COMPSCI 689
Lecture 6: Basis Function Expansion and Regularization

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Outline

Review

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- **Question:** What can we do when the data we are trying to model have non-linear relationships between inputs and outputs?

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- A simple solution to the linearity problem is to apply a set of functions $\phi_1,...,\phi_K$ to the raw feature vector $\mathbf{x}$ to map it in to a new feature space:

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- In the regression setting, we obtain the model $\hat{y} = \phi(\mathbf{x})\theta$.
- In the classification setting, we obtain the model $\hat{y} = \text{sign}(\phi(\mathbf{x})\theta)$.

Basis Function Expansion Examples

- **Univariate Functions:** We can set $\phi_k(\mathbf{x})$ to any univariate function of a single x_d to obtain mappings like $\phi(\mathbf{x}) = [x_1, x_2, \sin(x_1), \exp(x_2)]$, etc.

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"Interaction terms"

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- Don't forget that basis expansion still requires a bias term in the model!
- A key question is how complex should we let the basis expanded model be?

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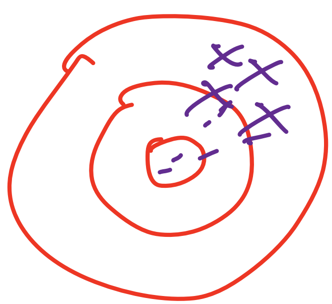
  [Illustration:]



High bias
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  [Illustration:]
- **Bias-Variance Dilemma:** To achieve low generalization error, we need models that are low-bias and low-variance, but this isn't possible for complex data.

Overfitting and Underfitting

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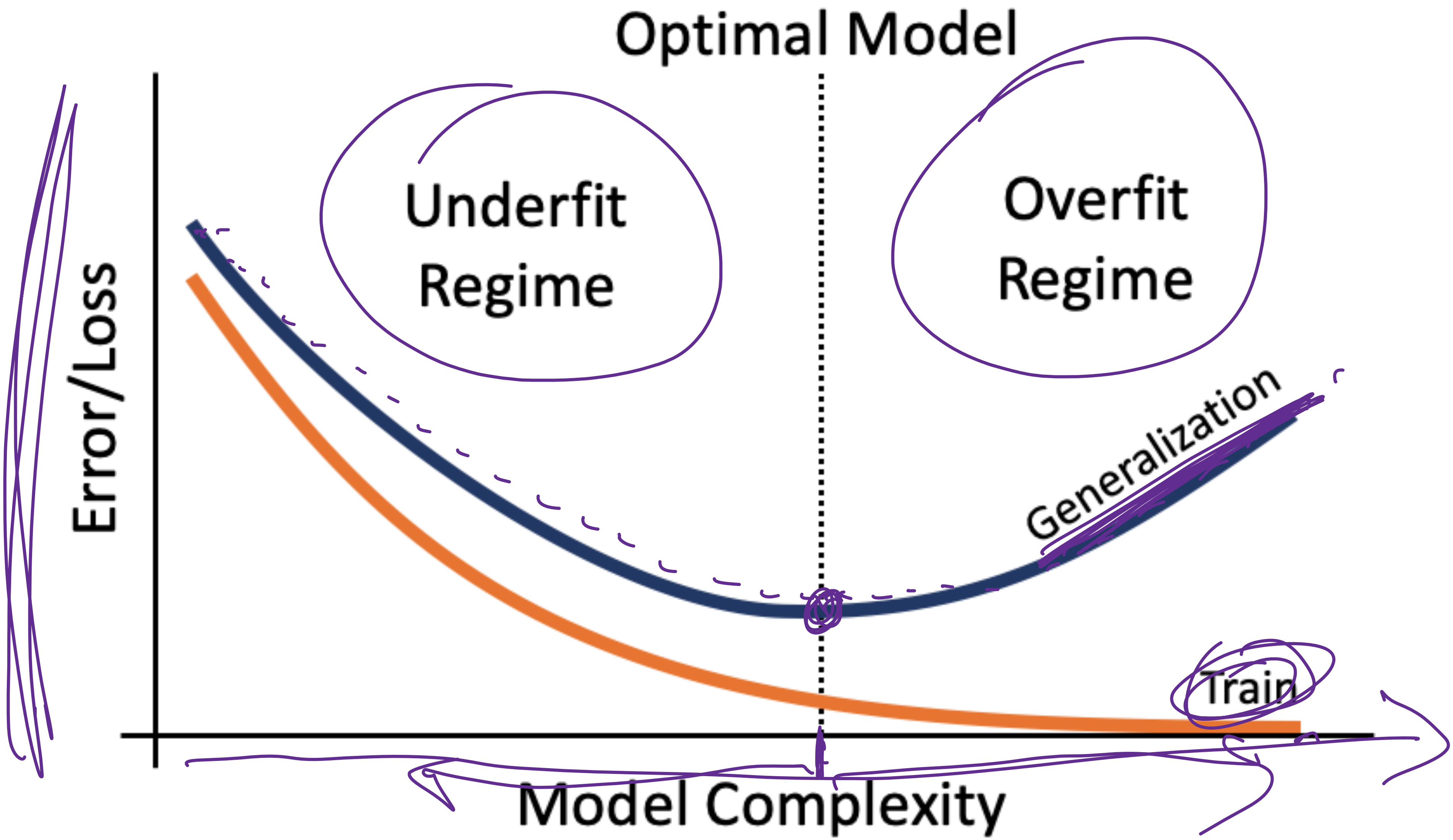
- **Overfitting:** Occurs when the complexity of the model is too high so the model is able to closely fit random variations in the data. Results is low training loss and much higher generalization loss.

