

Regularization

Lyle Ungar



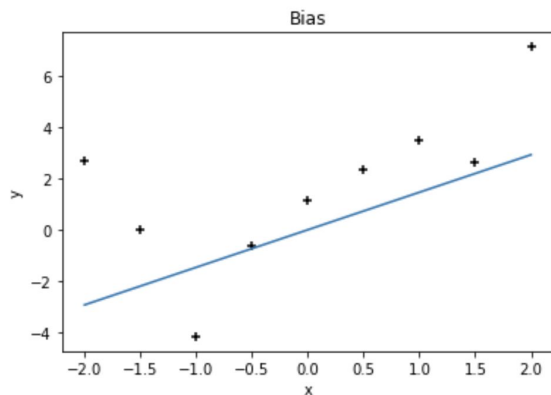
The goal of supervised learning is generalization

- **We minimize error on a training set**
 - using a *really* complex model
- **But we care about the error on a (future) test set**
 - want to fit the signal, not the noise
- **Why not use a simpler model?**
 - it doesn't work as well



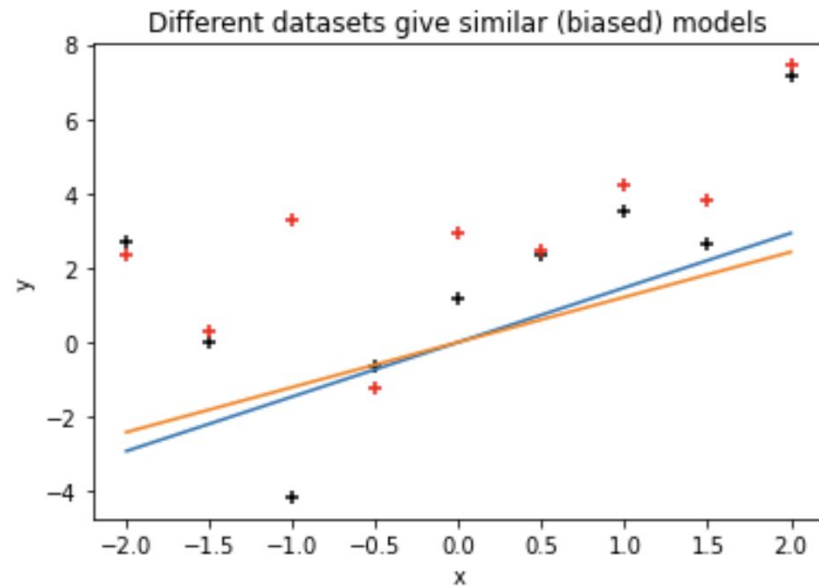
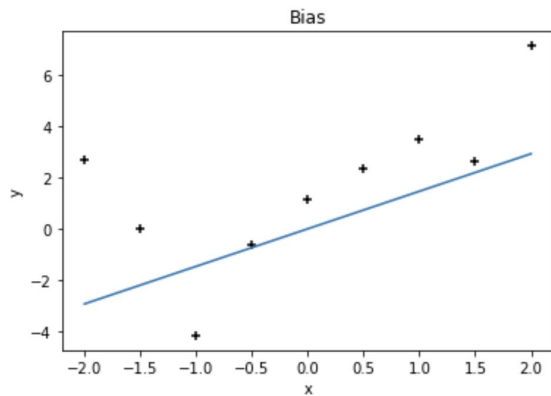
Model complexity matters

