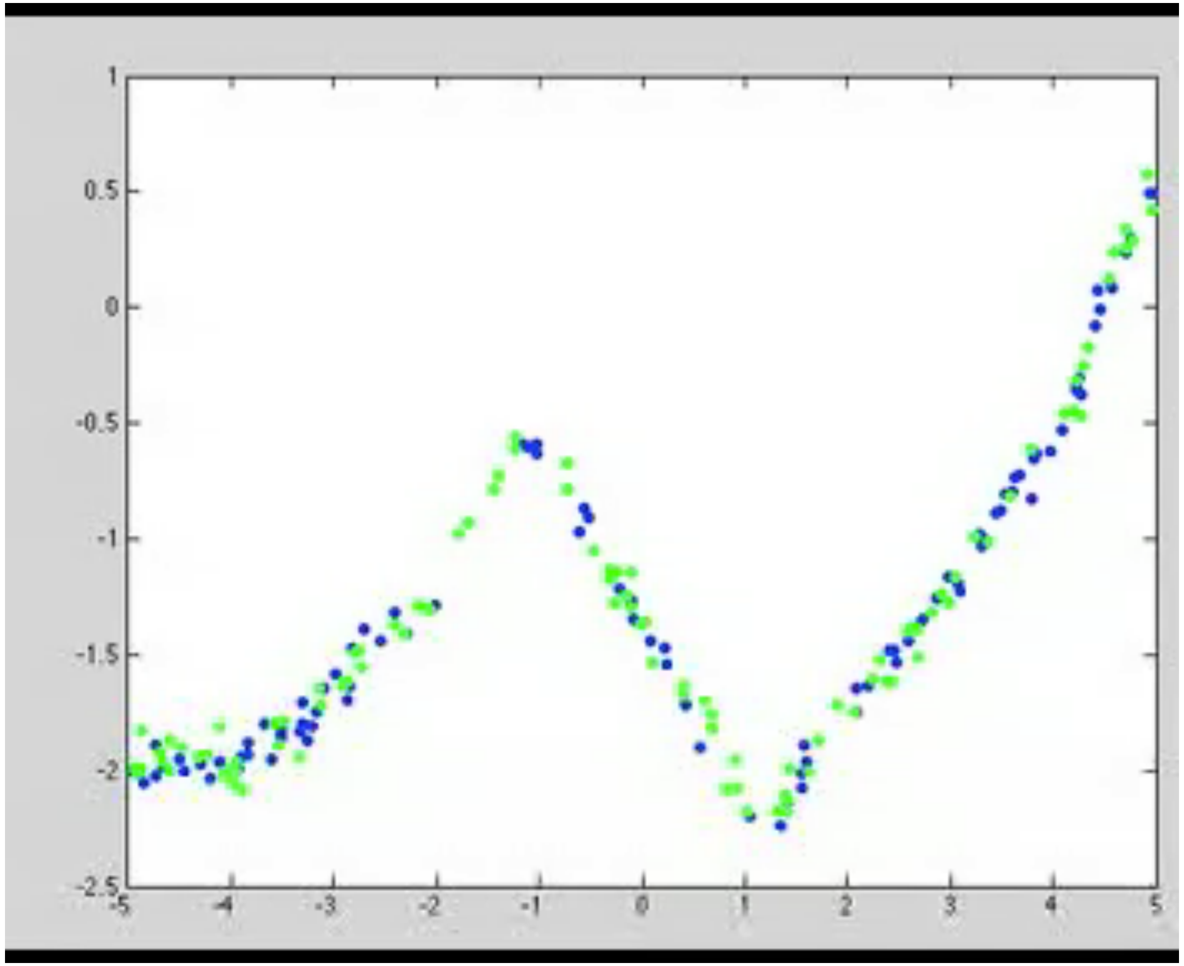

Could add <u>bias</u> and linear basis:

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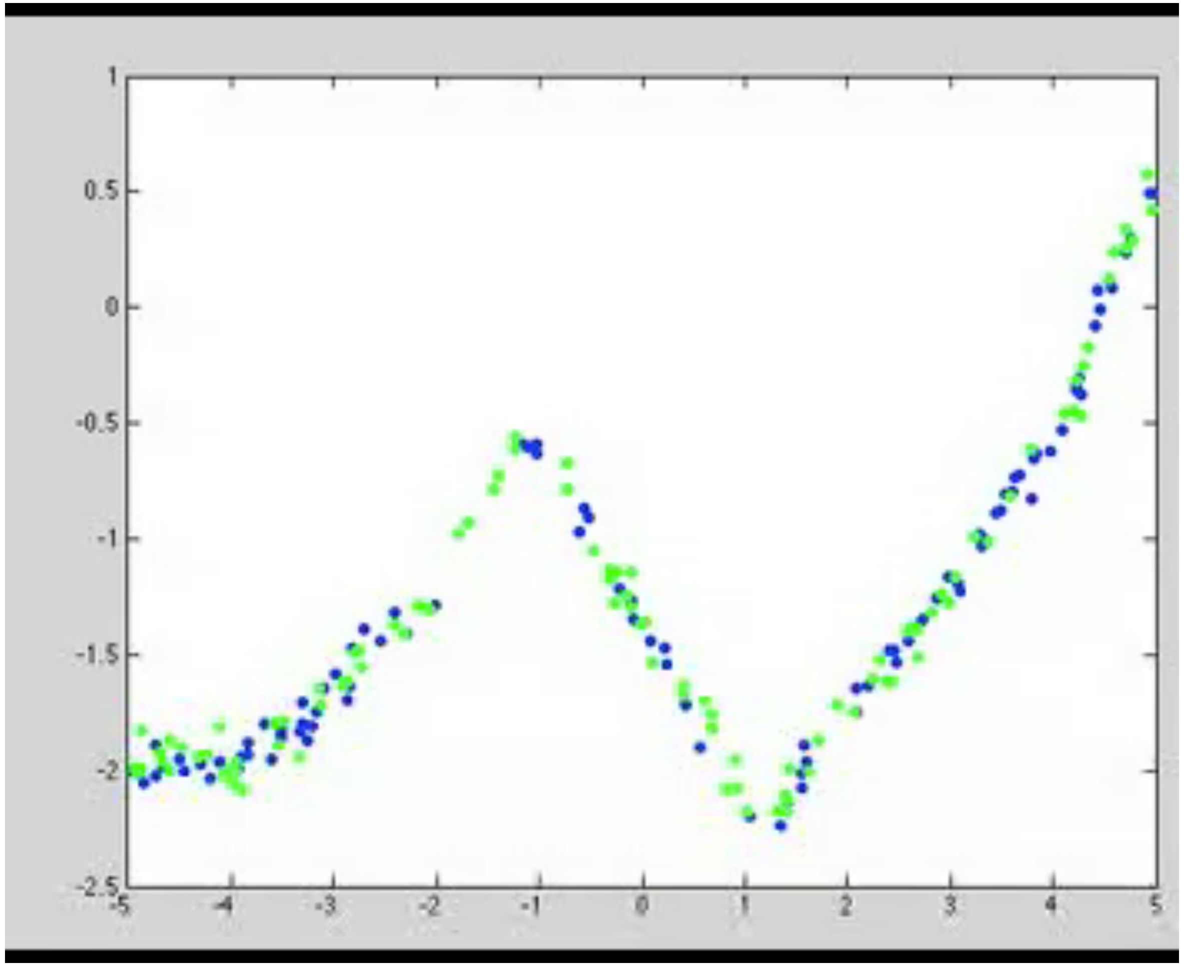

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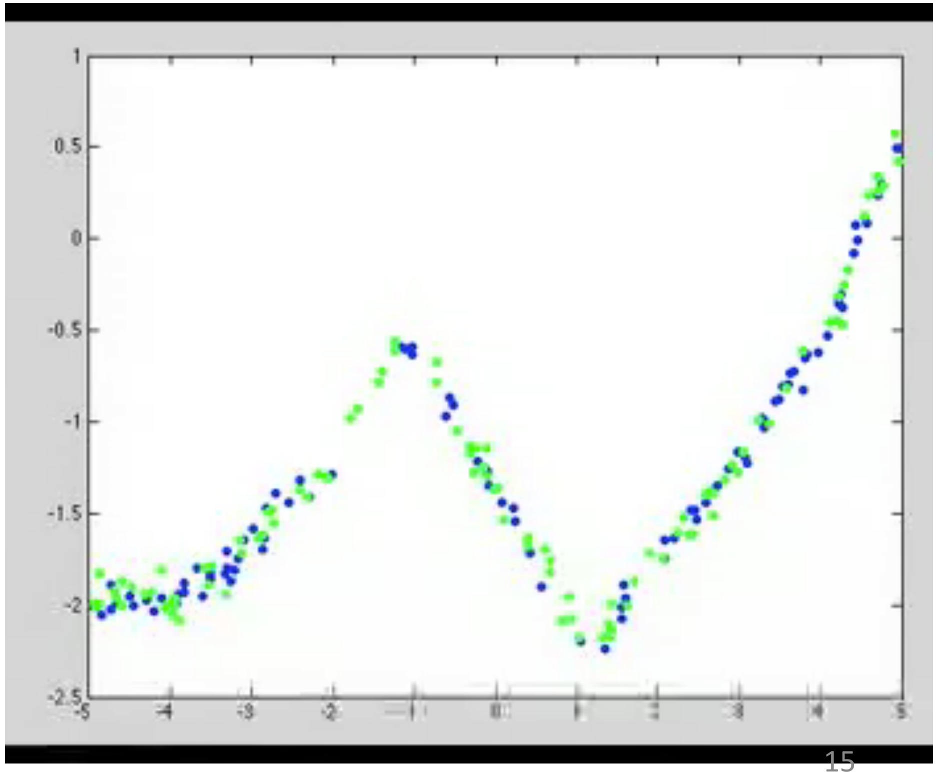

