

Machine Learning, Computer Vision & Open Source

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Alfred P. Sloan
FOUNDATION



What is machine learning?

Types of machine learning:

- supervised
- unsupervised
- reinforcement

Supervised Learning

$$(x_i, y_i) \propto p(x, y) \quad \text{i.i.d.}$$

$$x_i \in \mathbb{R}^n$$

$$y_i \in \mathbb{R}$$

$$f(x_i) \approx y_i$$

Examples of Supervised Learning

Classification and Regression

Classification:

- y discrete

Regression:

- y continuous

Generalization

Not only

$$f(x_i) \approx y_i$$

Also for new data:

$$f(x) \approx y$$

(regularized) Empirical Risk Minimization

Goal:

$$\min_{f \in F} \mathbb{E}_{x,y} \ell(f(x), y)$$

Empirical Risk Minimization

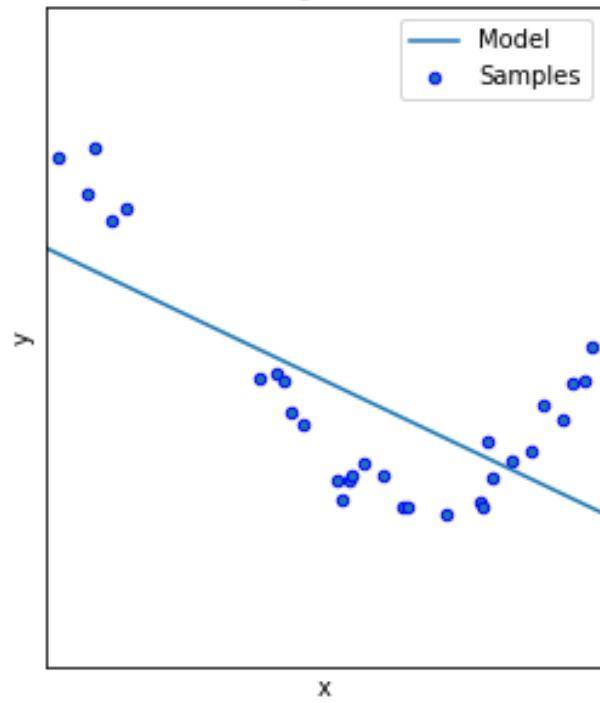
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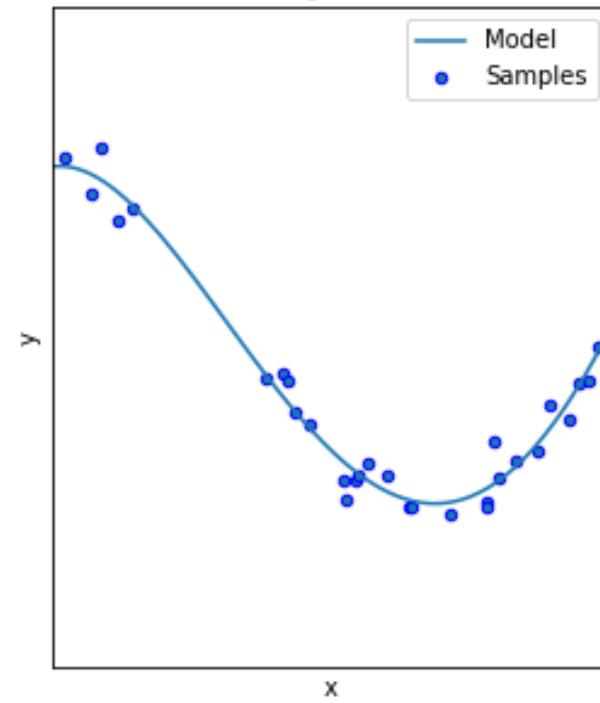
solvable:

$$\min_{f \in F} \sum_i \hat{\ell}(f(x_i), y_i)$$

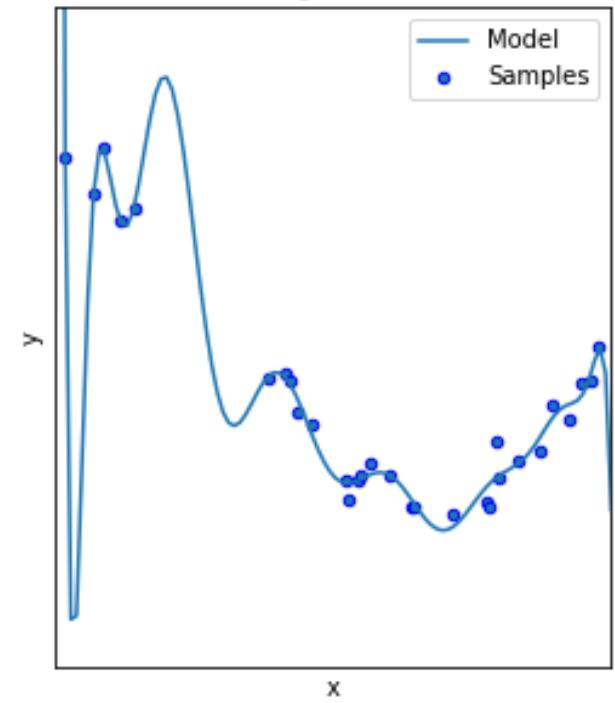
Degree 1



Degree 4



Degree 15



Regularized Empirical Risk Minimization

Goal:

$$\min_{f \in F} \mathbb{E}_{x,y} \ell(f(x), y)$$

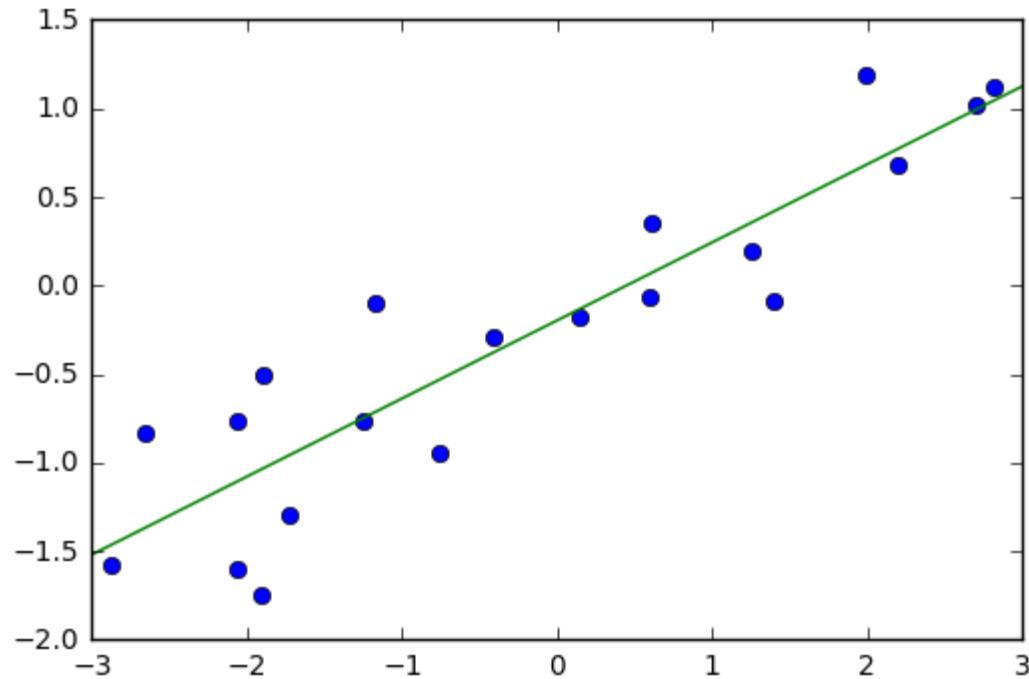
solvable:

$$\min_{f \in F} \sum_i \hat{\ell}(f(x_i), y_i)$$

better:

$$\min_{f \in F} \sum_i \hat{\ell}(f(x_i), y_i) + \lambda R(f)$$

Linear Regression as ERM



$$\min_{w \in \mathbb{R}^n} \sum_i ||w^T x_i - y_i||^2$$

Regularized Linear Regression: Ridge

$$\min_{w \in \mathbb{R}^n} \sum_i ||w^T x_i - y_i||^2 + \lambda ||w||^2$$

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Neural Networks

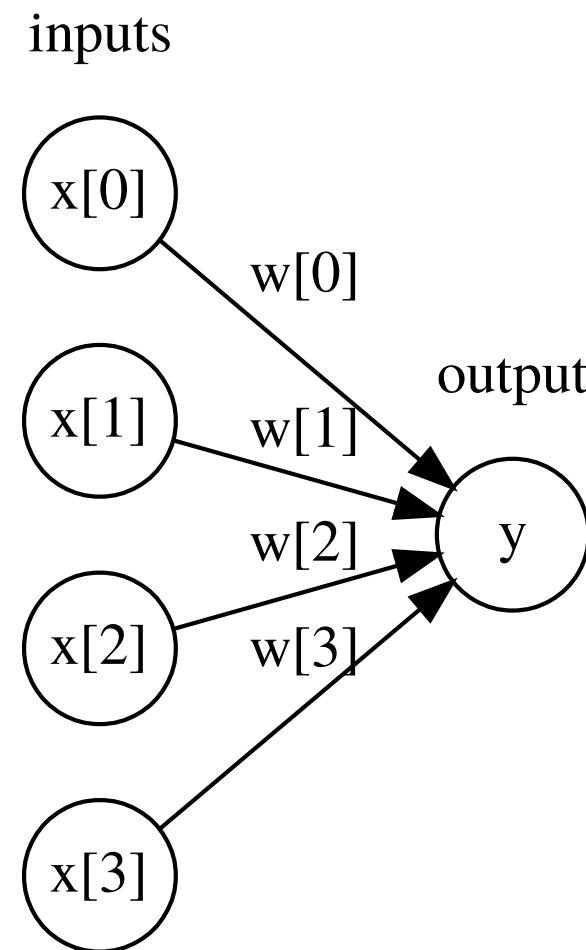
History

- Nearly everything we talk about today existed ~1990
- What changed?
 - More data
 - Faster computers (GPUs)
 - Some improvements in algorithms.