Overfitting and Underfitting



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Controlling Complexity

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- The first approach is to control the complexity of the terms used in the basis expansion.
- The second approach is to control the magnitude of the weights.

Control of the Basis Expansions

- Assume that the elements in a candidate basis expansion $\phi(\mathbf{x}) = [\phi_1(\mathbf{x}), ..., \phi_K(\mathbf{x})]$ are ordered in terms of increasing complexity (for example, increasing polynomial powers).

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- To select an appropriate complexity for the basis expanded model, we construct a sequence of models $f_\theta^1, \ldots, f_\theta^K$ where model f_θ^j uses the partial basis expansion $\phi^j(\mathbf{x}) = [\phi_1(\mathbf{x}), \ldots, \phi_j(\mathbf{x})]$.

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- We then select the model f_θ^k from this set of candidates that exhibits the best generalization loss.
- We refer to the parameter k as a model complexity *hyper-parameter*. The problem of selecting the optimal value of k is referred to as a *hyper-parameter* selection problem.

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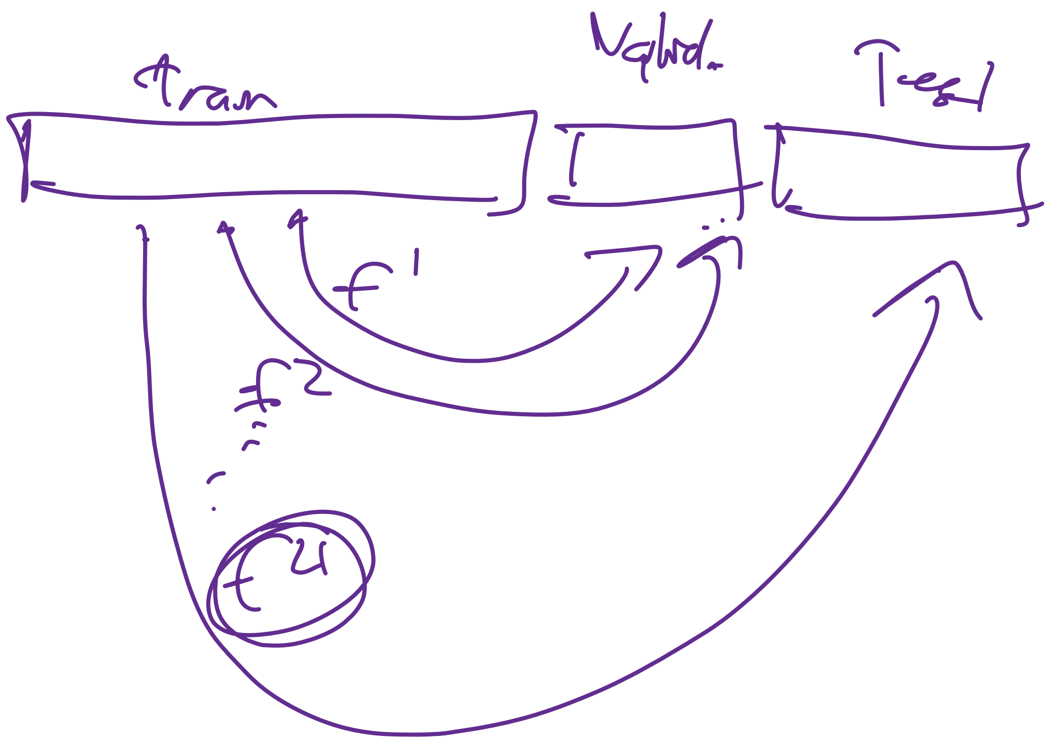