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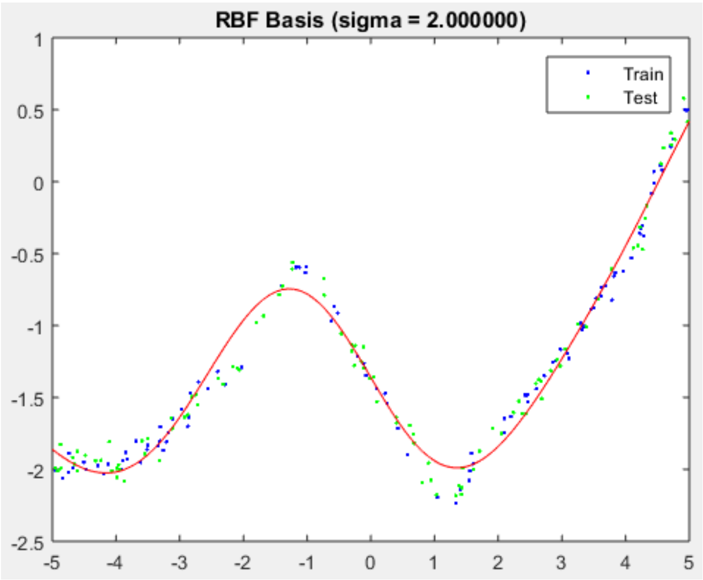

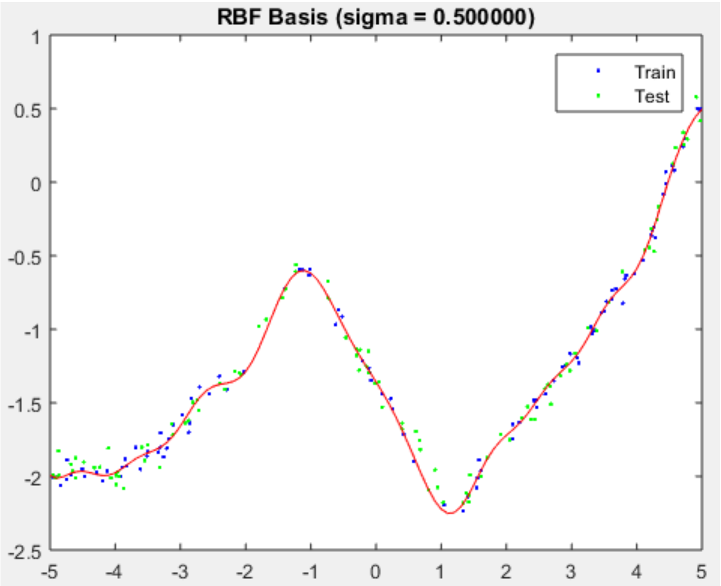

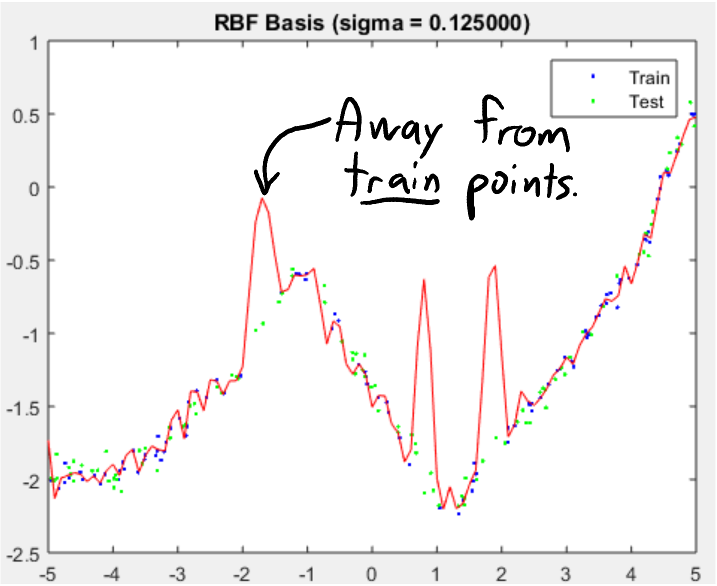

  - Expensive at test time: needs distance to all training examples.

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

bonus!

Hyper-Parameter Optimization

- Other common hyper-parameter optimization methods:
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    - Generic global optimization methods (simulated annealing, genetic algorithms, etc.).
  - Bayesian optimization (Mike's PhD research topic):
    - Use (e.g.) RBF regression to build model of how hyper-parameters affect validation error.
    - Try the best guess based on the model.

(pause)

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- But it's hard to find the 'w' minimizing this objective.
- We discussed forward selection, but requires fitting $O(d^2)$ models.

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- The situation is worse if we aren’t using basic least squares:
  - With regularization, for every lambda, we need to fit $O(d^2)$ models.

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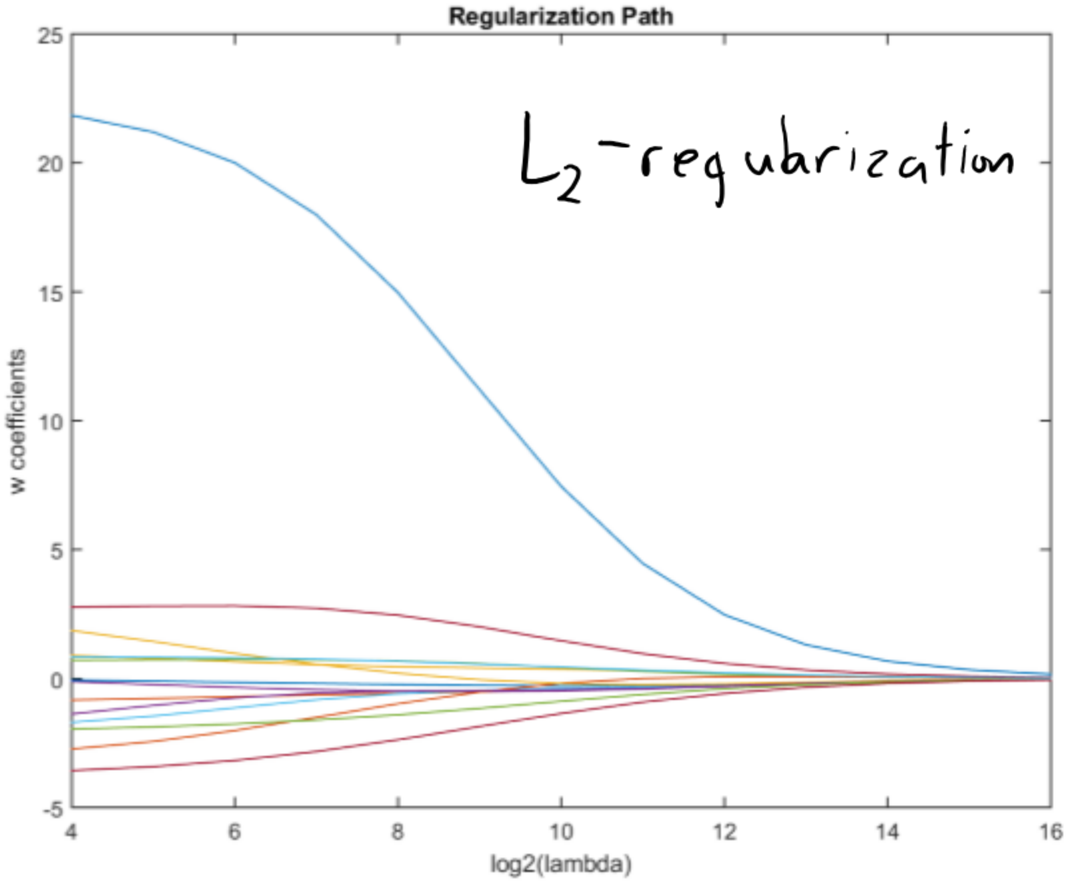
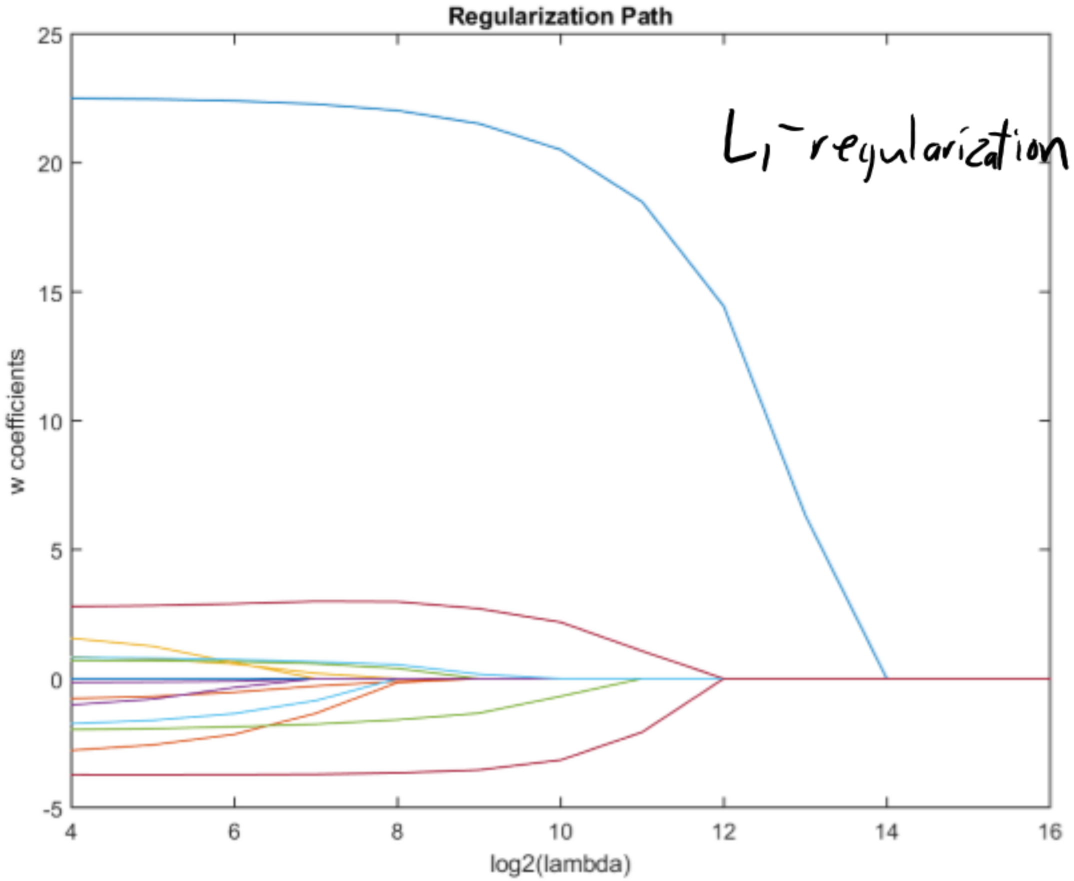
- L1-regularization simultaneously regularizes and selects features.
  - **Very fast alternative to search and score.**
  - Sometimes called "LASSO" regularization.