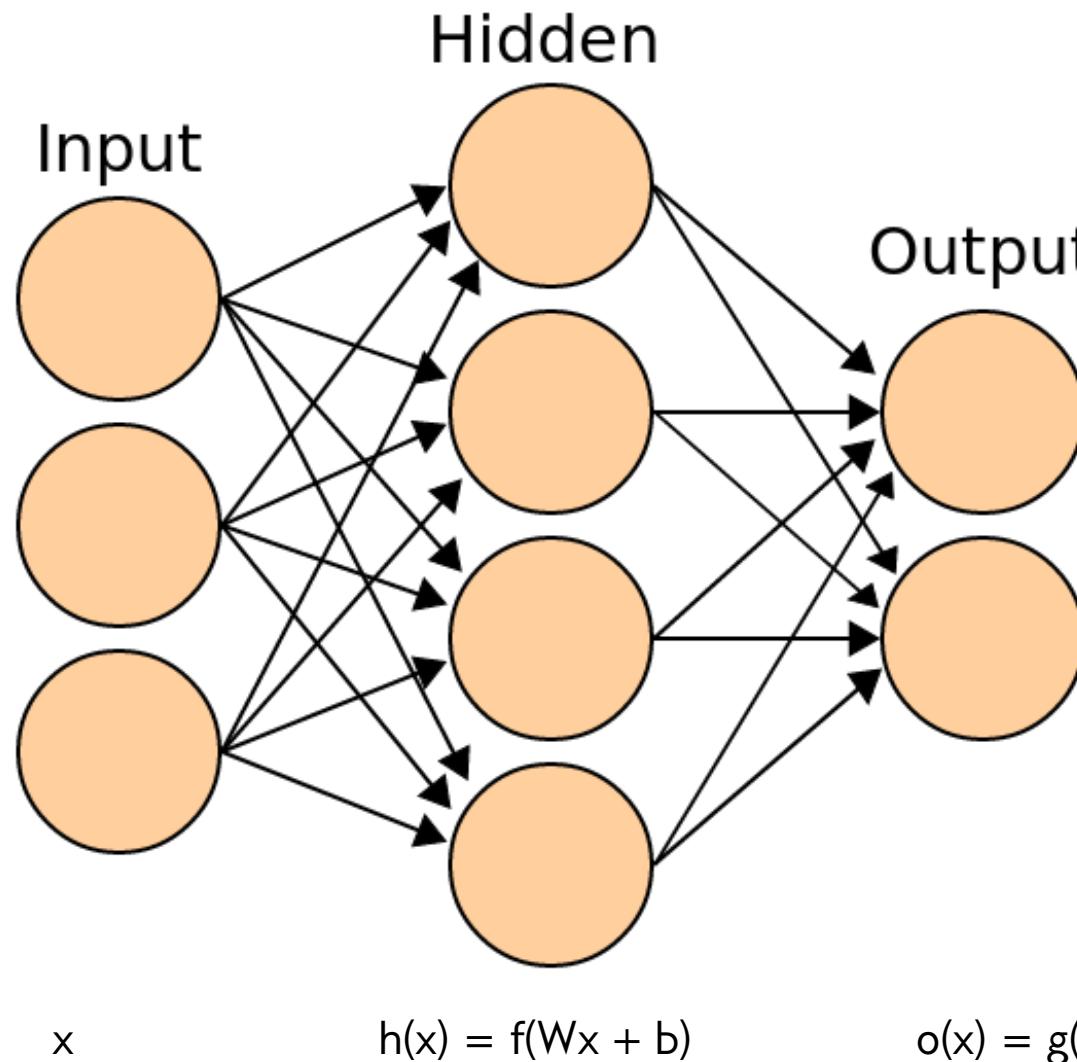
Supervised Neural Networks

- Non-linear models for classification and regression
- Work well for very large datasets
- Non-convex optimization
- Notoriously slow to train – need for GPUs
- Use dot products etc → require preprocessing, similar to SVM or linear models, unlike trees
- MANY variants (Convolutional nets, Gated Recurrent neural networks, Long-Short-Term Memory, recursive neural networks, variational autoencoders, general adversarial networks, neural turing machines...)

