# Foundations of Machine Learning
# AI2000 and AI5000

FoML-09
Underfitting and Overfitting
Regularized Least Squares


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భారతీయ సాంకేతిక విజ్ఞాన సంస్థ హైదరాబాద్
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# So far in FoML

- What is ML and the learning paradigms
- Probability refresher
- MLE, MAP, and fully Bayesian treatment
- Linear Regression with basis functions - geometric interpretation

# Under and Over fitting

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# Linear Regression

- Complex functions can be fit to the data
    - Using the basis functions

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- There are some choices (hyper parameters) to be made
  - What kind of basis functions?
  - How many of them?

# Linear Regression with basis functions

- Complex functions can be fit to the data
    - Using the basis functions
- There are some choices (hyper parameters) to be made
    - What kind of basis functions?
    - How many of them?
- They have consequences
    - over/under fitting

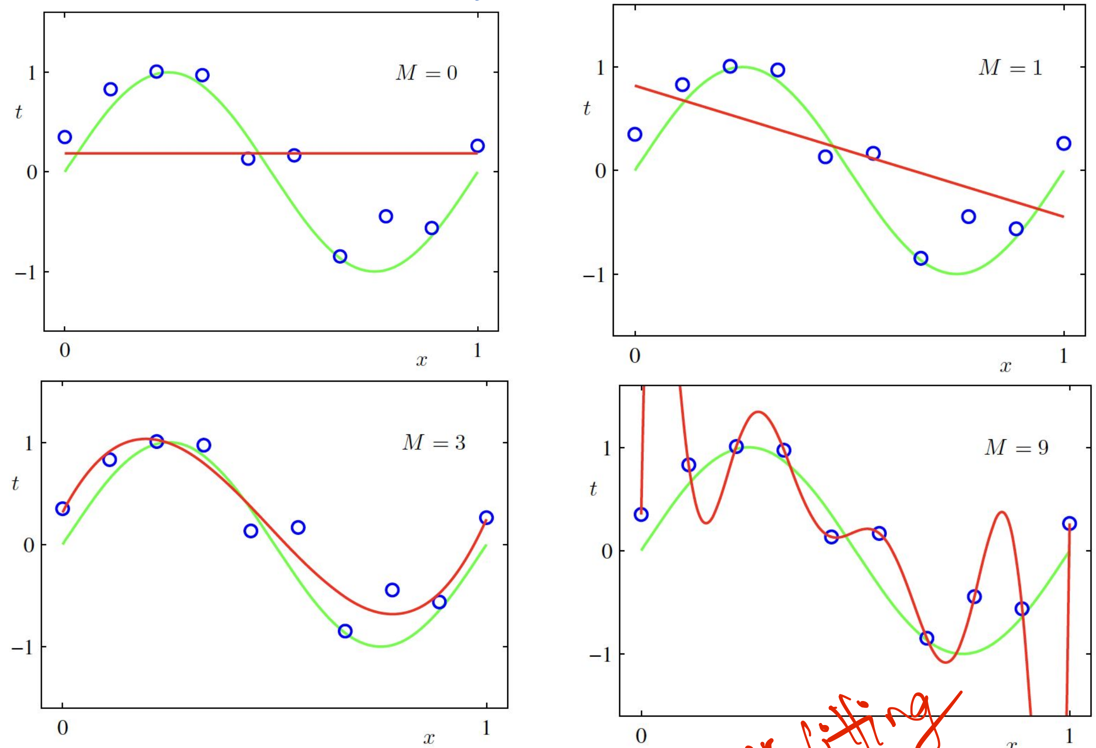
# Polynomial basis functions

underfitting

Target t = sin(2$\pi$x) + $\sigma.\epsilon$

Noise $\epsilon$ ~ N(0, 1)

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




Over fitting

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# How to spot Under/Over fitting?