L2-Regularization vs. L1-Regularization

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





- L1-Regularization sets values to exactly 0 (next slides explore why).

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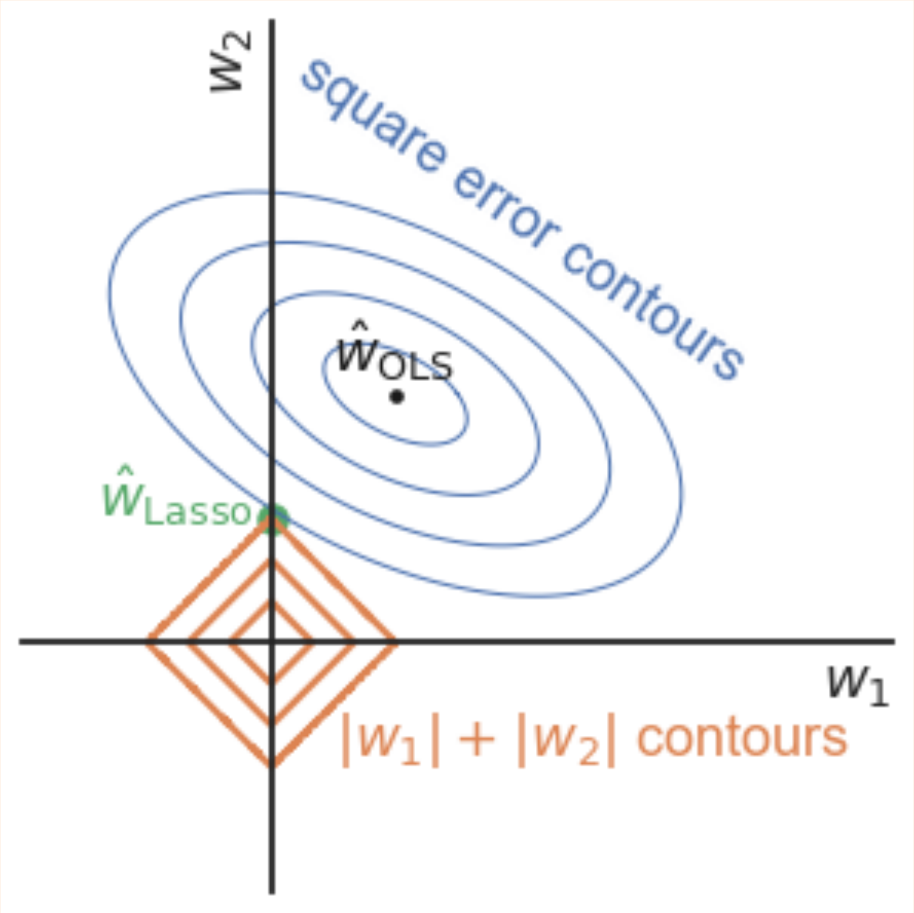
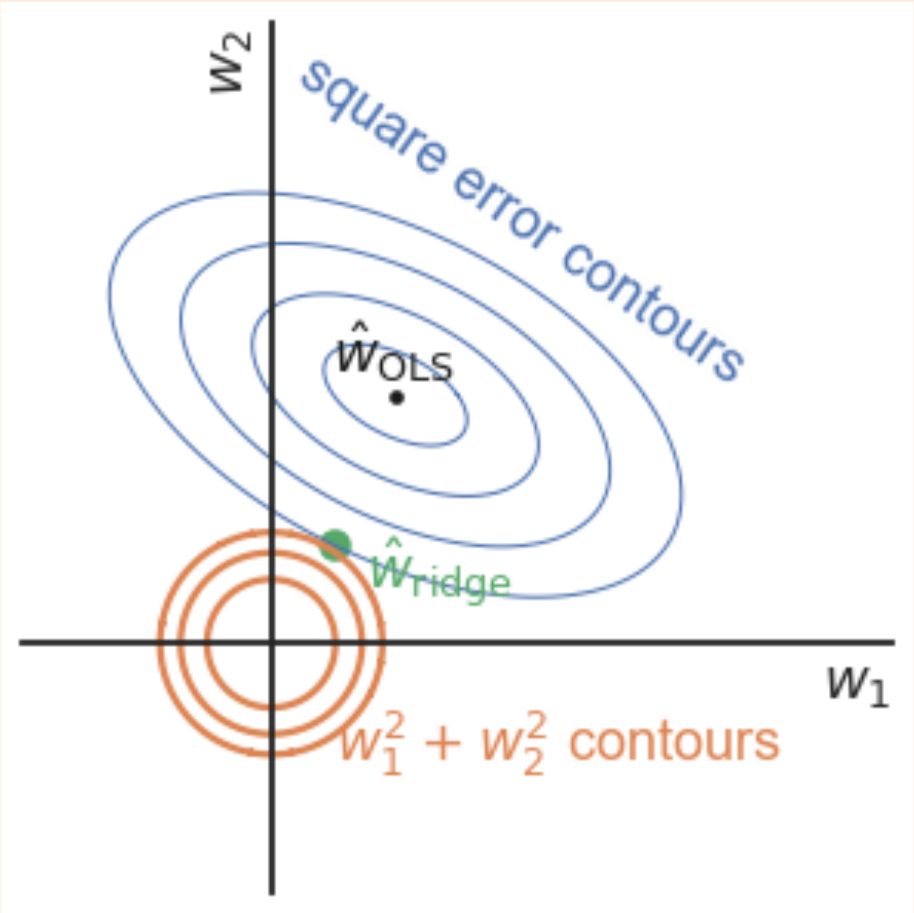
- L1-regularization: penalty of $\lambda|0.00001| = 0.00001\lambda$.
  - The penalty stays is proportional to how far away w_j is from zero.
  - There is still something to be gained from making a tiny value exactly equal to 0.

bonus!

Regularizers and Sparsity





Loss plus error usually minimized at "corners" (sparse points)

Minimizer moved towards 0, but axis-independently

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      Paper on this result by Andrew Ng

bonus!

L1-Regularization Applications

- Used to give super-resolution in imaging black holes.
  - Sparsity arises in a particular basis.

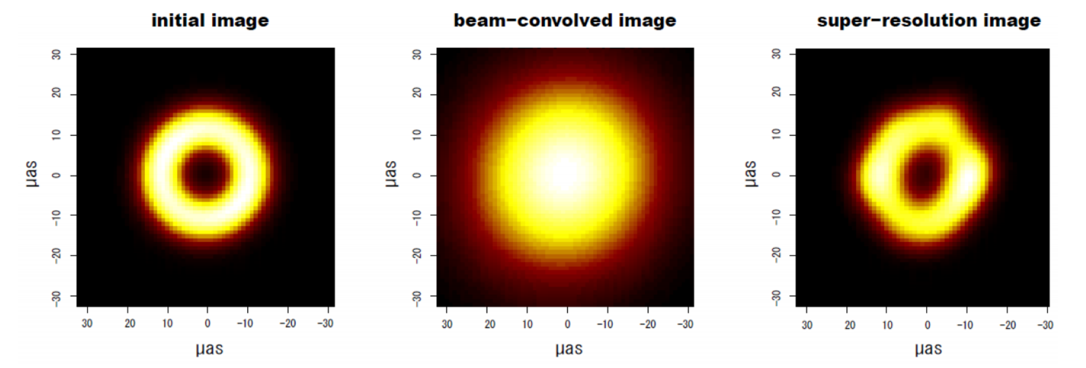

Figure 2. Simulated images of M87. From left to right, the initial model, the image with 0-filling, and the image with LASSO. Improvement of resolution in the LASSO image is significant.

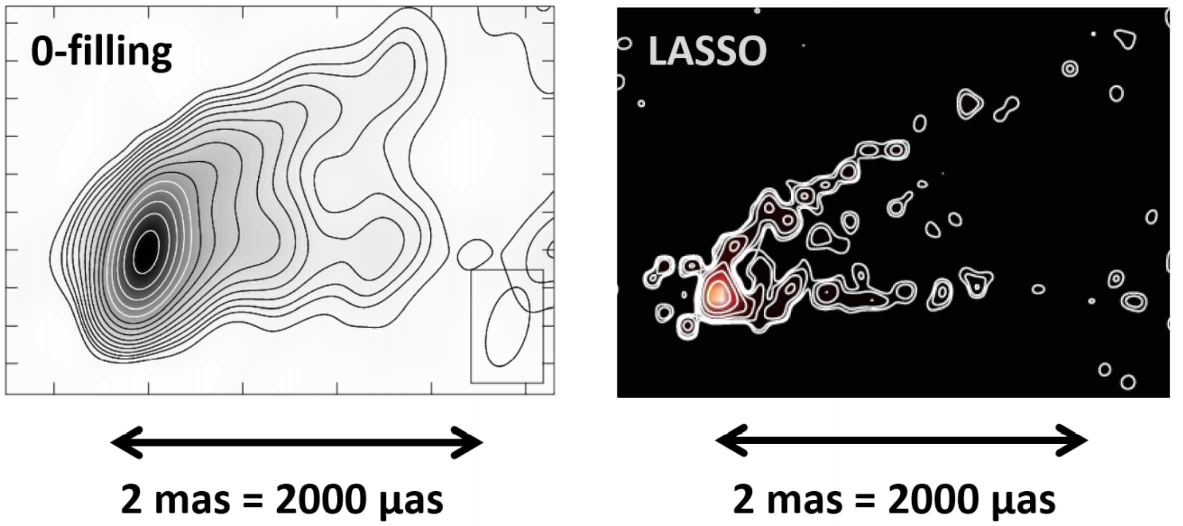

Figure 3. Standard and LASSO images of M87 observed with VLBA at a wavelength of 7 mm. In the two plots, exactly the same data are used. The angular resolution is better in the LASSO image, and the detailed structure of the M87 jet can be traced in more detail.

- Another application:
  - Use L1-regularization with Gaussian RBFs to reduce prediction time.

https://iopscience.iop.org/article/10.1088/1742-6596/699/1/012006/pdf

L1-loss vs. L1-regularization

- Don't confuse the L1 loss with L1-regularization!
  - L1-loss is robust to outlier data points.
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- Can we smooth and use "Huber regularization"?
  - Huber regularizer is still robust to irrelevant features.
  - But it's the non-smoothness that sets weights to exactly 0.