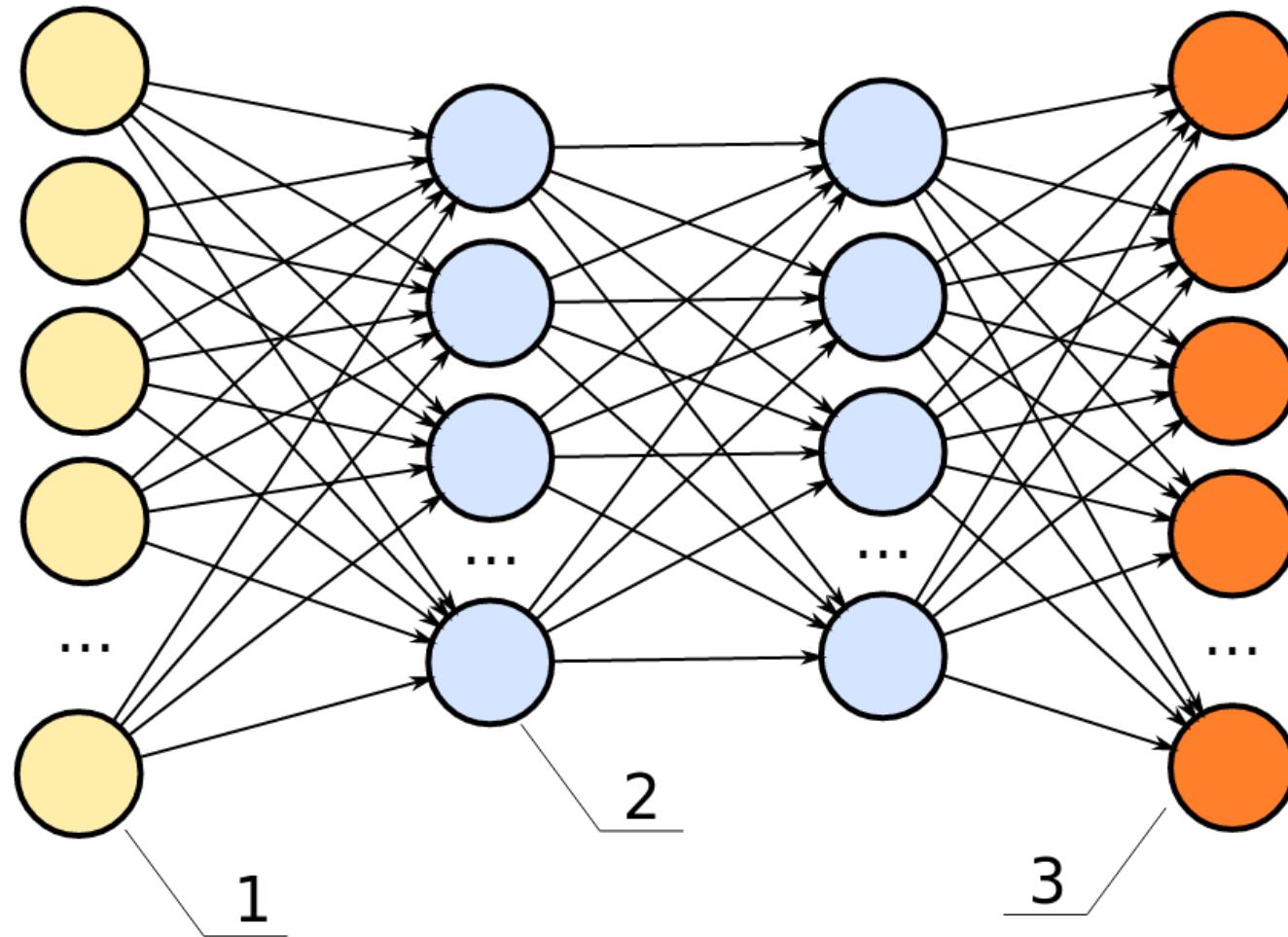
Linear regression drawn as neural net



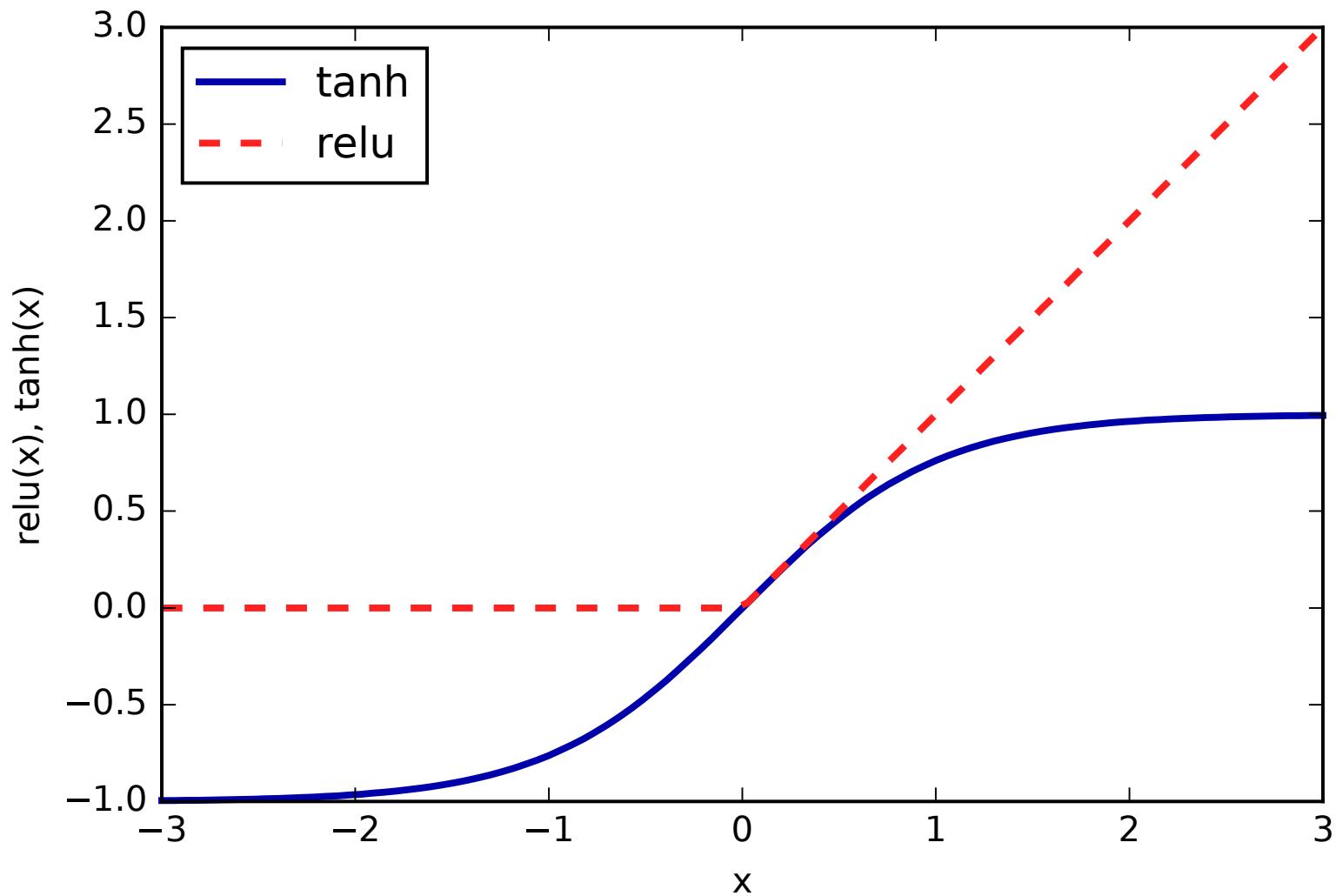
Basic Architecture (for making predictions)



Can have arbitrary many layers



Nonlinear activation function



Training objective

$$h(\mathbf{x}) = f(W_1 \mathbf{x} + \mathbf{b}_1)$$

$$o(\mathbf{x}) = g(W_2 h(\mathbf{x}) + \mathbf{b}_2) = g(W_2 f(W_1 \mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2)$$

$$\min_{W_1, W_2, \mathbf{b}_1, \mathbf{b}_2} \sum_{i=1}^N \ell(y_i, o(\mathbf{x}_i)) \quad \text{Could add regularization}$$

$$= \min_{W_1, W_2, \mathbf{b}_1, \mathbf{b}_2} \sum_{i=1}^N \ell(y_i, g(W_2 f(W_1 \mathbf{x}_i + \mathbf{b}_1) + \mathbf{b}_2))$$

ℓ squared loss for regression
cross-entropy loss (multi-class log-loss) for classification

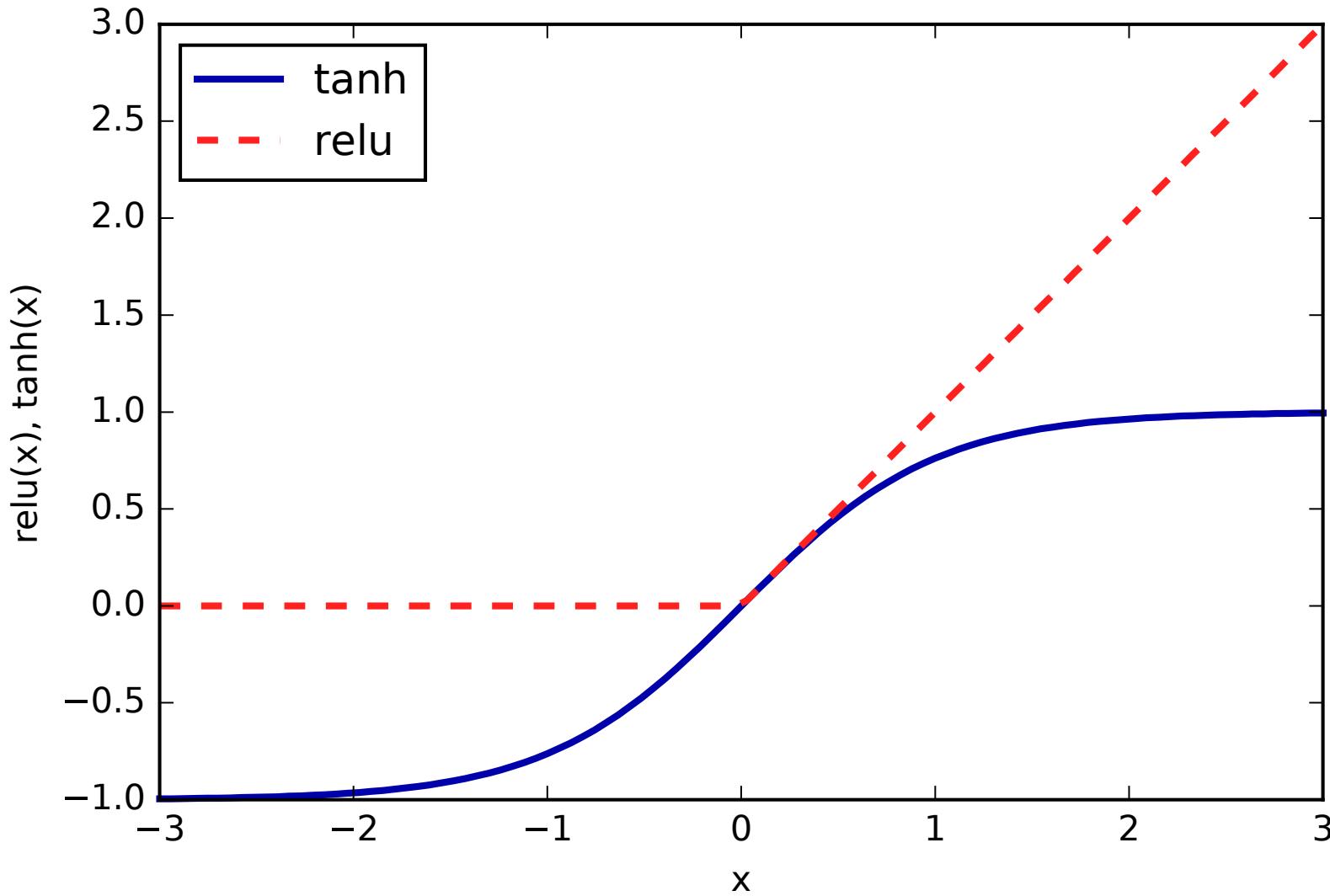
Backpropagation

- For gradient based-method need $\frac{\partial o(\mathbf{x})}{\partial W_i}$ $\frac{\partial o(\mathbf{x})}{\partial \mathbf{b}_i}$
 $\text{net}(\mathbf{x}) := W_1 \mathbf{x} + b_1$

$$\frac{\partial o(\mathbf{x})}{\partial W_1} = \underbrace{\frac{\partial o(\mathbf{x})}{\partial h(\mathbf{x})}}_{\text{backpropagation of gradient of layer above.}} \underbrace{\frac{\partial h(\mathbf{x})}{\partial \text{net}(\mathbf{x})}}_{\text{Gradient of Non-linearity } f} \underbrace{\frac{\partial \text{net}(\mathbf{x})}{\partial W_1}}_{\text{Input to 1}^{\text{st}} \text{ layer } \mathbf{x}}$$

Backpropagation = Chain Rule + Dynamic Programming

But wait!