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| | $M = 0$ | $M = 1$ | $M = 3$ | $M = 9$ |
|---|---|---|---|---|
| $w_0^\star$ | 0.19 | 0.82 | 0.31 | 0.35 |
| $w_1^\star$ | | -1.27 | 7.99 | 232.37 |
| $w_2^\star$ | | | -25.43 | -5321.83 |
| $w_3^\star$ | | | 17.37 | 48568.31 |
| $w_4^\star$ | | | | -231639.30 |
| $w_5^\star$ | | | | 640042.26 |
| $w_6^\star$ | | | | -1061800.52 |
| $w_7^\star$ | | | | 1042400.18 |
| $w_8^\star$ | | | | -557682.99 |
| $w_9^\star$ | | | | 125201.43 |

very Big

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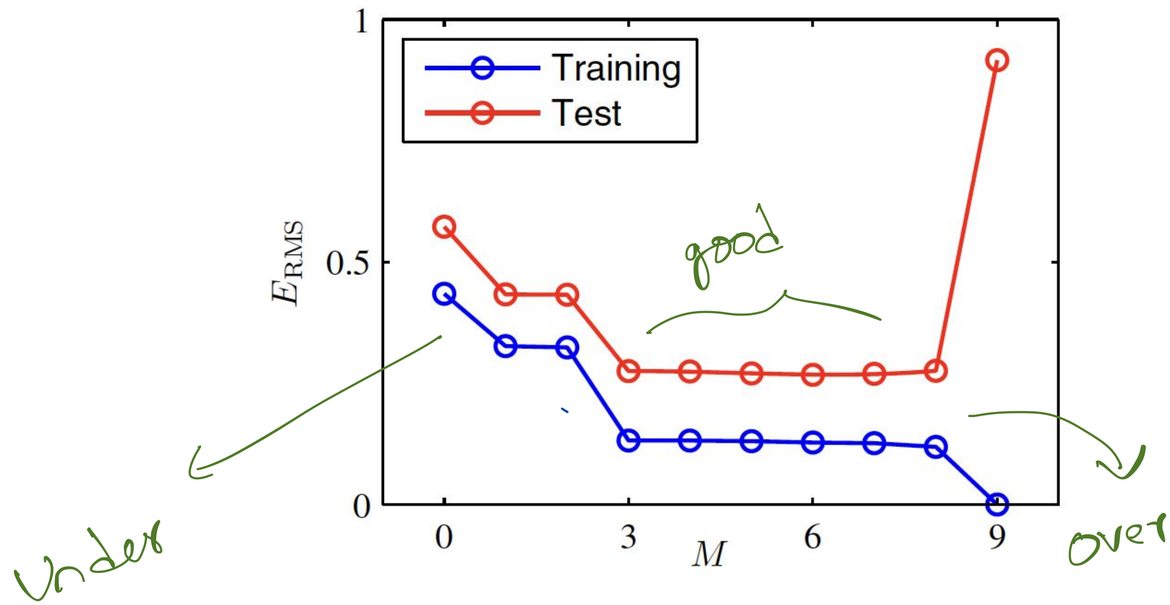
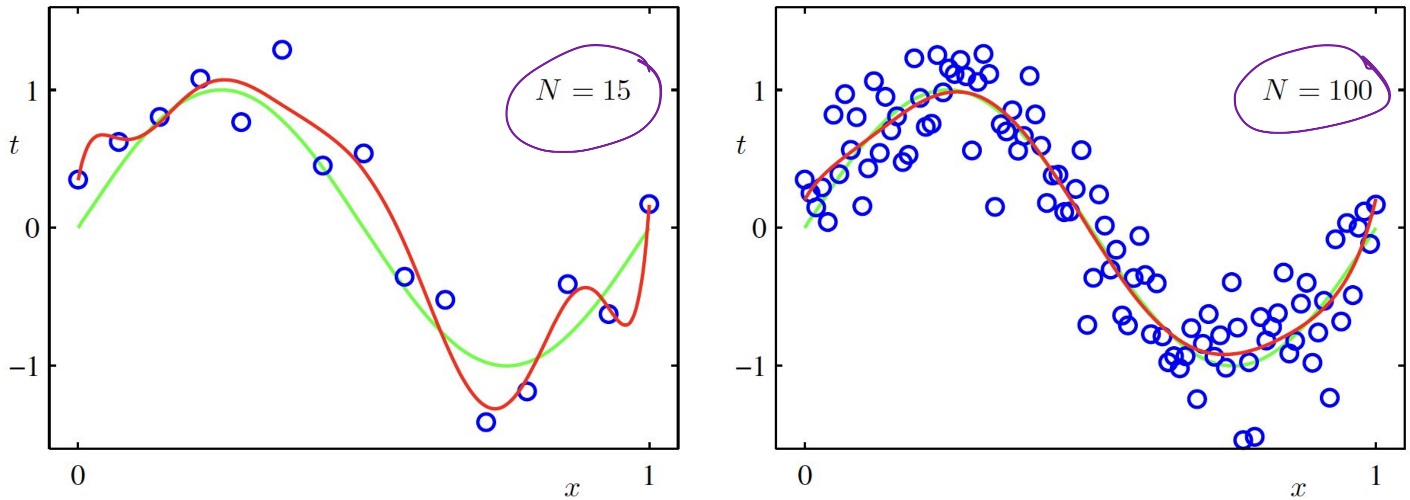
Why didn’t our M = 9 model realize a mapping similar to that of M = 3 model?