L*-Regularization

- L0-regularization (AIC, BIC, Mallow's Cp, Adjusted R^2, ANOVA):
  - Adds penalty on the number of non-zeros to select features.

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- L1-regularization (LASSO):
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L0- vs. L1- vs. L2-Regularization

	Sparse 'w' (Selects Features)	Speed	Unique 'w'	Coding Effort	Irrelevant Features
L0-Regularization	Yes	Slow	No	Few lines	Not Sensitive
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- Using L0+L2 does not give a unique solution.

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  - 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?

bonus!

Regularizers and Sparsity

- L1-regularization gives sparsity but L2-regularization doesn't.
  - But don't they both shrink variables to zero?

bonus!

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- Consider problem where 3 vectors can get minimum training error:

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

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

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$$= 10000.0004$$

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Regularizers and Sparsity

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

bonus!

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

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

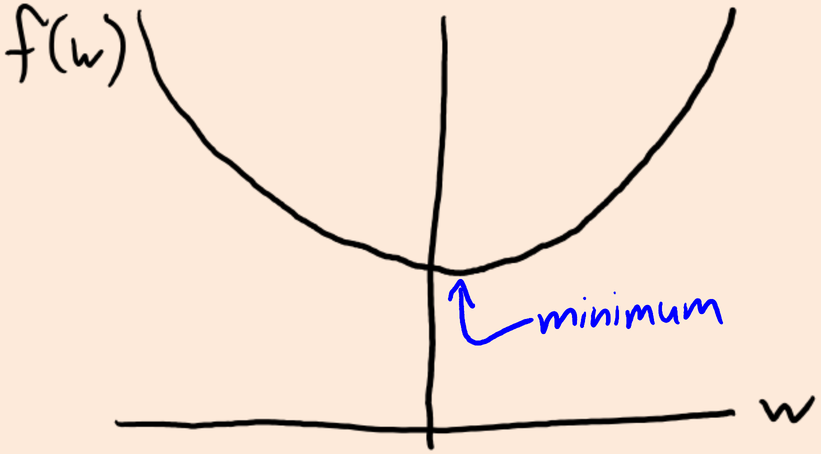
bonus!

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):



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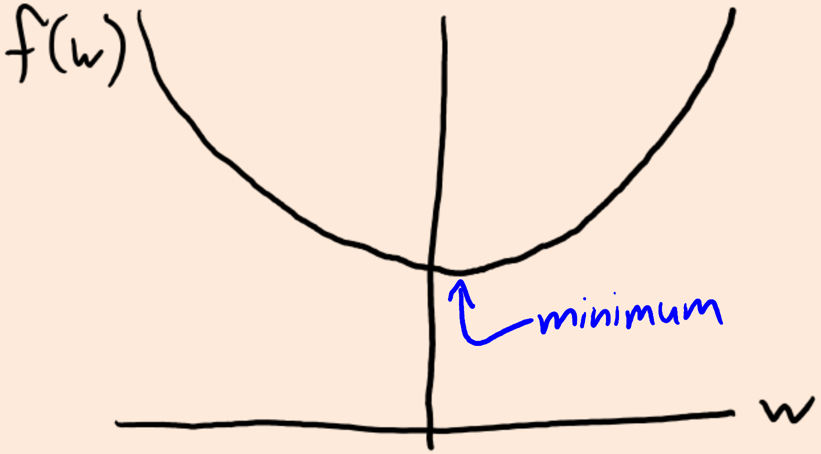

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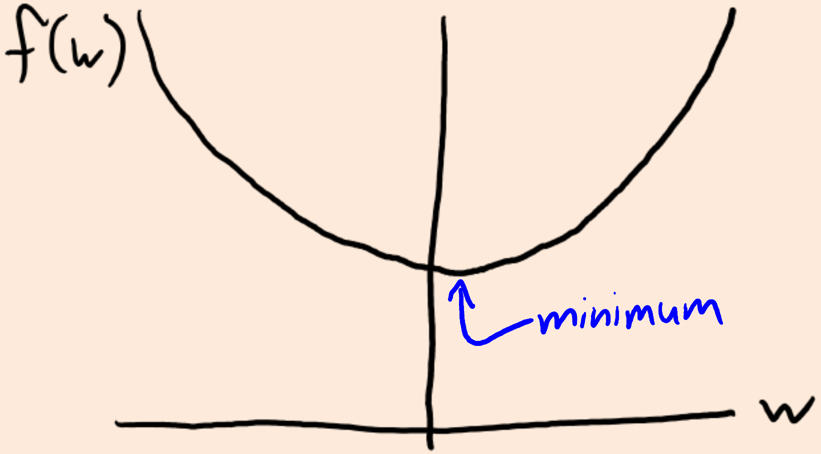

$f'(0) = 0$ only happens if $\sum_{i=1}^{n} y_i x_i = 0$. (bonus)

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Sparsity and L0-Regularization

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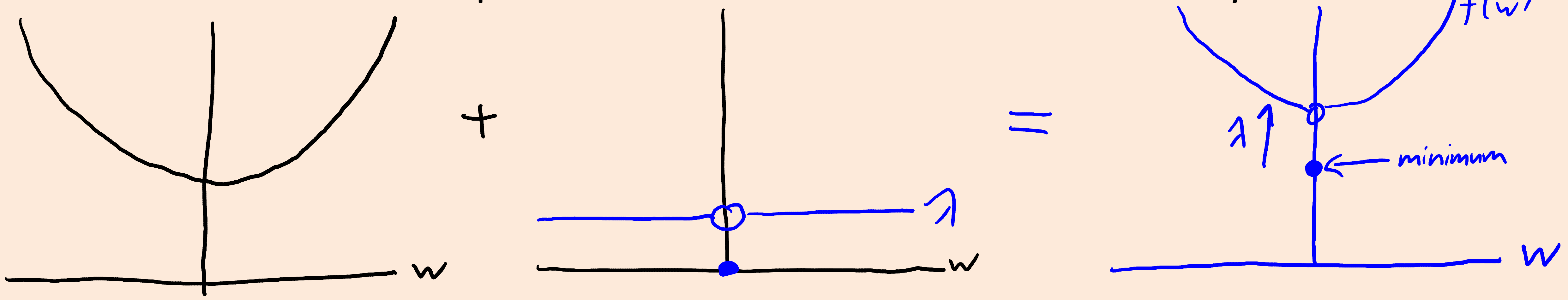

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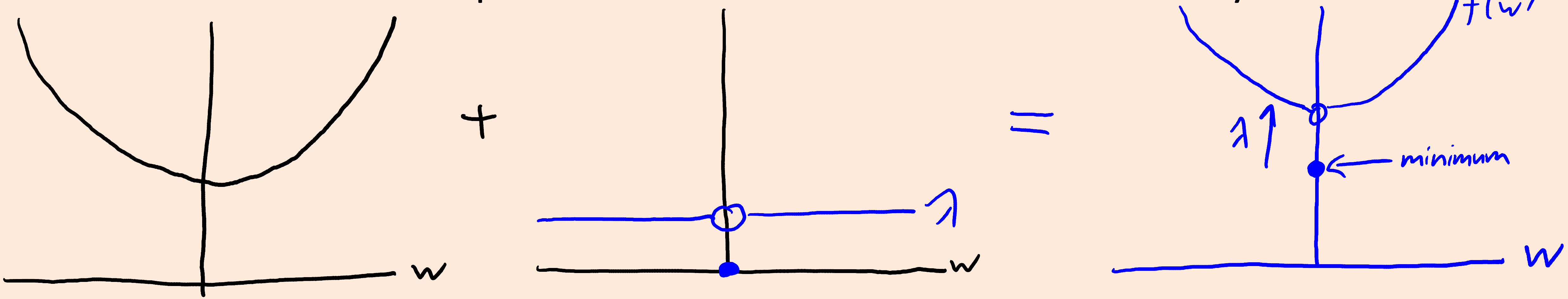

- L0-regularized minimum is often exactly at the 'discontinuity' at 0:
  - Sets the feature to exactly 0 (does feature selection), but is non-convex.

bonus!

Sparsity and L2-Regularization

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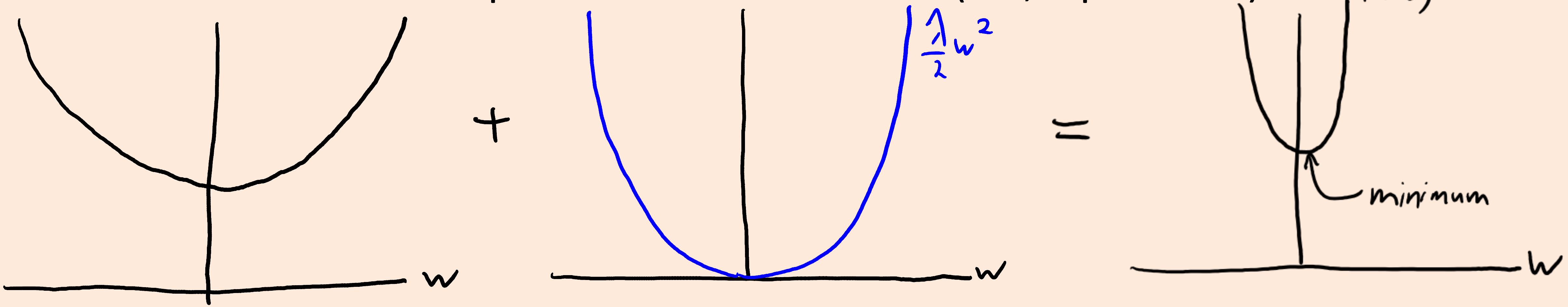