Optimizing W, b

$$W_i \leftarrow W_i - \eta \sum_{j=1}^n \frac{\ell(\mathbf{x}_j, y_j)}{W_i} \quad \text{batch}$$

$$W_i \leftarrow W_i - \eta \sum_{j=k}^{k+m} \frac{\ell(\mathbf{x}_j, y_j)}{W_i} \quad \text{minibatch}$$

$$W_i \leftarrow W_i - \eta \frac{\ell(\mathbf{x}_j, y_j)}{W_i} \quad \text{Online / stochastic}$$

Learning Heuristics

- Constant η not good
- Can decrease η
- Better: adaptive η for each entry if W_i
- State-of-the-art: adam (with magic numbers)

<https://arxiv.org/pdf/1412.6980.pdf>

<http://sebastianruder.com/optimizing-gradient-descent/>

Open Questions in Neural Networks

- Why are they so effective?
- When are they effective?
- What are good learning methods and architectures?
- What role does optimization play?
- How can we implement memory or algorithms in neural networks?

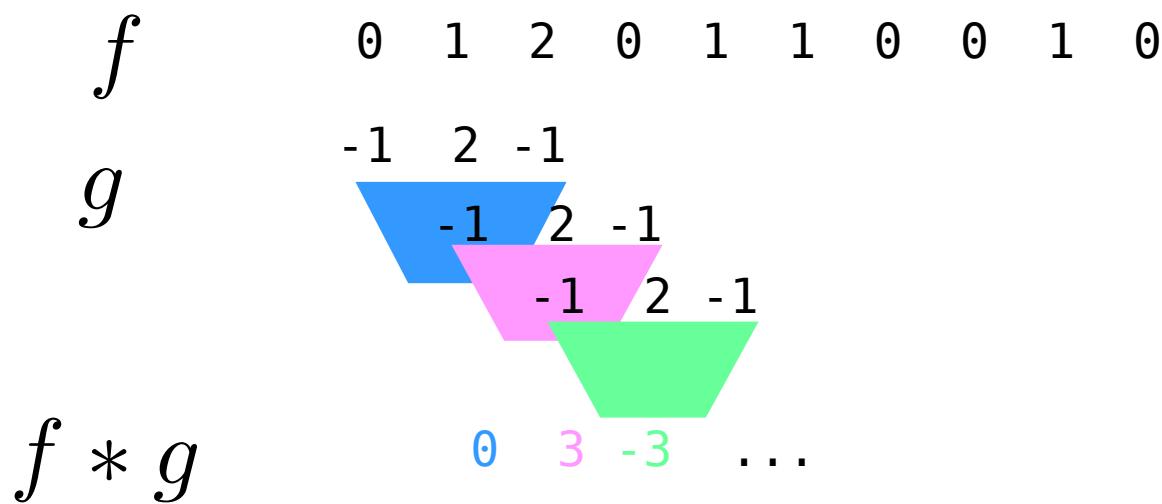
Convolutional Neural Networks

Idea

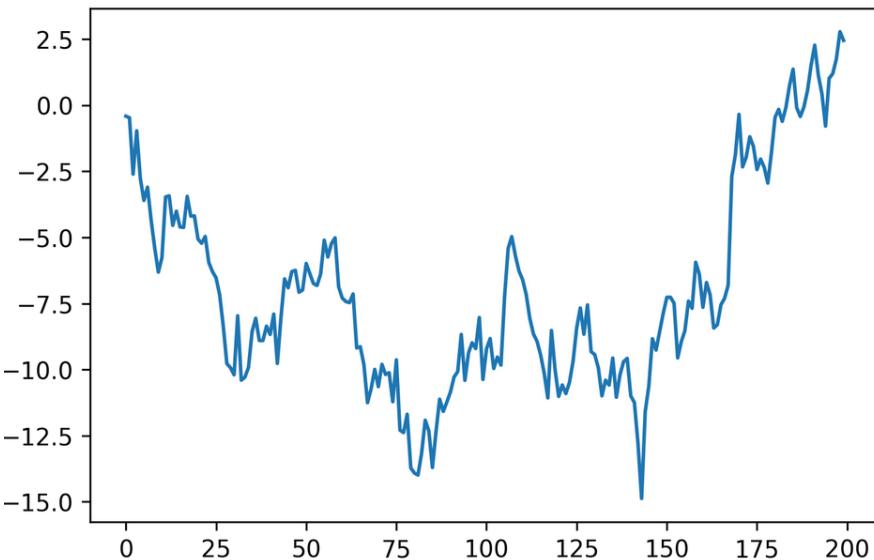
- Translation invariance
- Weight sharing

Definition of Convolution

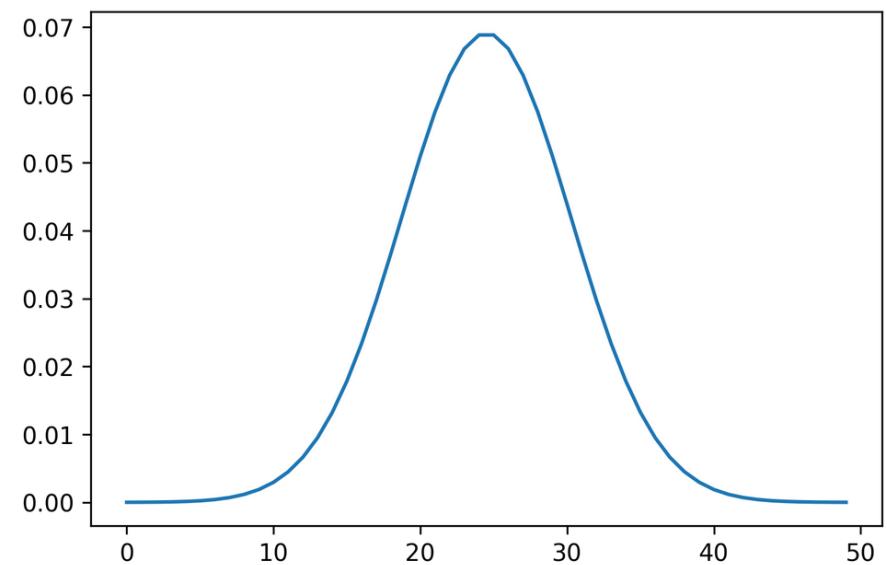
$$\begin{aligned}(f * g)[n] &= \sum_{m=-\infty}^{\infty} f[m] g[n - m] \\&= \sum_{m=-\infty}^{\infty} f[n - m] g[m].\end{aligned}$$