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- We learn the model parameters using the training set for each model f^j_θ.
- We then estimate the generalization loss of each fit model $f^j_{\hat{\theta}}$ using the validation set and select the value of j with the lowest estimated value of the generalization loss.

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- This experiment design is referred to as *Train-Validation-Test* experiment.

Controlling Weights

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- In linear model, smaller magnitude weights usually represent “smoother" functions.
- Controlling model complexity via weight magnitudes gives us a complementary approach to selecting from a discrete set of models of different complexity.

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$\sum_d |w_d|$

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- Note that we typically do not regularize the bias term in the model.

Visualization: L_p norm regularization

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Regularized Risk Minimization

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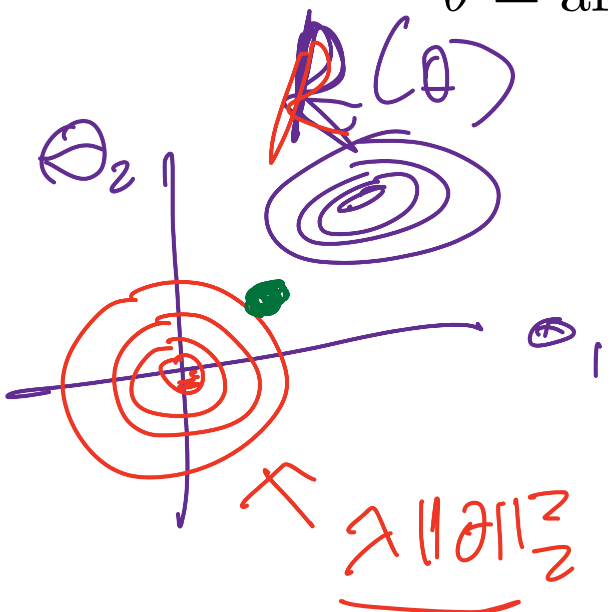
$$\hat{\theta} = \underset{\theta \in \Theta}{\arg\min} \left(\underbrace{\left(\sum_{n=1}^{N} L(y_n, f_\theta(\mathbf{x}_n)) \right)}_{\text{Train loss}} + \lambda \sum_{k=1}^{K} w_k^2 \right)$$



$\lambda = 0 \Rightarrow$ no regul. (OLS)

$\lambda = 1000 \Rightarrow \vec{w} \approx 0$

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- When $\lambda = 0$, we recover ERM and the weights are free to take arbitrary values.

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- When running such an experiment with a given range of values for λ, it is important to check that the optimal value over the range is not achieved at the minimum or maximum value tested (if it is, the range needs to be extended and the experiment re-run).
- As noted previously, to get a valid estimate of the generalization performance of the model with the optimal hyper-parameters, it is necessary to run a Train-Validation-Test experiment.

Nested optimization

When considering held-out loss and parameters vs. hyperparameters, the broader learning problem is quite complex. Typically only the parameters for training loss are differentiable.

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- A key property of this approach is that we need to have prior knowledge of a good set of potential basis expansion elements.
- Importantly, we also need to apply model complexity control methodology to balance bias and variance and thus optimize generalization performance.
- The main drawback with this approach is that while it can select from pre-specified elements, it can not learn useful basis expansion elements directly from data.