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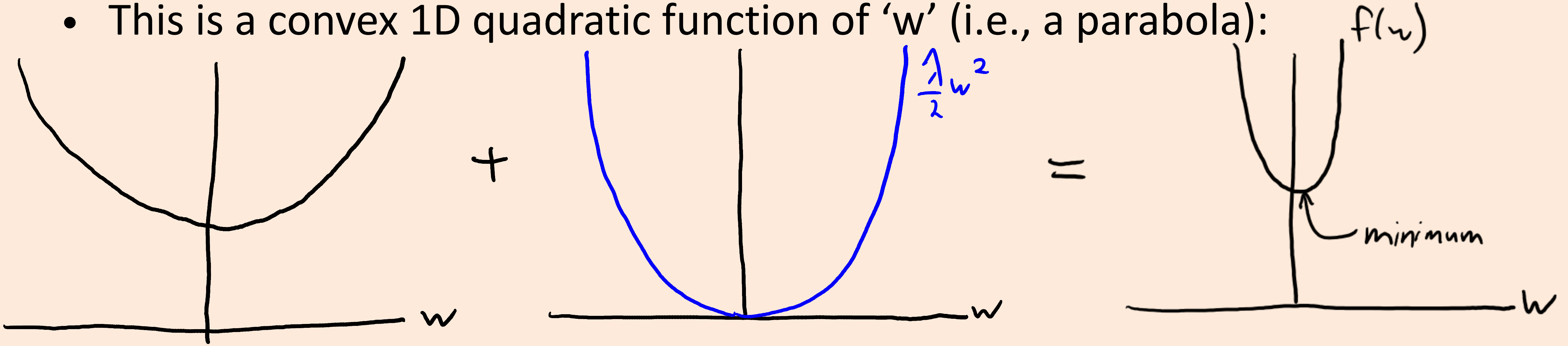

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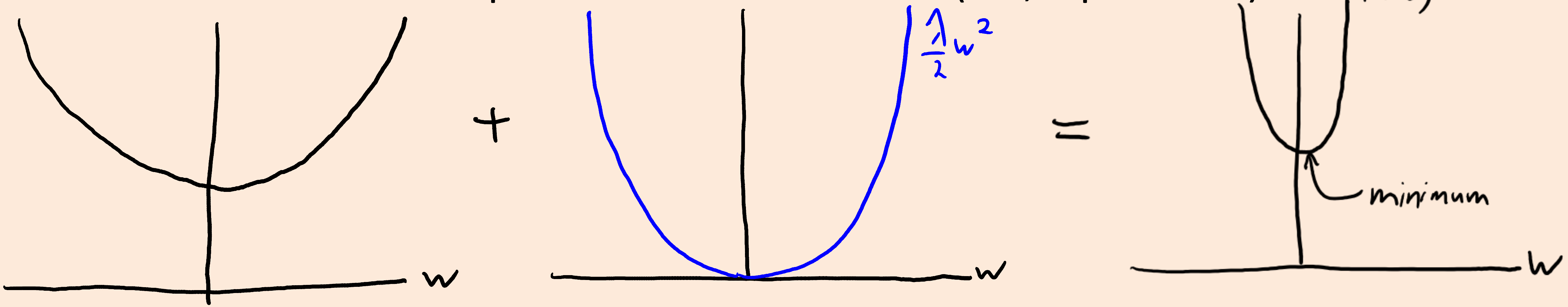

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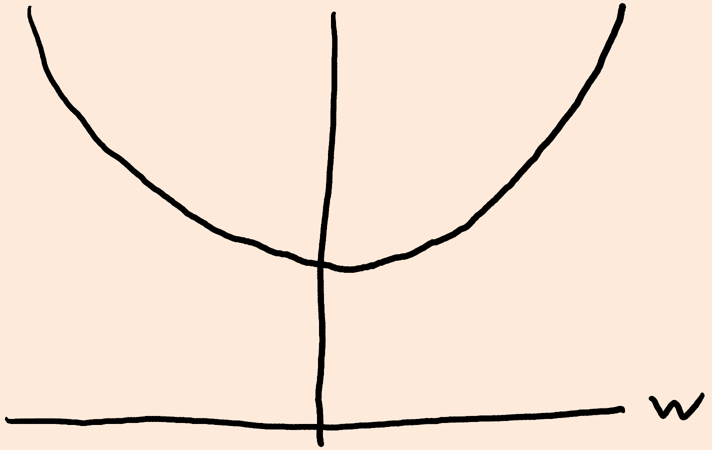

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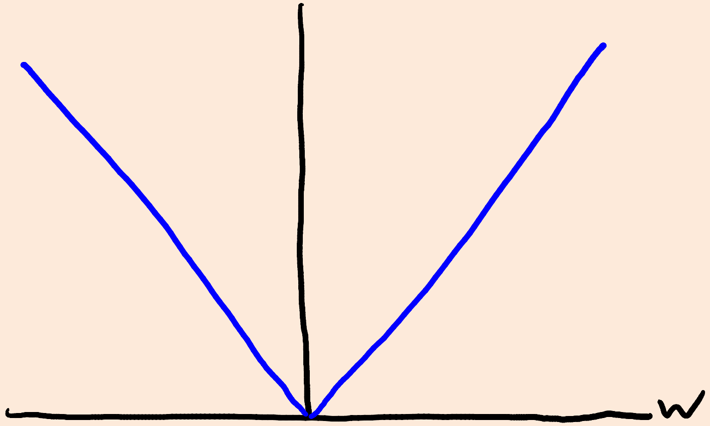

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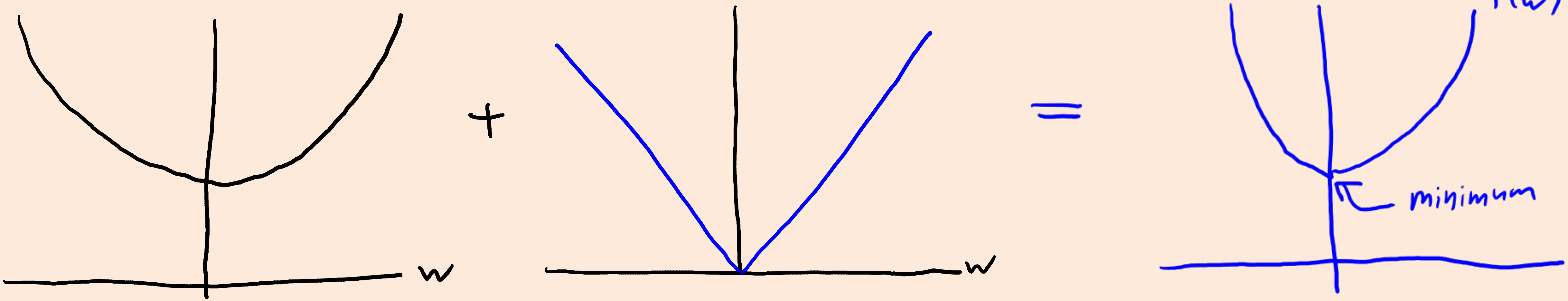

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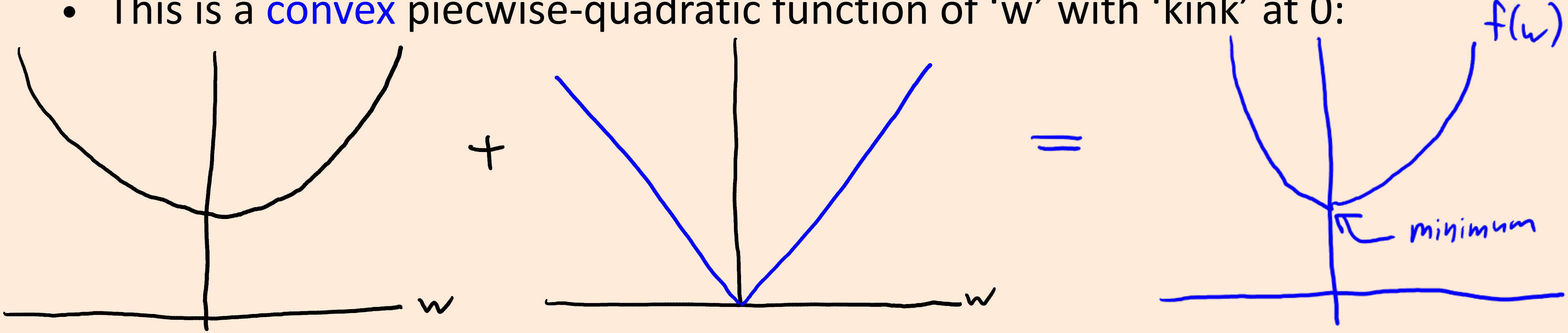

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bonus!

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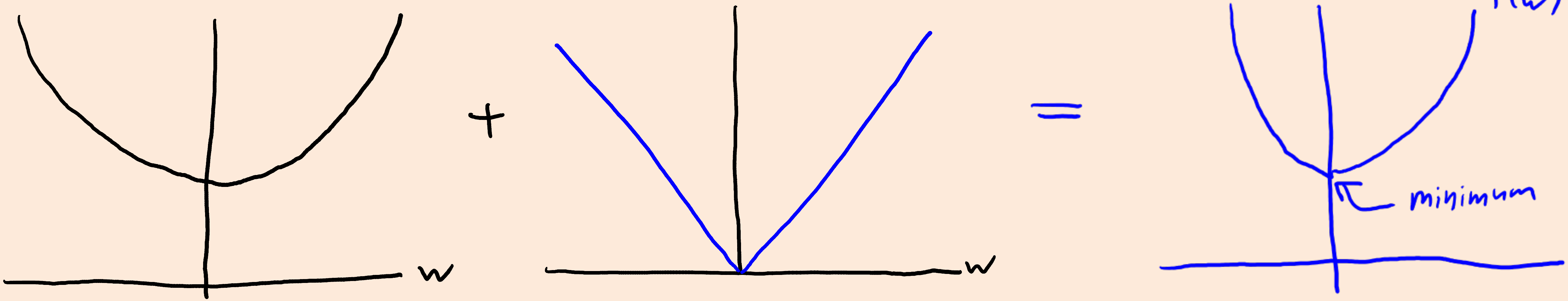