# Better way to spot under/over fitting

- Plot the error ($E_{RMS}$)



# Effect of dataset size on overfitting




M = 9 model fitting to dataset of different sizes

$\underline{w} = \hat{y} \approx y$

$\Phi$

$\underline{N \times M}$

N

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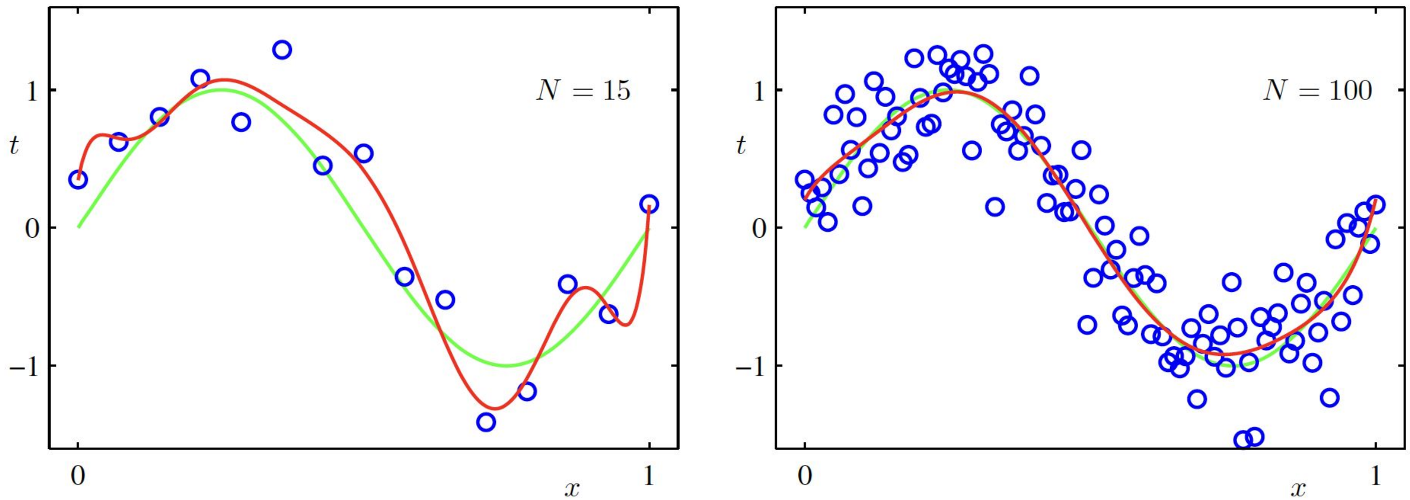


M = 9 model fitting to dataset of different sizes

For a given model complexity, the overfitting problem becomes less severe as the dataset size increases

# What if it is not easy to collect a lot of data?

- More data helps to avoid overfitting
- But, it may be challenging to collect a lot of data
- Then, what?

# Regularization

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# How to spot Under/Over fitting?

- Large weight values indicate overfitting
- Higher complexity models lead to overfitting

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# Regularized least squares

- In case of smaller datasets, instead of manually restricting the number of parameters
  - Add a penalty to avoid large weight values → 'weight decay' regularization

Called

# Regularized least squares

- In case of smaller datasets, instead of manually restricting the number of parameters
  - Add a penalty to avoid large weight values → 'weight decay' regularization

$$\tilde{E}(\mathbf{w}) = \frac{1}{2}\underbrace{\sum_{i=1}^{N}\{\mathbf{t_i} - \mathbf{w^T}\phi(\mathbf{x_i})\}^2}_{\text{MSE}} + \lambda \sum_{i=1}^{M} w_i^2$$

New objective

regularization

✓ weight decay
or
parameter shrinkage

# Regularized least squares

- In case of smaller datasets, instead of manually restricting the number of parameters
  - Add a penalty to avoid large weight values