- Too simple a model “underfits”
 - It fails to capture the signal in the data



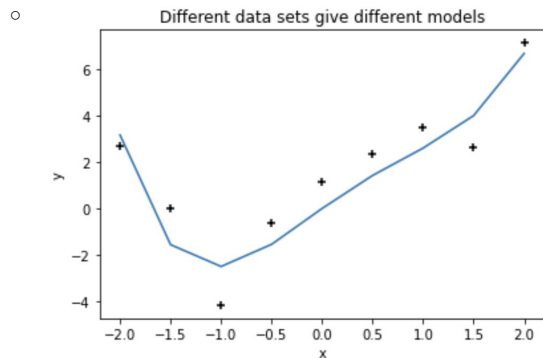
Bias

- Simple models can underfit
 - weights are systematically too small



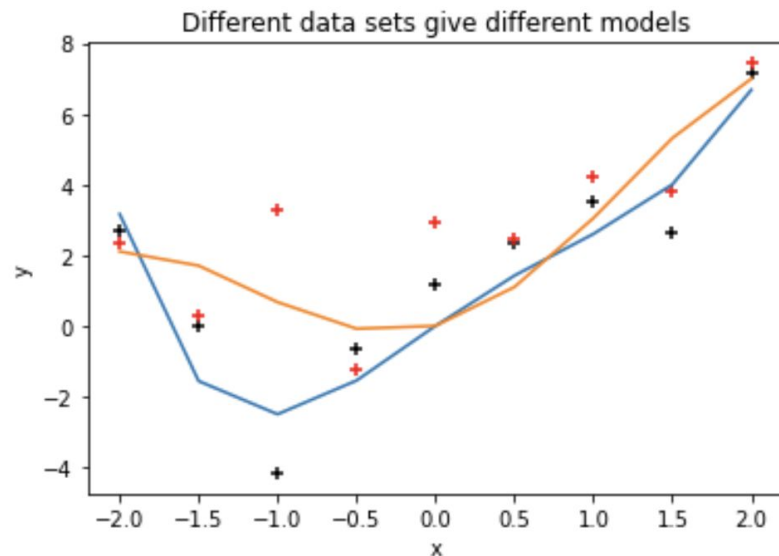
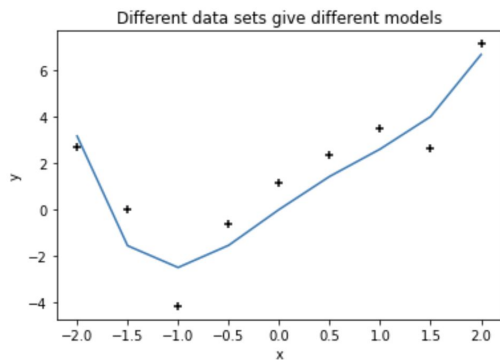
Model complexity matters

- Too complex a model “overfits”
 - It fits the noise in the data, and so generalizes poorly