- L1-regularization tends to set variables to exactly 0 (feature selection). Happens when $\left|\sum_{i=1}^{n} x_i y_i\right| \leq \lambda$ (bonus)
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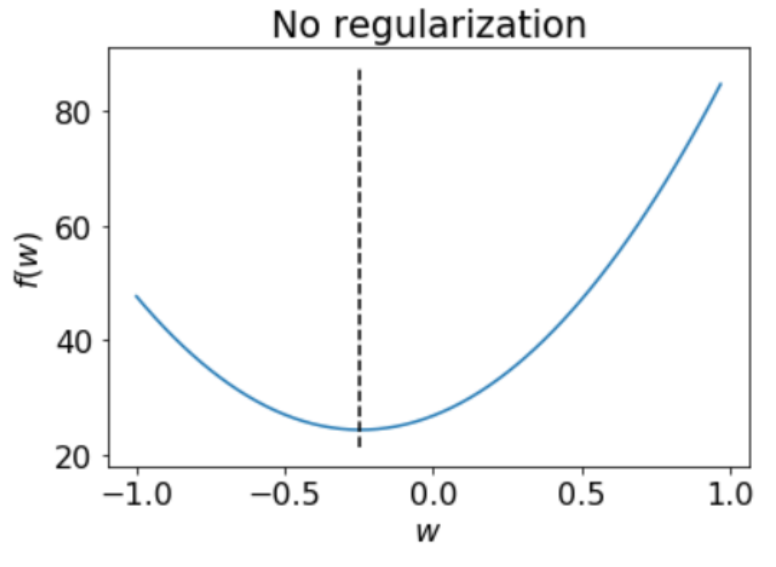
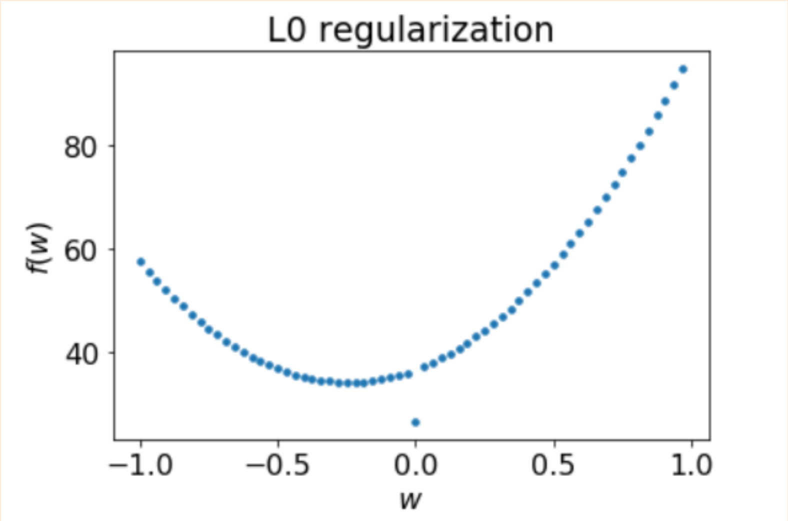
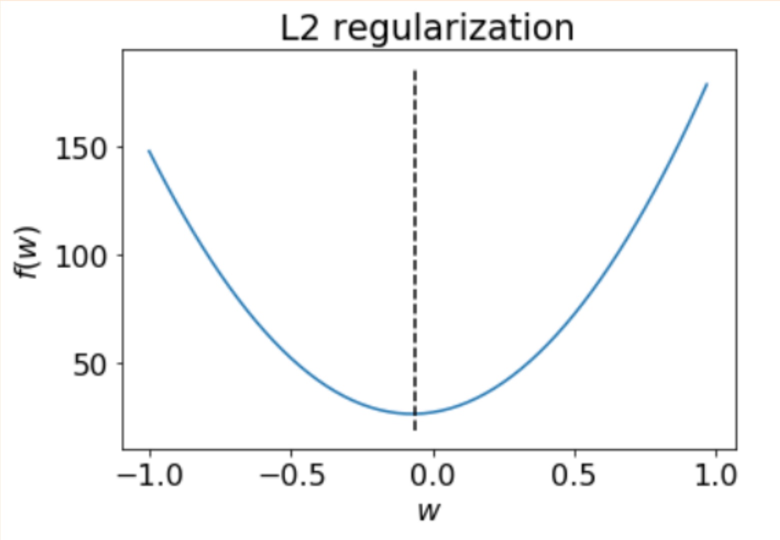
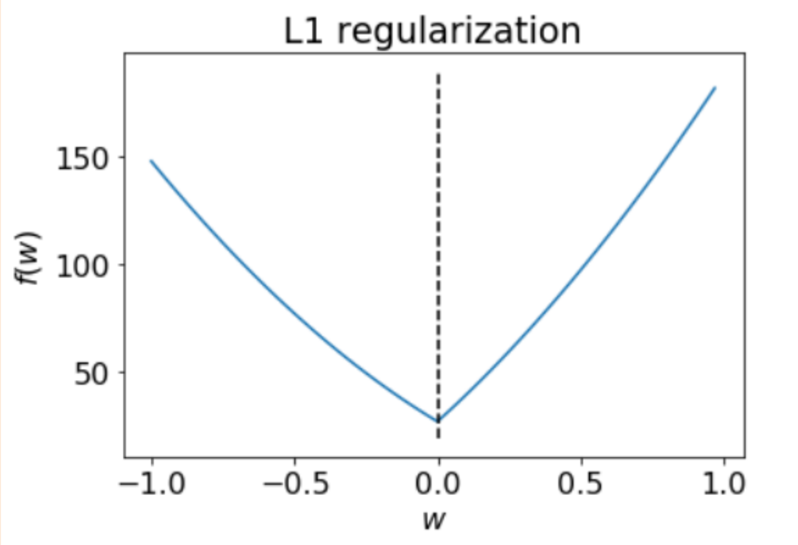
Sparsity and Regularization (with d=1)

bonus!









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

bonus!

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

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

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

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

bonus!

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

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

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Set equal to 0: $\sum_{i=1}^{n} x_i^2 w - \sum_{i=1}^{n} x_i y_i + \lambda w = 0$ $\xrightarrow{\text{re-arrange}}$ $w\left(\sum_{i=1}^{n} x_i^2 + \lambda\right) = \sum_{i=1}^{n} x_i y_i$

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re-arrange

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

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

- So as λ gets bigger, 'w' converges to 0.

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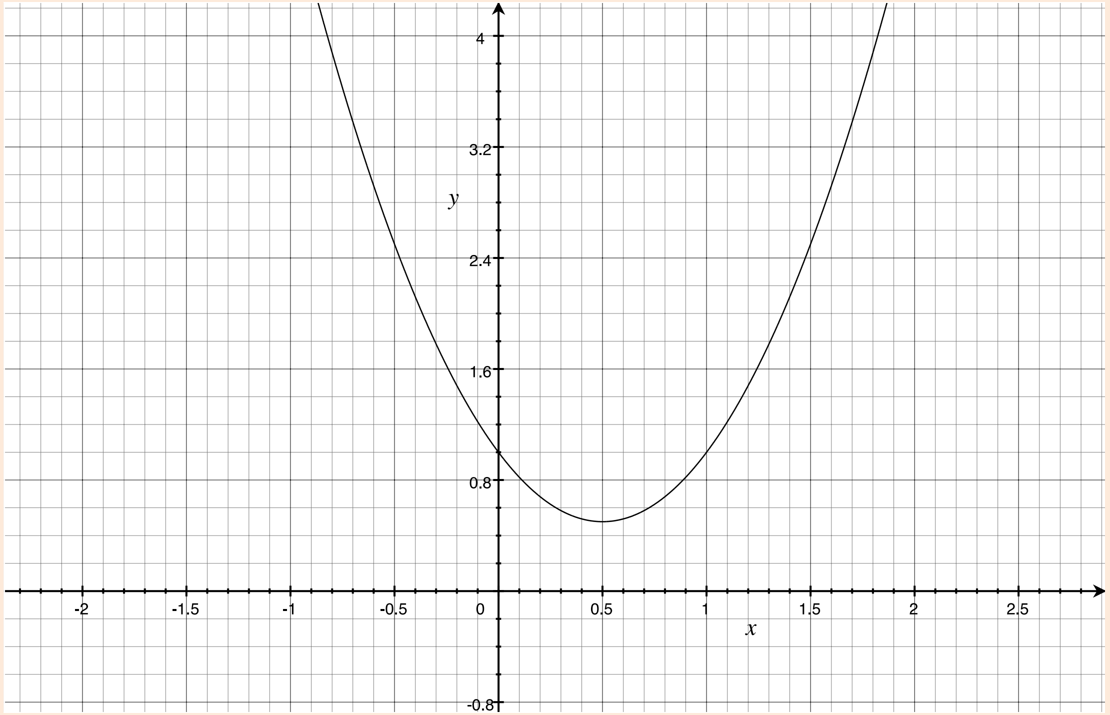
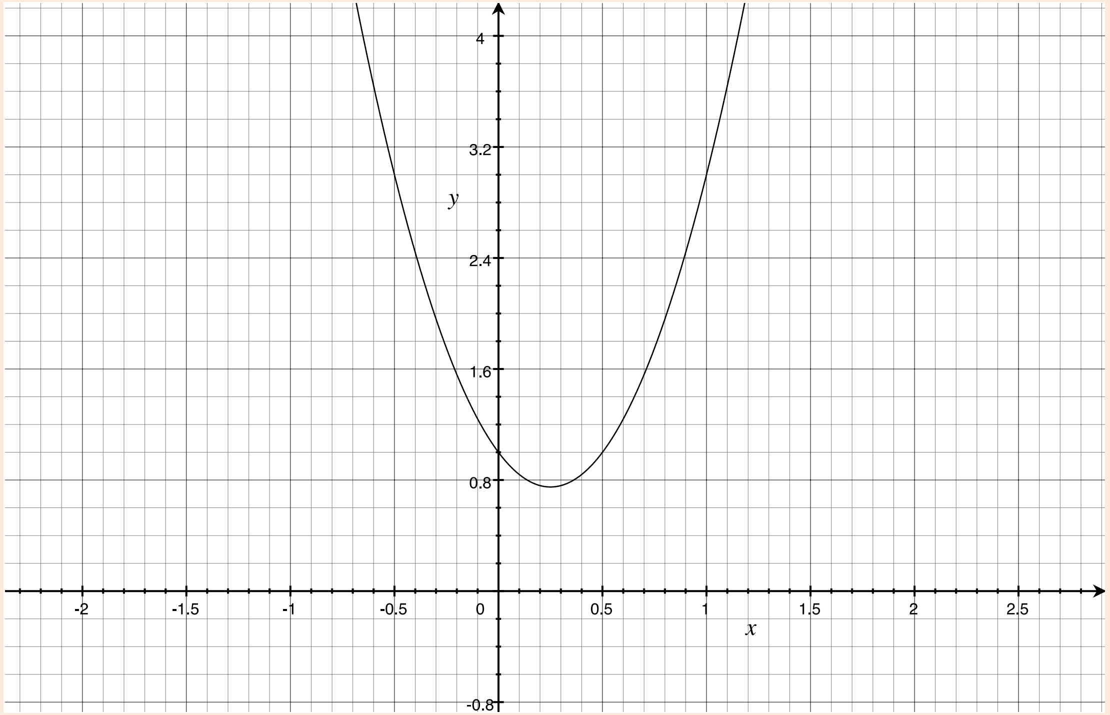
- So as λ gets bigger, 'w' converges to 0.
- However, for all finite λ 'w' will be non-zero unless $y^Tx = 0$ exactly.
  - But it's very unlikely that y^Tx will be exactly zero.

bonus!