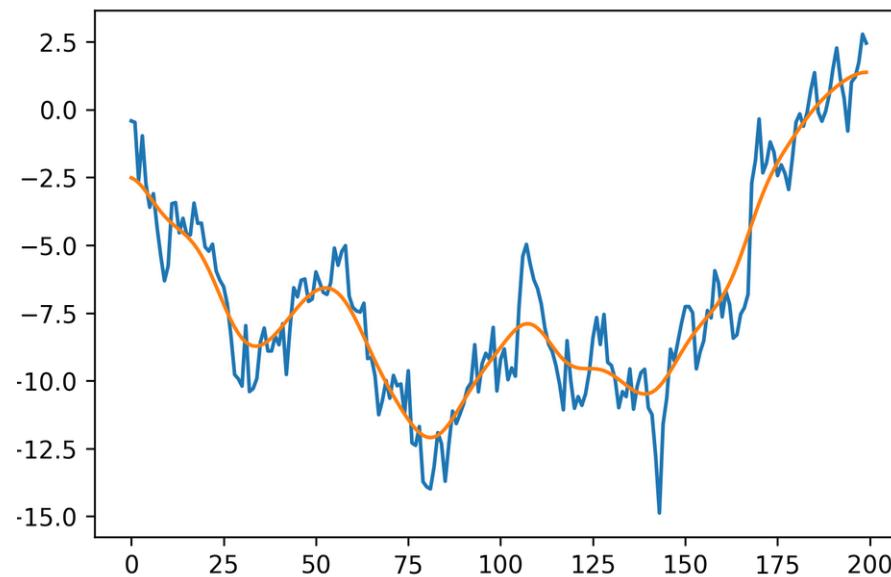
1d example: Gaussian smoothing



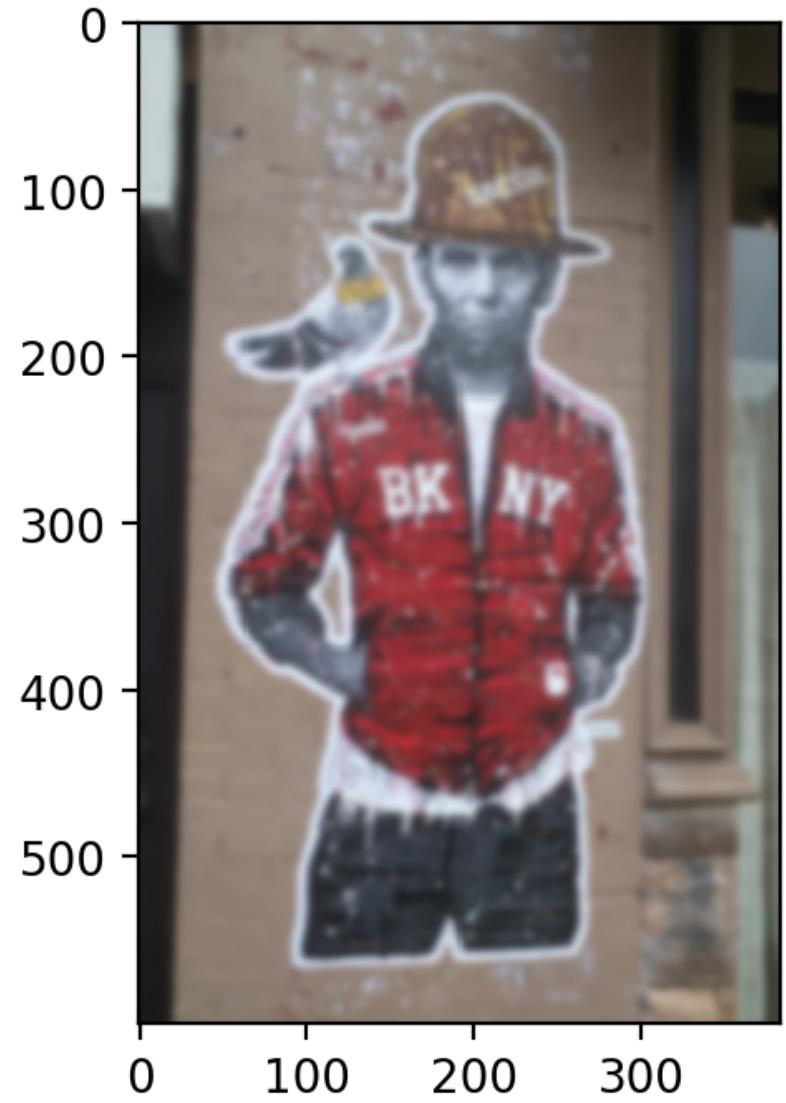
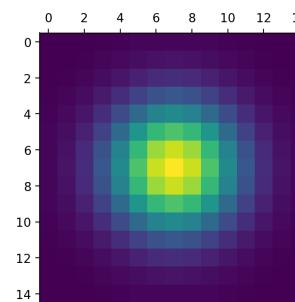
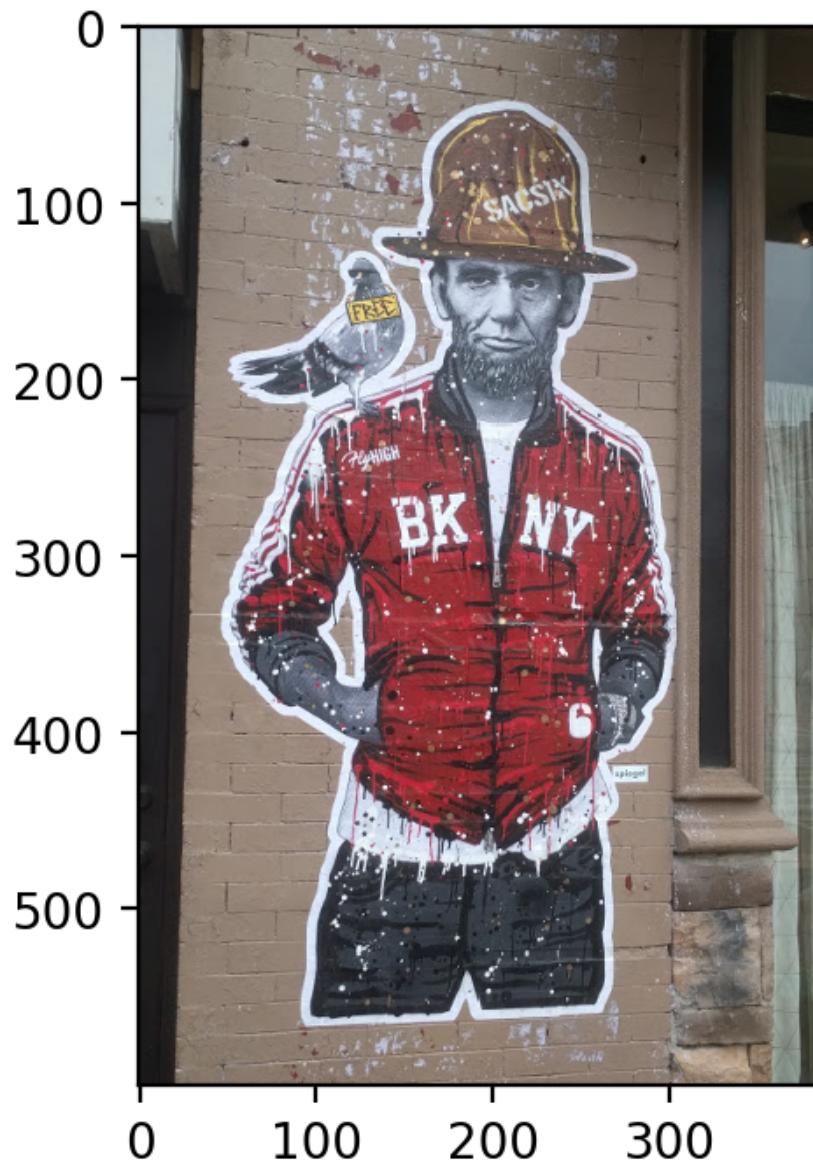
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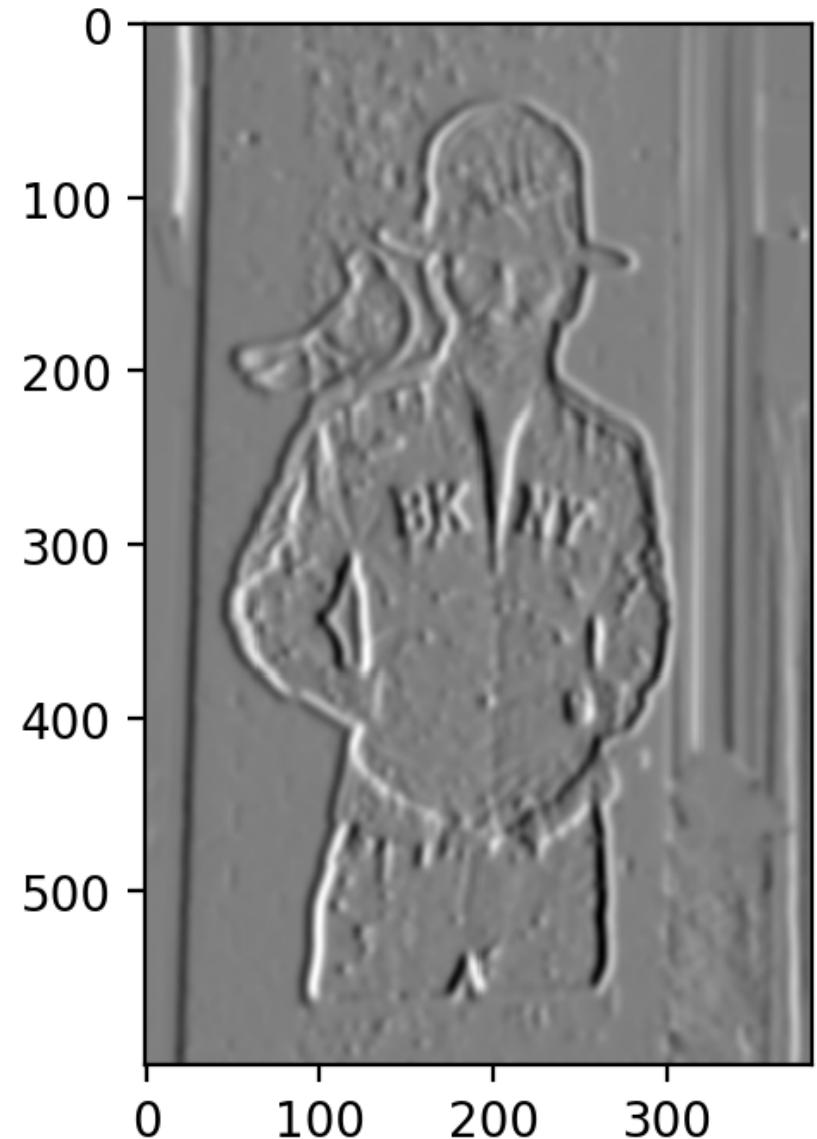
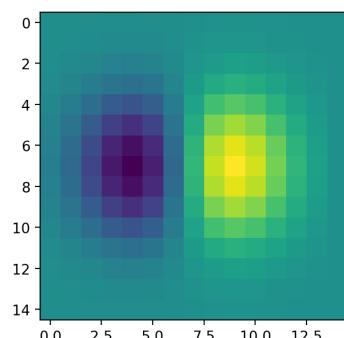
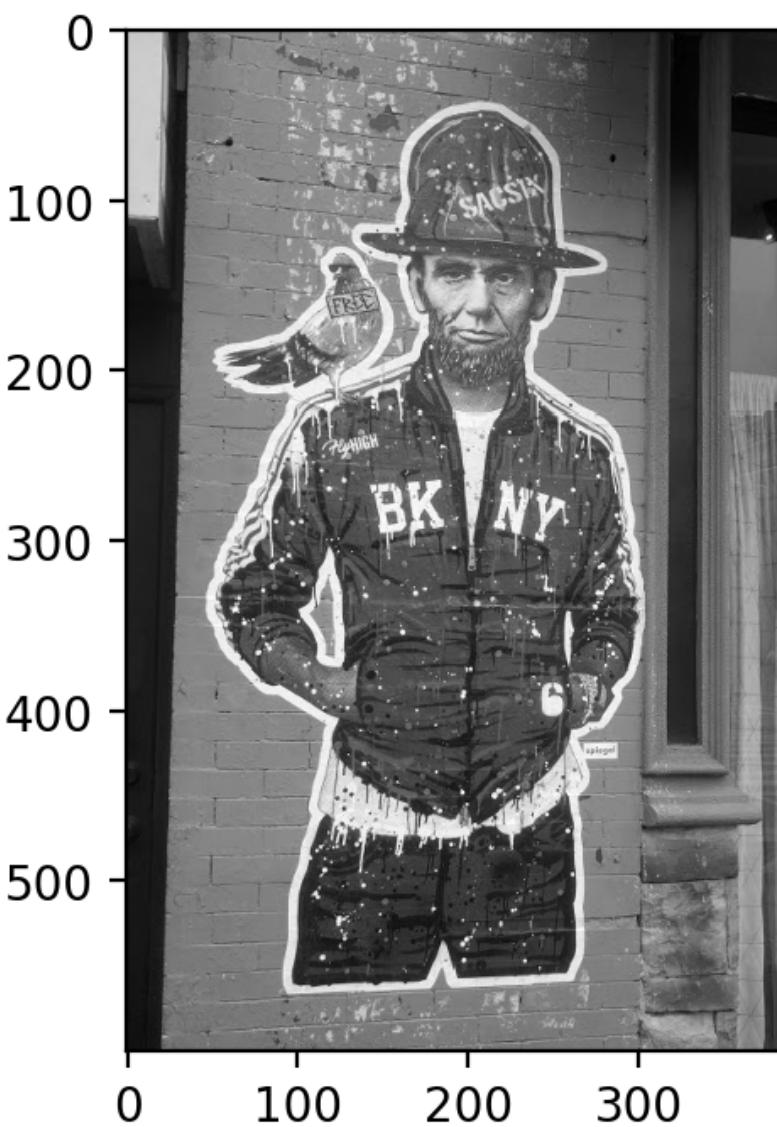
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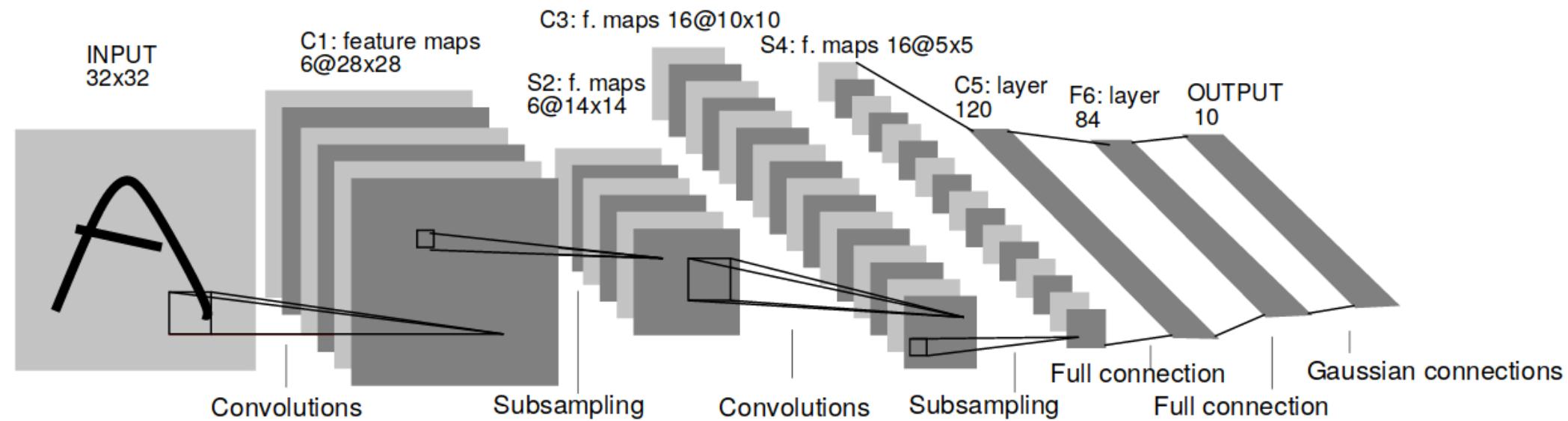
2d smoothing