Ridge Regression

$$\tilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}\{t_i - \mathbf{w}^T\phi(\mathbf{x}_i)\}^2 + \frac{\lambda}{2}\sum_{i=1}^{M-1} w_i^2$$

Bias term $w_0$ may not be included in the regularization

# Regularized least squares

$$\tilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}\{t_i - \mathbf{w}^T\phi(\mathbf{x}_i)\}^2 + \frac{\lambda}{2}\sum_{i=1}^{M-1} w_i^2$$

- Looks similar to what we saw during the MAP discussion

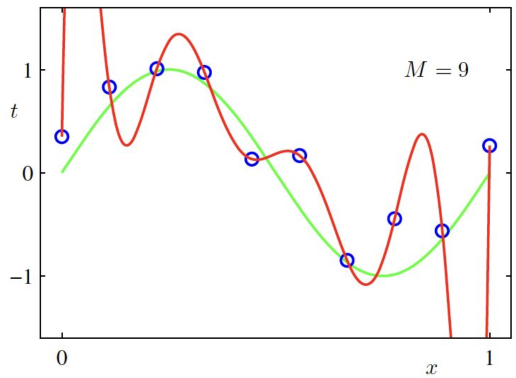
MAP objective $= \frac{\beta}{2}\sum_{i=1}^{N}\left[\;\;\right]^2 + \frac{\alpha}{2}\underline{w}^T\underline{w}$

$\lambda = \alpha/\beta$

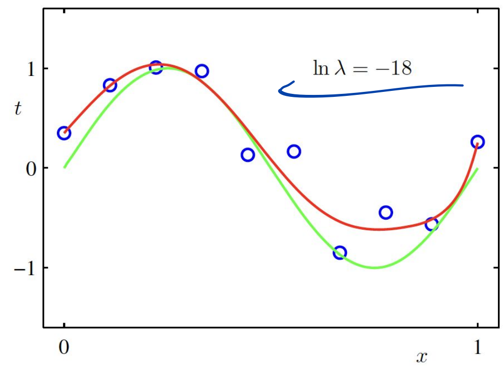
$= \beta\left[ MSE + \frac{\lambda}{2}\underline{w}^T\underline{w}\right]$

$= \beta\,\tilde{E}(\underline{w})$

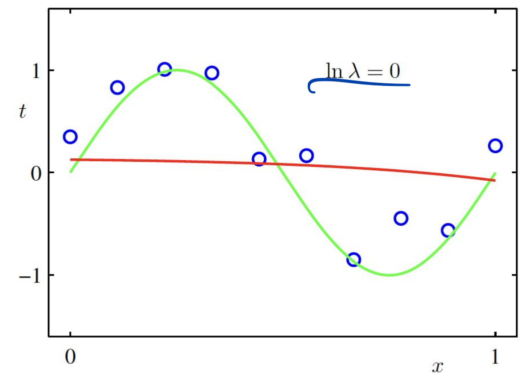
# Regularized Least Squares




w/o regularization




moderate regularization




Heavy regularization

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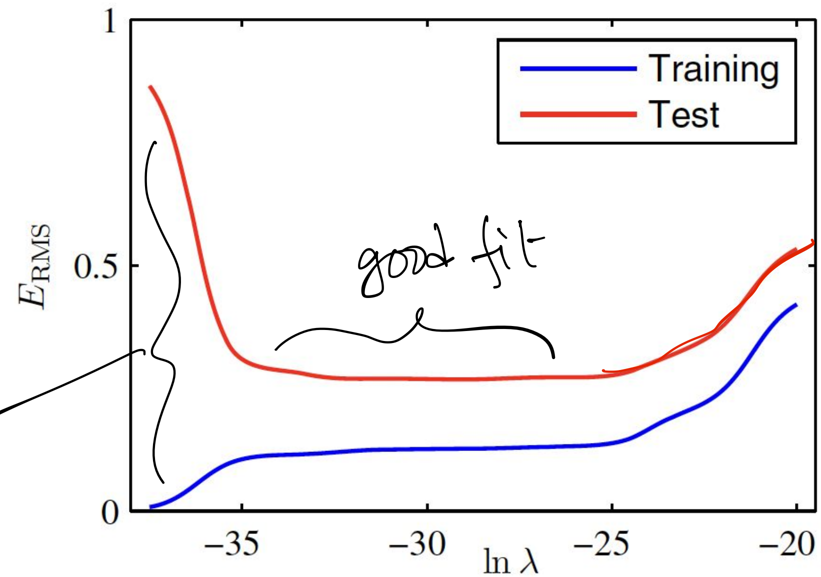
# Regularized Least Squares




good fit

over fitting

under fitting

strength of regularization

# More general form of the regularization

$$\tilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}\{\mathbf{t_i} - \mathbf{w^T}\phi(\mathbf{x_i})\}^2 + \frac{\lambda}{2}\sum_{i=1}^{M-1}|\mathbf{w_i}|^{\mathbf{q}}$$