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

- Small λ — Big λ





- Solution further from zero — Solution closer to zero (but not exactly 0)

Why does L1-Regularization set things to 0?

bonus!

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

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

bonus!

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

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

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$-f^-(0) = -y^Tx + \lambda$

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

bonus!

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$$\left.\begin{aligned} -f^-(0) &= -y^Tx + \lambda \\ -f^+(0) &= -y^Tx - \lambda \end{aligned}\right\}$$ If these are positive $(-y^Tx > \lambda)$, we can improve by increasing 'w'.

$-y^Tx - \lambda$ in the second line has a brace under it: If these are negative $(y^Tx > \lambda)$, we can improve by decreasing 'w'.

Why does L1-Regularization set things to 0?

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

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

$-f^+(0) = -y^Tx - \lambda$

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

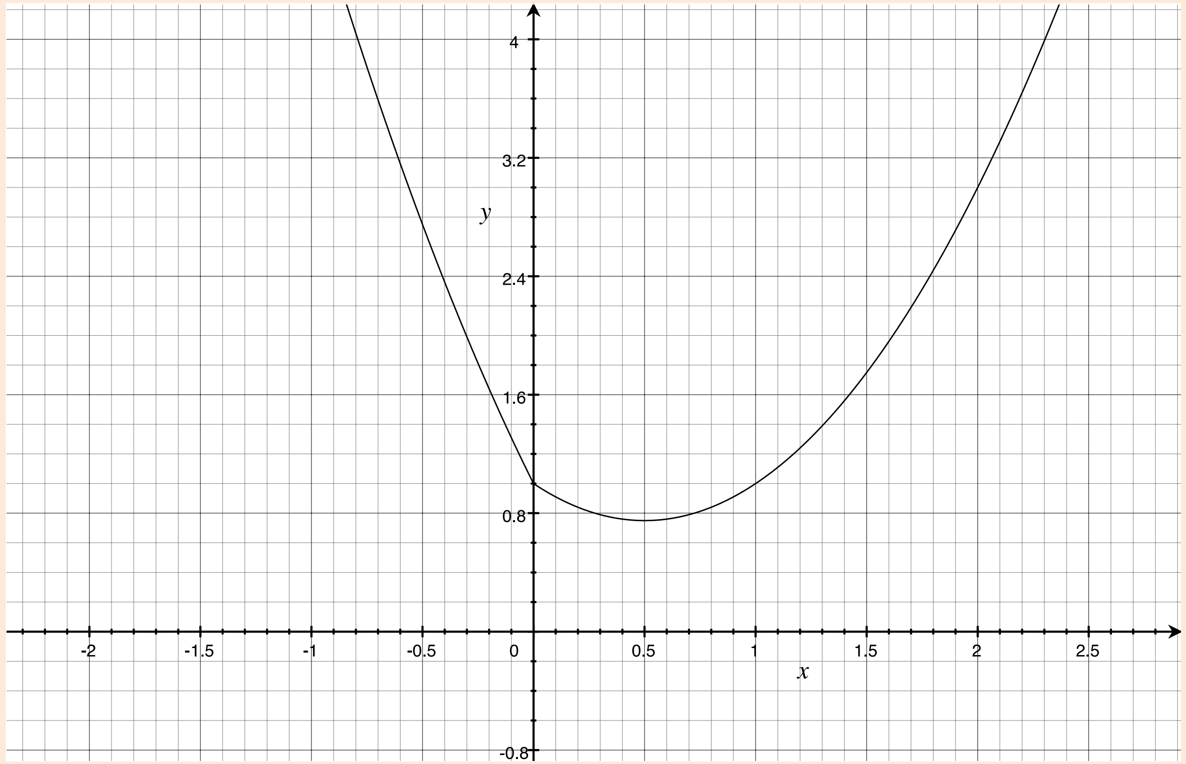
But if left and right "gradient descent" directions point in opposite directions ($|y^Tx| \leq \lambda$), minimum is 0.

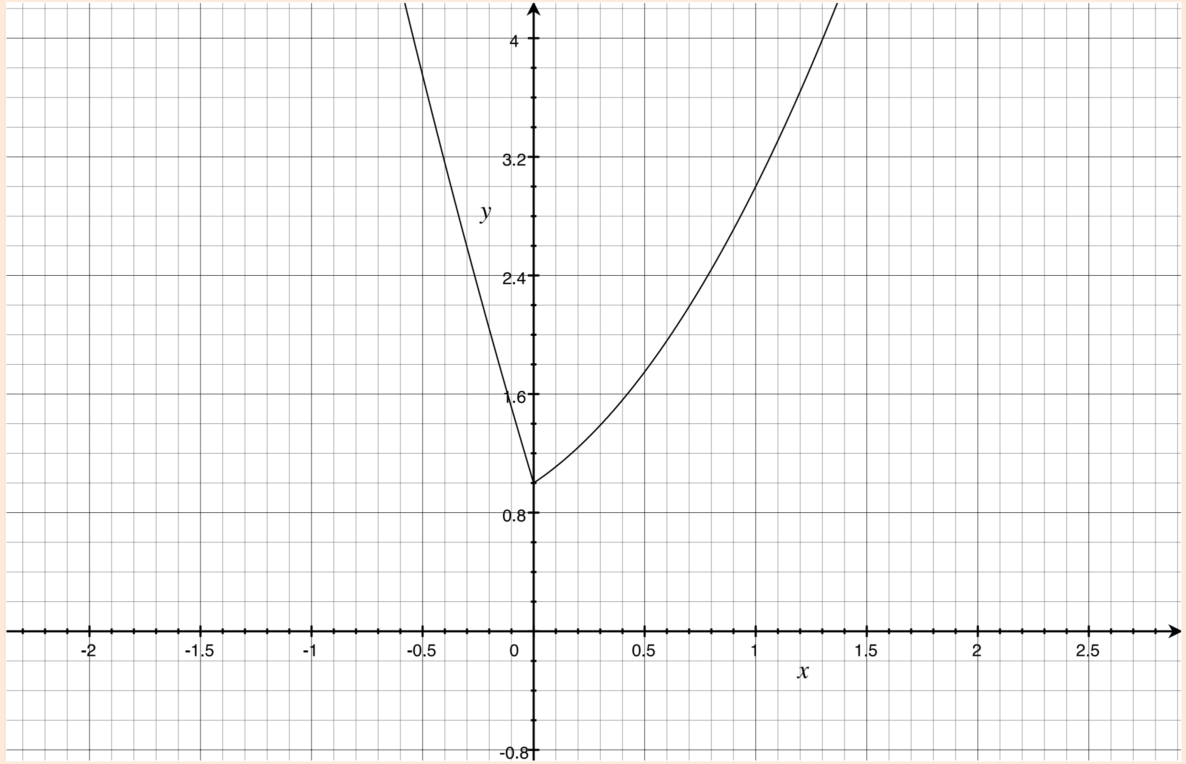
Why does L1-Regularization set things to 0?

bonus!

- Small λ

Big λ





- Solution nonzero

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

Solution exactly zero

(minimum of both parabola are past the origin)

bonus!

L2-regularization vs. L1-regularization

- So with 1 feature:
  - L2-regularization only sets 'w' to 0 if $y^T x = 0$.
    - There is a only a single possible $y^T x$ value where the variable gets set to zero.
    - And λ has nothing to do with the sparsity.

bonus!

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  - 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.
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    - 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.

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.

bonus!

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:

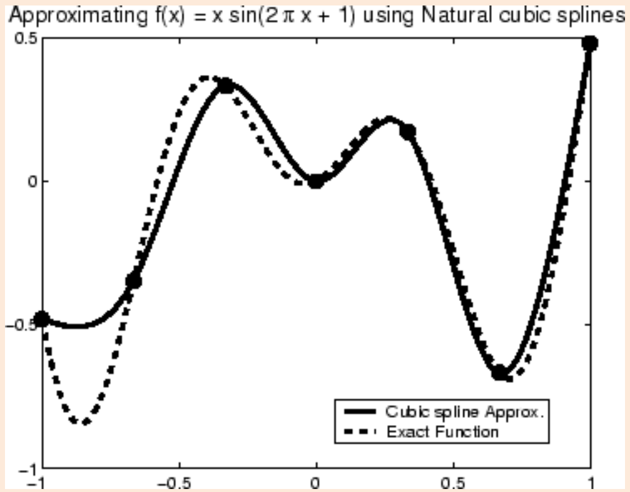
$$\hat{y}_i = w_1 x_{i1} + w_2 x_{i2} = w_1 x_{i1} + w_2 x_{i1} = (w_1 + w_2) x_{i1}$$

- 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.

bonus!

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*.

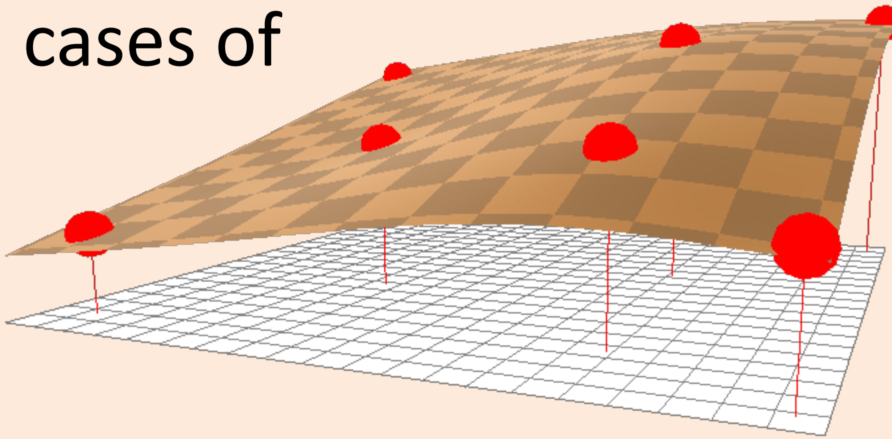


http://www.physics.arizona.edu/~restrepo/475A/Notes/sourcea-/node35.html

bonus!