2d Gradients



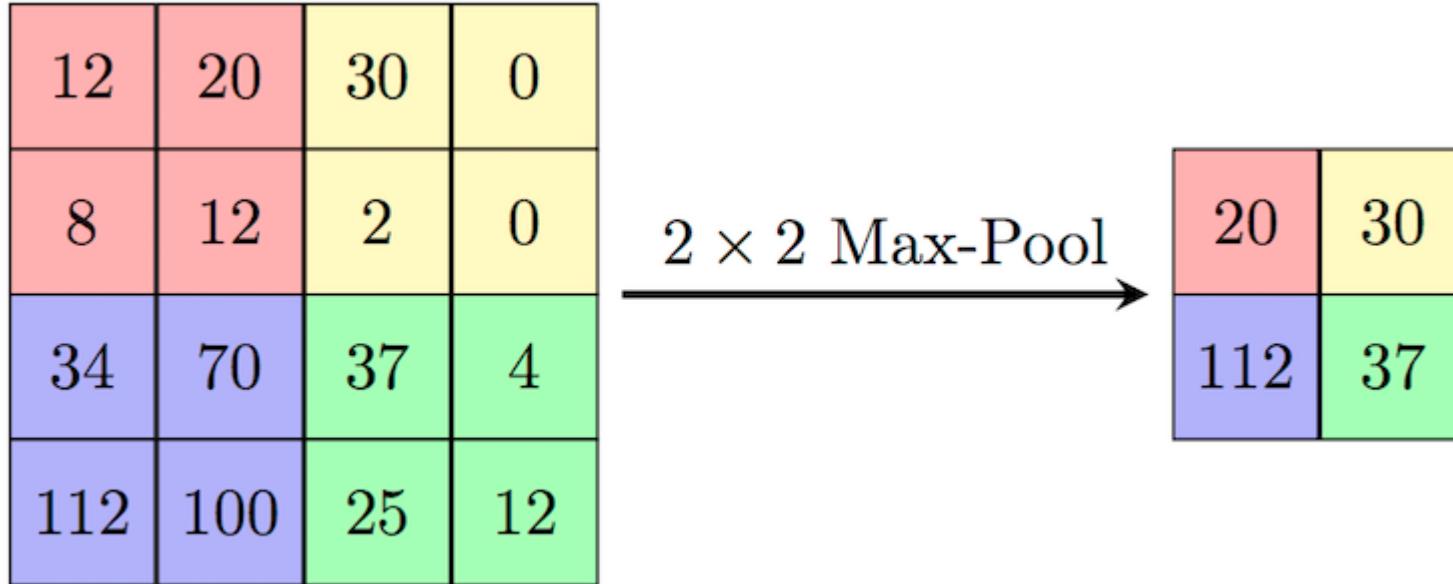
Convolutional Neural Networks



Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner.

Gradient-based learning applied to document recognition

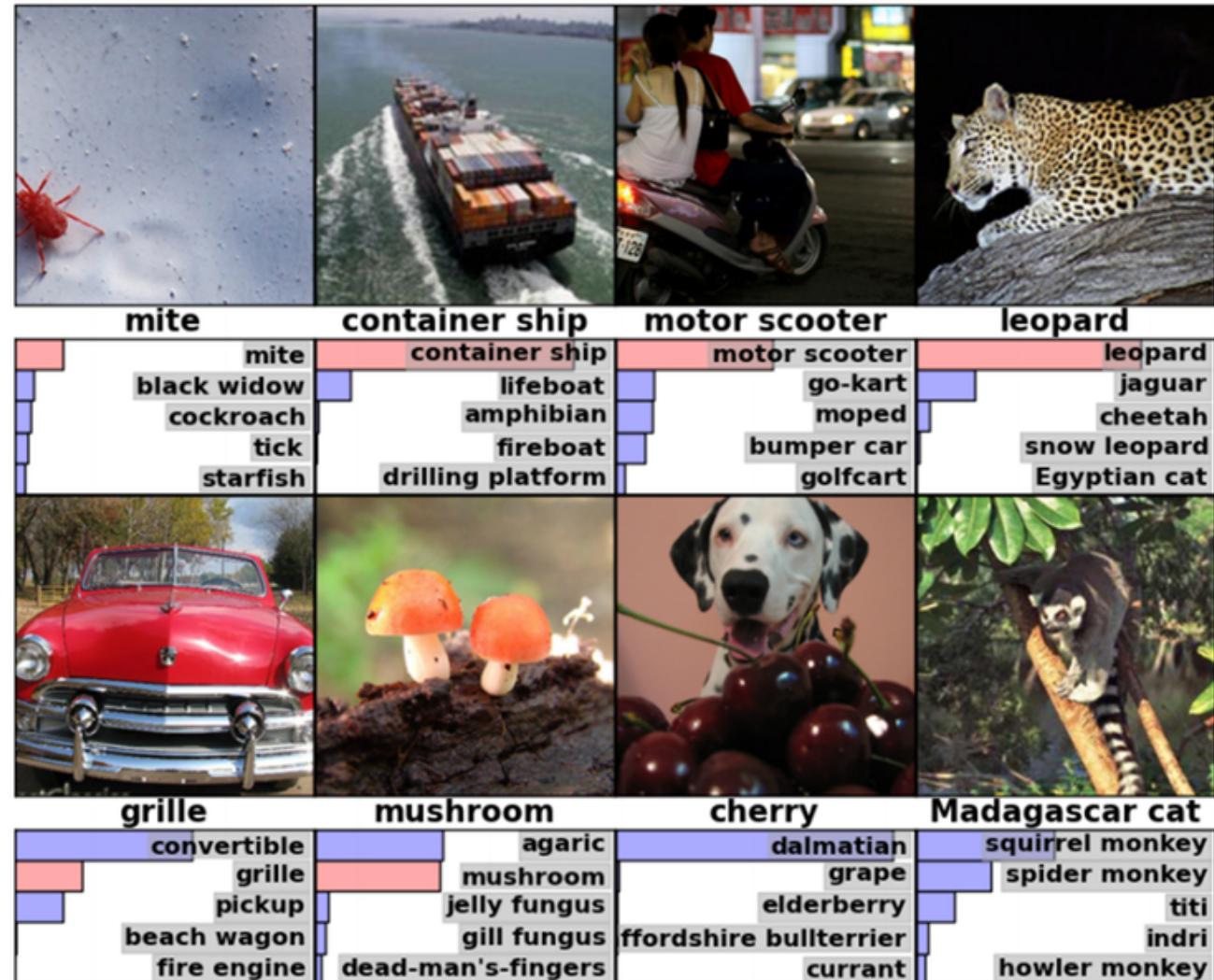
Max pooling



Need to remember position of maximum for back-propagation.
Again not differentiable → subgradient descent