- When q = 2 → $l_2$ norm penalty on the parameters

# More general form of the regularization

$$\tilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}\{\mathbf{t_i} - \mathbf{w}^{\mathbf{T}}\phi(\mathbf{x_i})\}^2 + \frac{\lambda}{2}\sum_{i=1}^{M-1}|\mathbf{w_i}|^{\mathbf{q}}$$

square

- When q = 2 → $l_2$ norm penalty on the parameters
- When q = 1 → $l_1$ norm penalty (also, called Lasso)

# Geometric interpretation

Equivalent to minimizing

$$\frac{1}{2}\sum_{i=1}^{N}\{t_i - \mathbf{w}^T\phi(\mathbf{x}_i)\}^2 \quad \text{with} \quad \sum_{j=1}^{M}|w_j|^q \leq \eta$$

objective

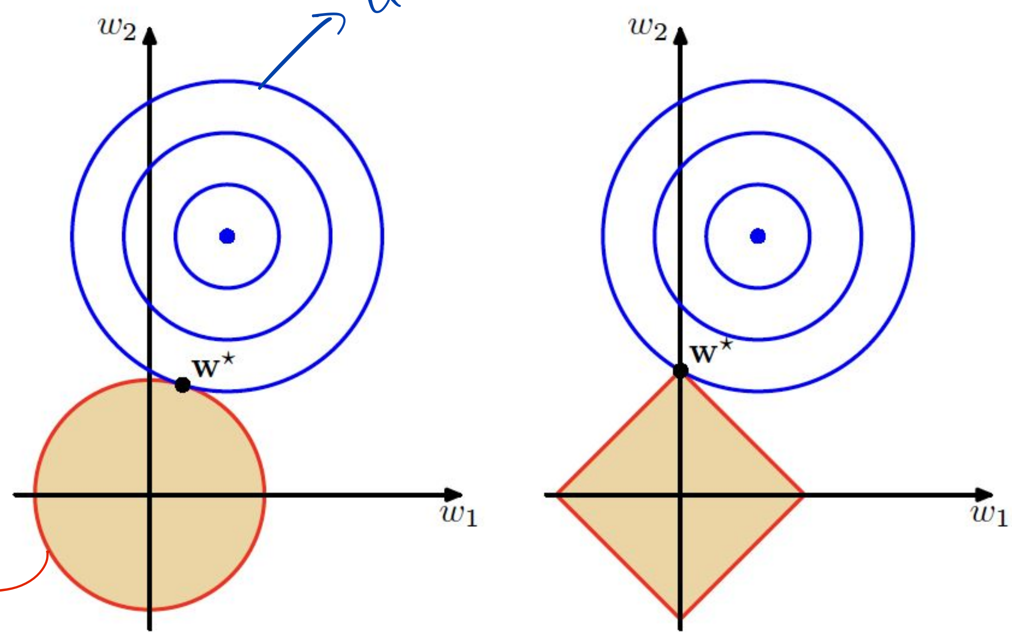
feasible set

# Geometric interpretation

unregularized error (MSE)