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.

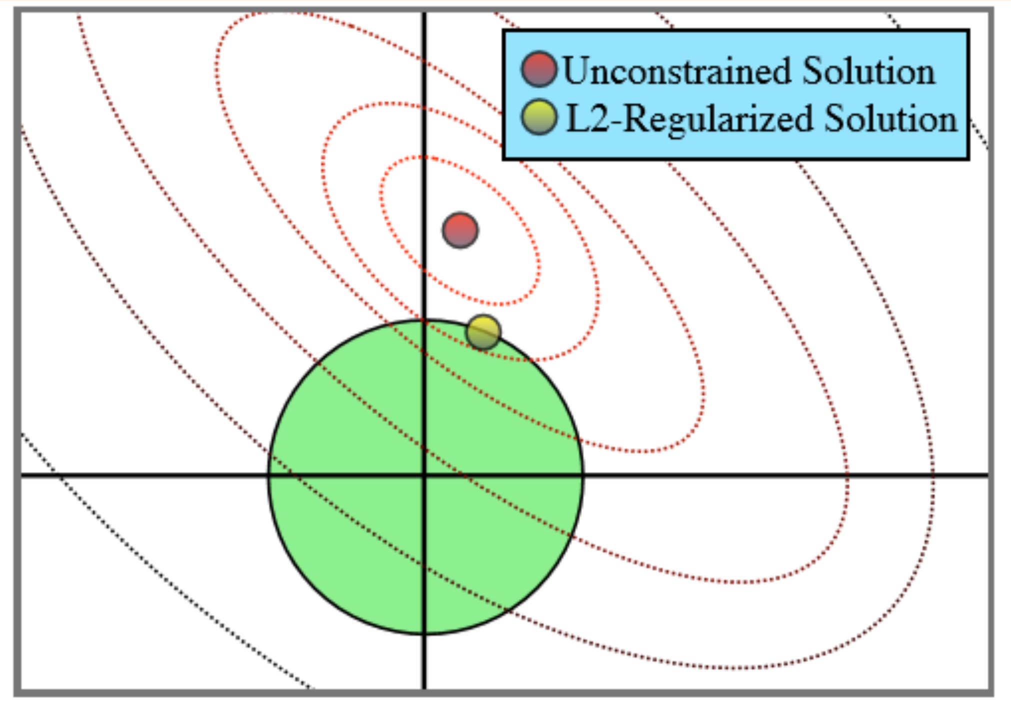


http://step.polymtl.ca/~rv101/thinplates/

bonus!

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'

bonus!

L2-Regularization vs. L1-Regularization

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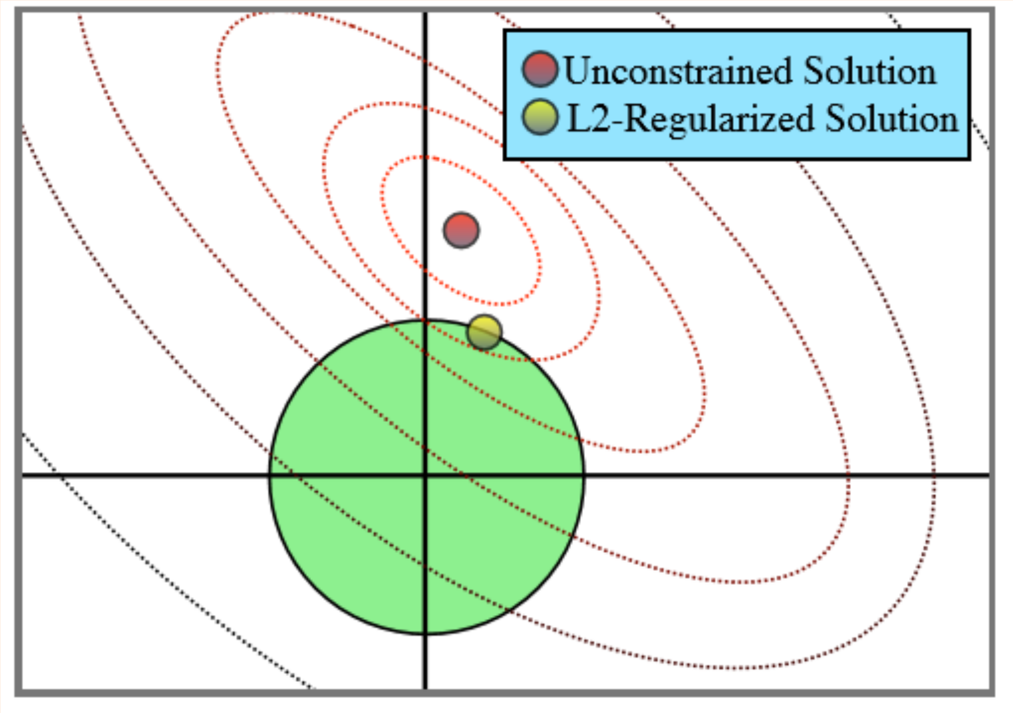

Related Infinite Series video

L2-Regularization vs. L1-Regularization

bonus!

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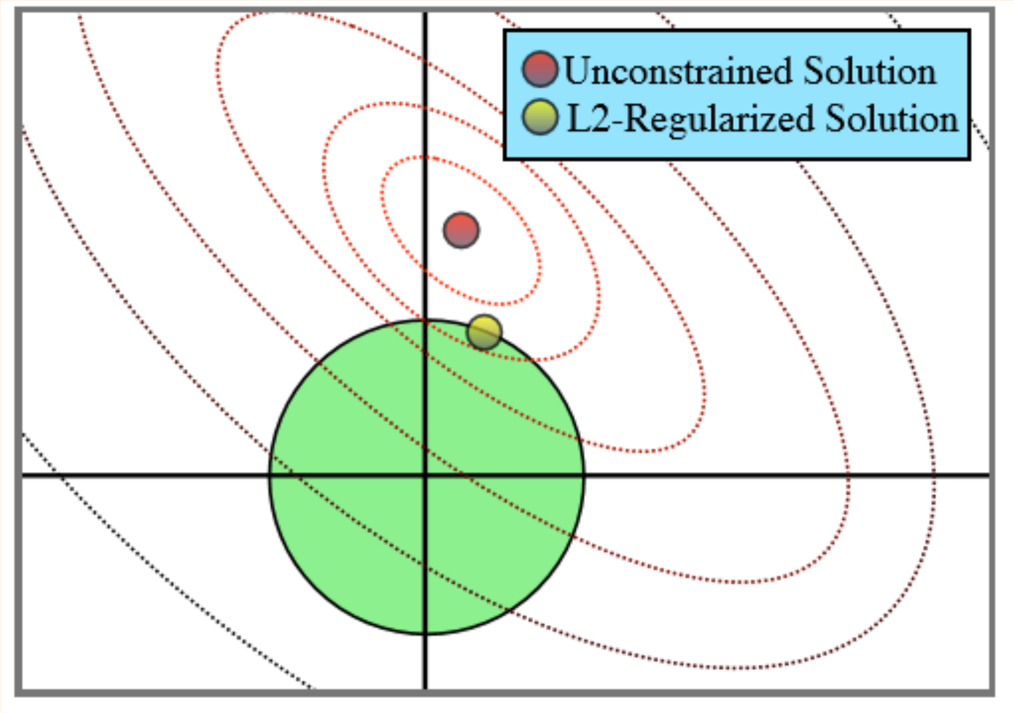

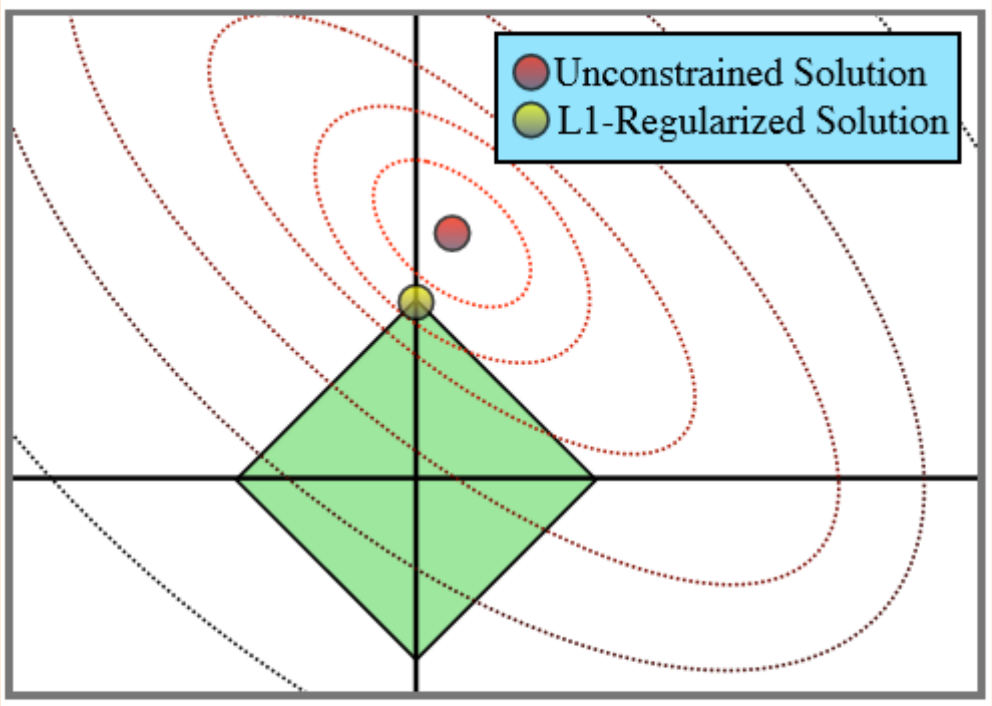

- L1-regularization restricts to the L1 “ball”:
  - Solutions tend to be at corners where w_j are zero.

[Related Infinite Series video]