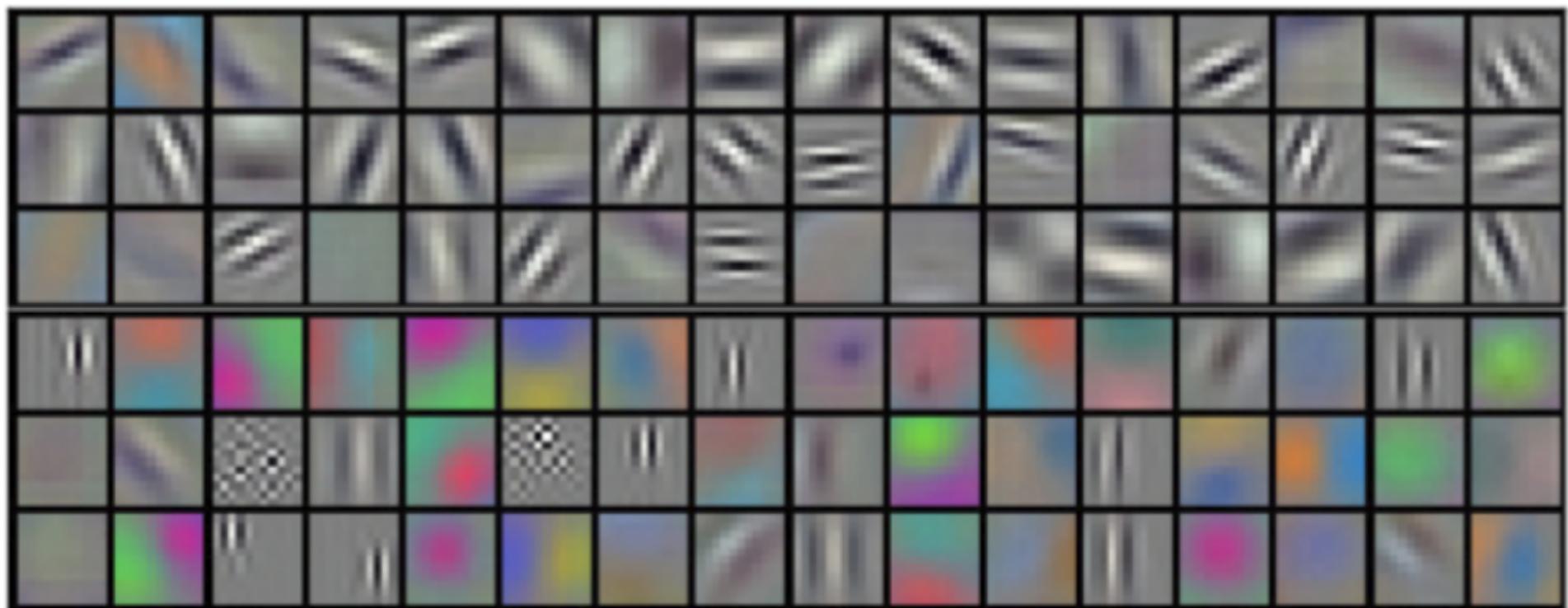
ImageNet Challenge

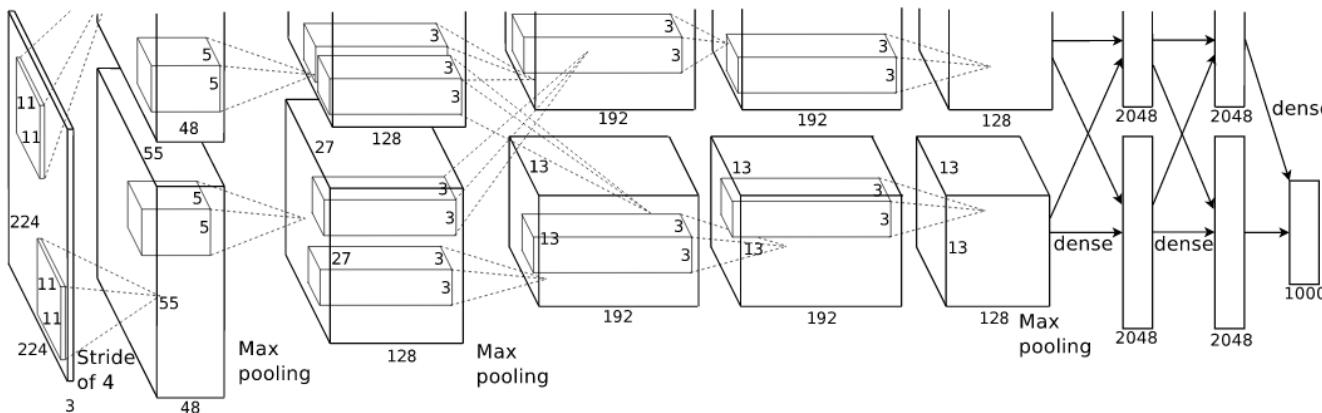
IMAGENET



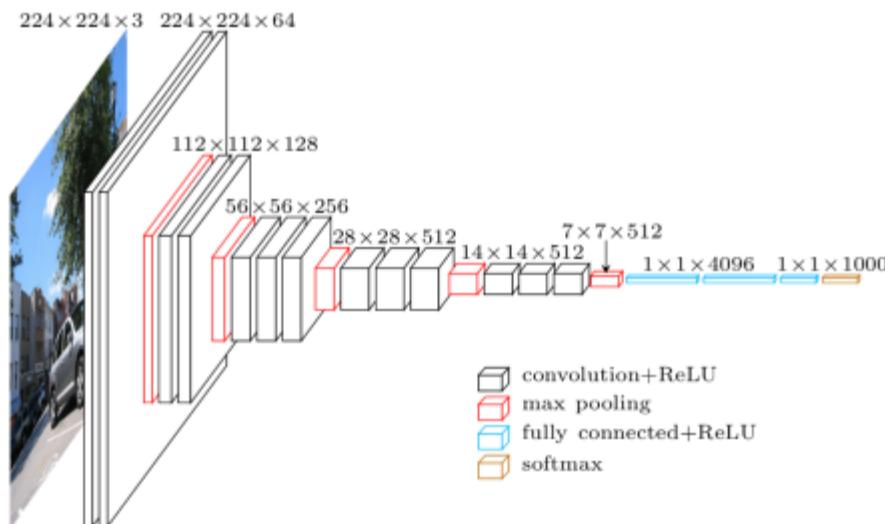
- 1,000 object classes (categories).
 - Images:
 - 1.2 M train
 - 100k test.

Typical first layer filters





Alex Net



VGG 16

ConvNet Configuration					
A	A-LRN	B	C	D	E
11 weight layers	11 weight layers	13 weight layers	16 weight layers	16 weight layers	19 weight layers
input (224 × 224 RGB image)					
conv3-64	conv3-64 LRN	conv3-64 conv3-64	conv3-64 conv3-64	conv3-64 conv3-64	conv3-64 conv3-64
maxpool					
conv3-128	conv3-128	conv3-128 conv3-128	conv3-128 conv3-128	conv3-128 conv3-128	conv3-128 conv3-128
maxpool					
conv3-256 conv3-256	conv3-256 conv3-256	conv3-256 conv3-256	conv3-256 conv3-256 conv1-256	conv3-256 conv3-256 conv3-256	conv3-256 conv3-256 conv3-256
maxpool					
conv3-512 conv3-512	conv3-512 conv3-512	conv3-512 conv3-512	conv3-512 conv3-512 conv1-512	conv3-512 conv3-512 conv3-512	conv3-512 conv3-512 conv3-512
maxpool					
conv3-512 conv3-512	conv3-512 conv3-512	conv3-512 conv3-512	conv3-512 conv3-512 conv1-512	conv3-512 conv3-512 conv3-512	conv3-512 conv3-512 conv3-512
maxpool					
FC-4096	FC-4096	FC-4096	FC-1000	FC-1000	soft-max

conv <receptive field size>-<number of channels>

Open Questions in Convolutional Neural Networks

- What are good learning methods and architectures?
- Where else could they be applied?
- When to use CNN vs Recurrent networks?