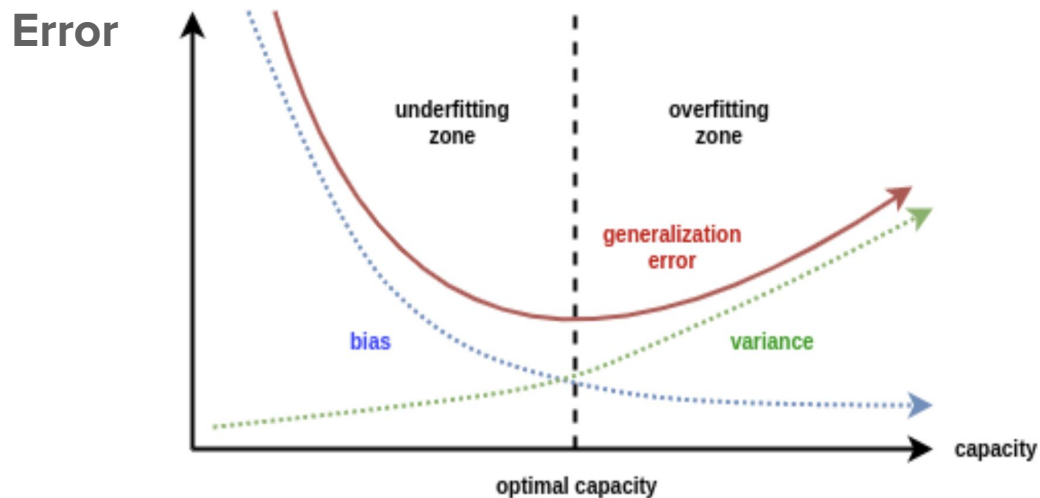


Variance

- Complex models can overfit
 - Fits the noise in the data



Picking the right model complexity



<https://images.deepai.org/>

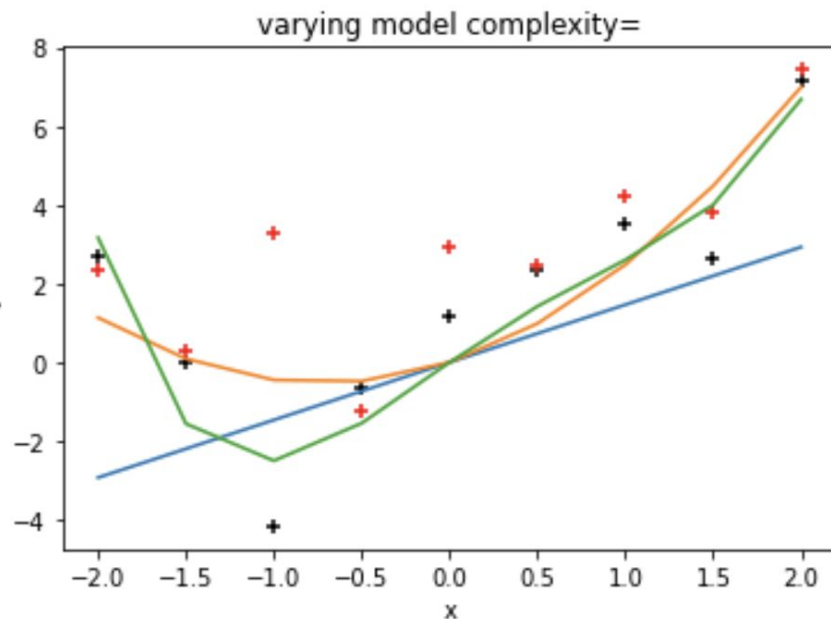


The “right” complexity generalizes best

- Too simple a model “underfits”
 - It fails to capture the signal in the data
- Too complex a model “overfits”
 - It fits the noise in the data, and so generalizes poorly

linear, quadratic and quartic models
train and test data

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Generalization and Overfitting

- Deep learning often uses more parameters than observations
 - 'should' massively overfit
- Deep learning on images (Zhang, Bengio, Hardt, Recht, and Vinyals 2017)
 - gives 0 training error -- and small test error
 - gives 0 training error with randomized labels
- GPT-3 (175B params trained on 500B words) seems to memorize a lot
 - Q. What do you call a droid that takes the long way around?
 - A. R2 detour.



Regularization is key

- **Modern neural nets don't overfit as much as one might expect**
 - often trained with similar numbers of weights and observations
- **Best accuracy from giant networks with lots of regularization**
 - best: combine many different regularizations



Today: Regularization

- Regularization controls overfitting in overparameterized models
- Regularization by
 - shrinking: L1, L2, early stopping
 - data augmentation
 - SGD
 - dropout
- Hyperparameter tuning is critical and expensive
- Adversarial attacks
 - defense via regularization



Overparameterization and Overfitting

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Overparameterization

- If you have more adjustable parameters than you have observations, you can generally fit the training data perfectly
 - E.g. 100 patients, each with an image with 40,000 voxels
- What happens when to try to use linear regression with more features than observations?