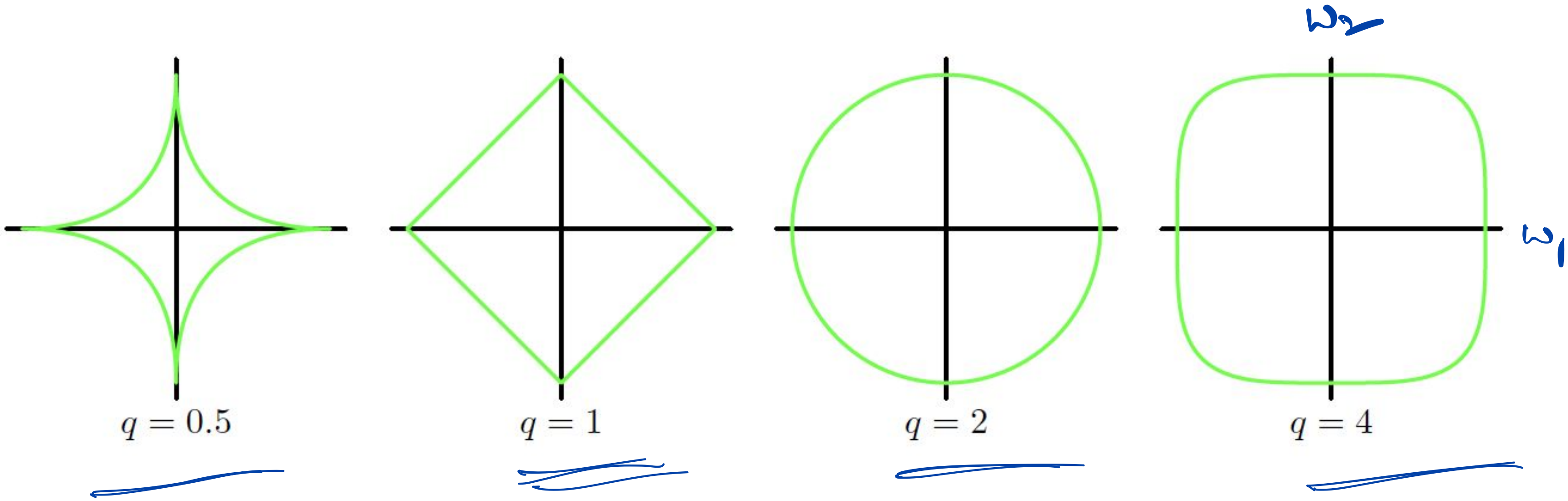
Equivalent to minimizing

$$\frac{1}{2}\sum_{i=1}^{N}\{t_i - \mathbf{w}^T\phi(\mathbf{x}_i)\}^2 \quad \text{with} \quad \sum_{j=1}^{M}|w_j|^q \leq \eta$$



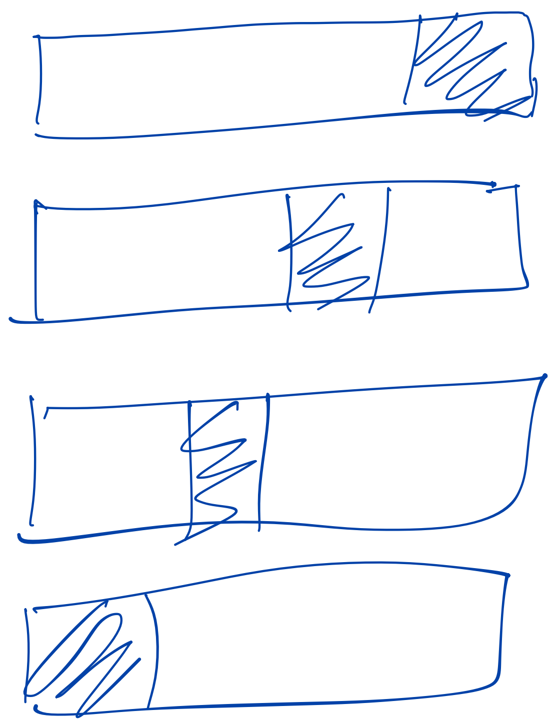

Plots of the 'unregularized' error and the 'regularization' term for q =1 and 2

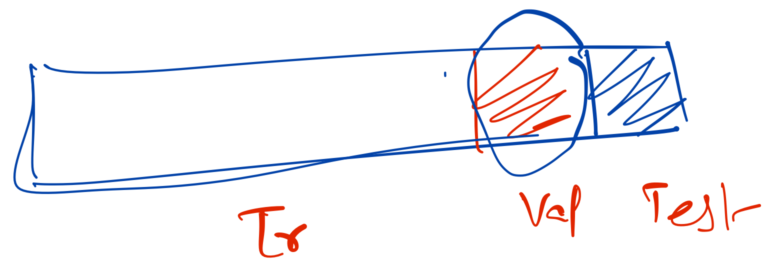
# Geometric interpretation




Contours of regularization term for different values of q

# Rough work






Model selection via
Cross validation

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# Next
# Model selection