Regularization is Shrinkage

Lyle Ungar



Shrinkage is Regularization

- We'll see many ways to shrink parameters
 - L2 penalties
 - set some of them to zero
- Smaller weights
 - *regularize* more
 - give smoother models
 - give models with lower “capacity”
 - fit the noise less well



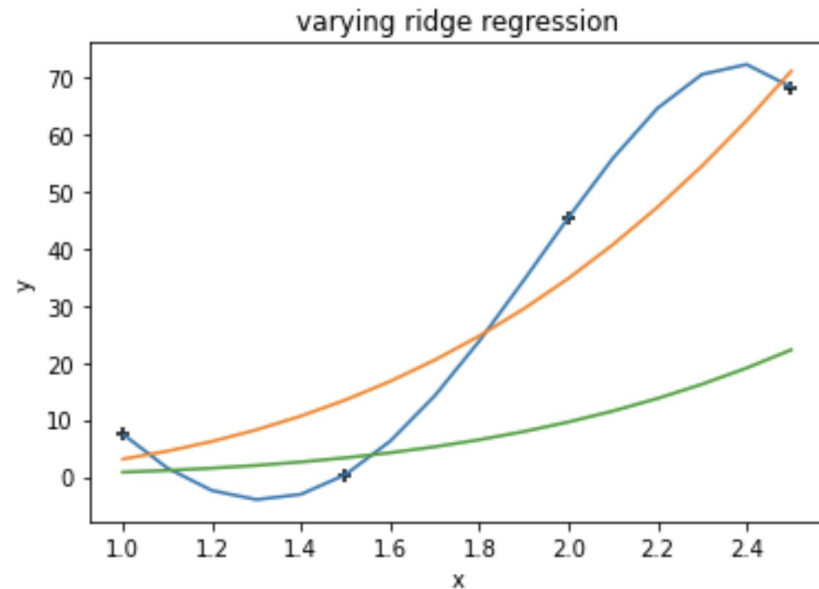
Shrinkage is Regularization

Fit $y = c_0 + c_1x + c_2x^2 + c_3x^3$

with a ridge penalty of 0, 0.5, or 5,000

higher penalty = smoother prediction

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Shrinkage is Regularization

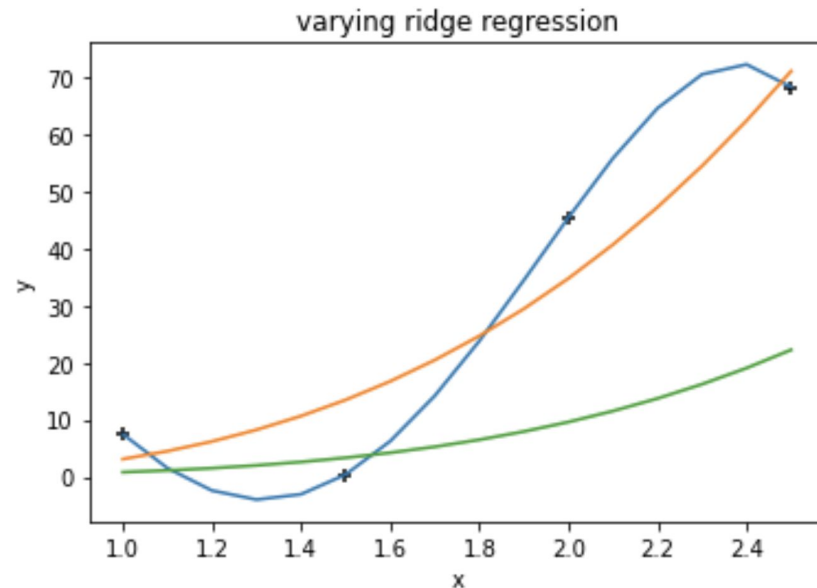
Fit $y = c_0 + c_1x + c_2x^2 + c_3x^3$

with a ridge penalty of 0, 0.5, or 5,000

$\|c\|_2$ 518, 17 0.5

higher penalty = smaller weights

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Generalization and overfitting

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Generalization and Overfitting

- Deep learning often uses more parameters than observations
 - 'should' massively overfit
- Deep learning on CIFAR10 and IMAGENET
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Zhang, Bengio, Hardt, Recht, and Vinyals 2017



Regularization via early stopping

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Early stopping

- Initialize with small weights
- These get bigger as you do gradient descent
- Stop when they are the 'optimal' size