Structured Prediction

Structured Prediction

$$y = (y_1, y_2, \dots y_{n_k})$$

Applications: Multi-Label Classification

	Politics	Sports	Finance	Domestic	Religion
News Story1	1	0	0	1	1
News Story2	0	1	0	1	0
News Story3	0	0	1	0	0

Applications: Multi-Label Classification

	Politics	Sports	Finance	Domestic	Religion
News Story1	1	0	0	1	1
News Story2	0	1	0	1	0
News Story3	0	0	1	0	0

	Owns Car	Smokes	Married	Self-Employed	Has Kids
Customer1	1	0	1	0	1
Customer2	1	1	0	1	0
Customer3	0	1	1	0	0

Applications: Sequence Tagging



Applications: Sequence Tagging



Stroke cat.



Stroke cat.



Stroke cat.

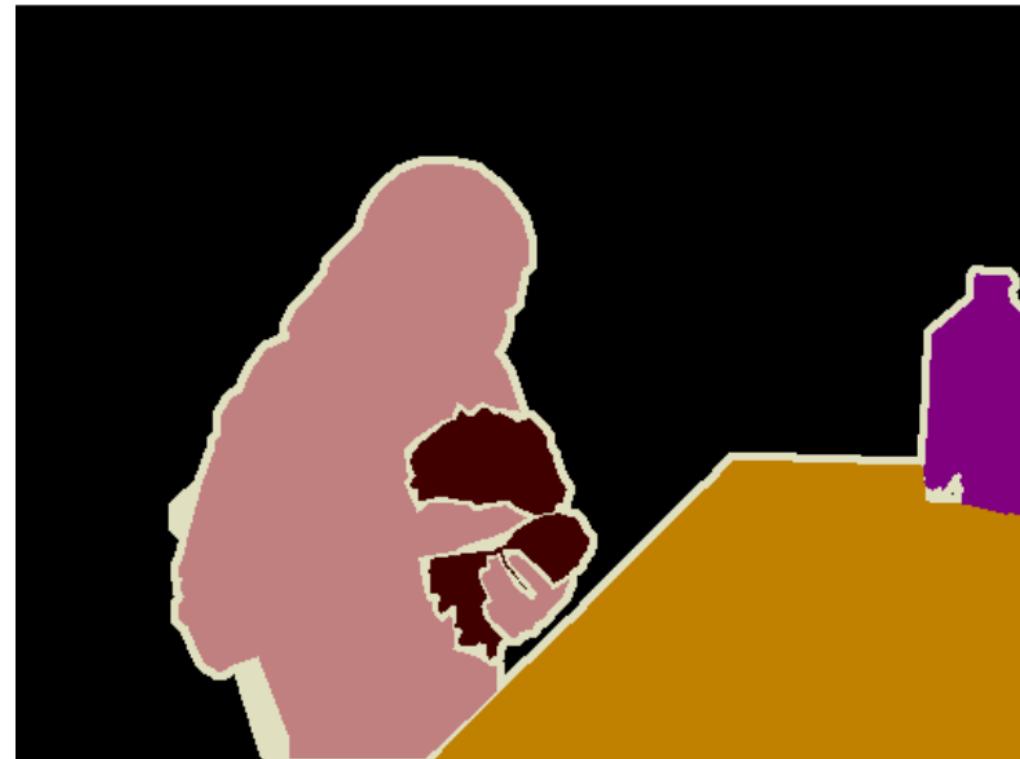


Open trash can.



Put cat in trash can.

Applications: Image Segmentation



The Essence of Structured Prediction

$$f(x, w) := \arg \max_{y \in \mathcal{Y}} g(x, y, w)$$

The Essence of Structured Prediction

$$f(x, w) := \arg \max_{y \in \mathcal{Y}} g(x, y, w)$$

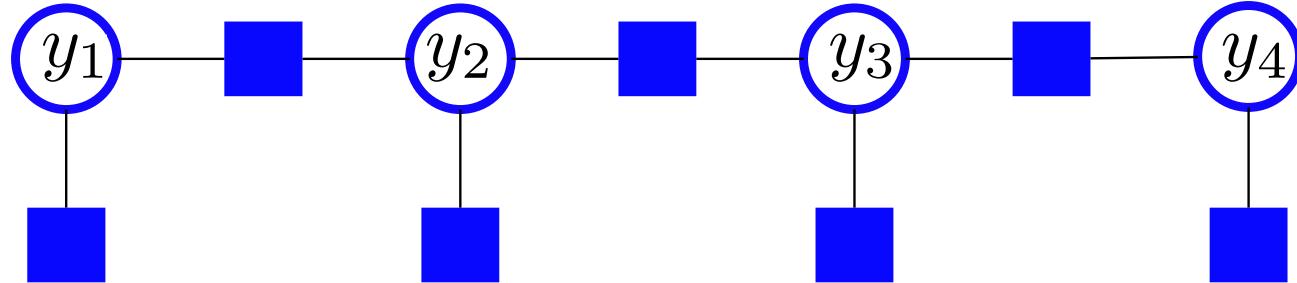
If you like:

$$\arg \max_{y \in \mathcal{Y}} p(y|x, w)$$

Pairwise Structured Models

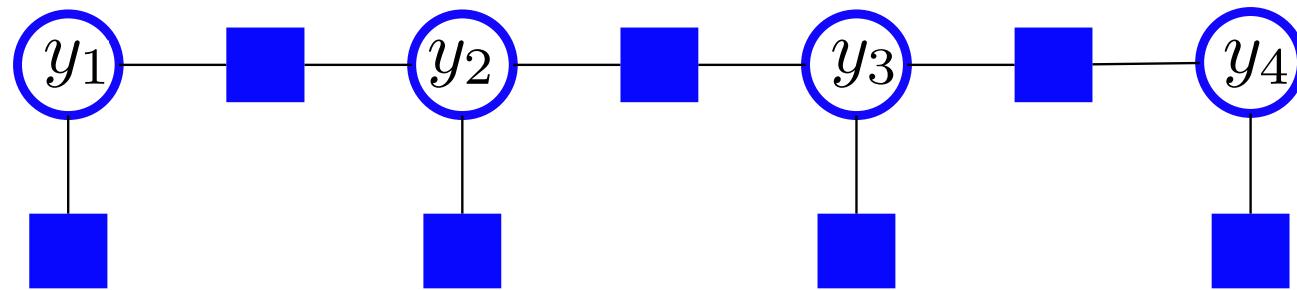
$$\arg \max_{y_1, y_2, \dots, y_n} w^T \psi(x, y)$$

$$= \arg \max_{y_1, y_2, \dots, y_n} \sum_I w_i^T \psi(x, y_i) + \sum_{(i,j) \in E} w_{i,j}^T \psi(x, y_i, y_j)$$



The Devil is in the Inference

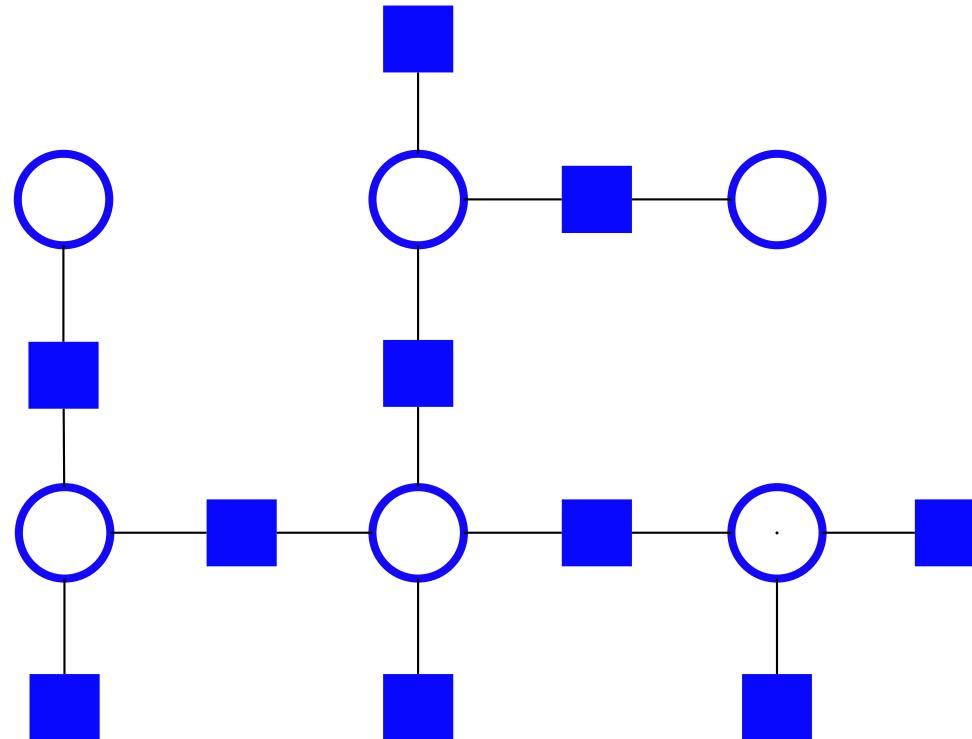
$$\arg \max_{y_1, y_2, \dots, y_n} \sum_I w_i^T \psi(x, y_i) + \sum_{(i,j) \in E} w_{i,j}^T \psi(x, y_i, y_j)$$



Easy: Dynamic Programming

The Devil is in the Inference

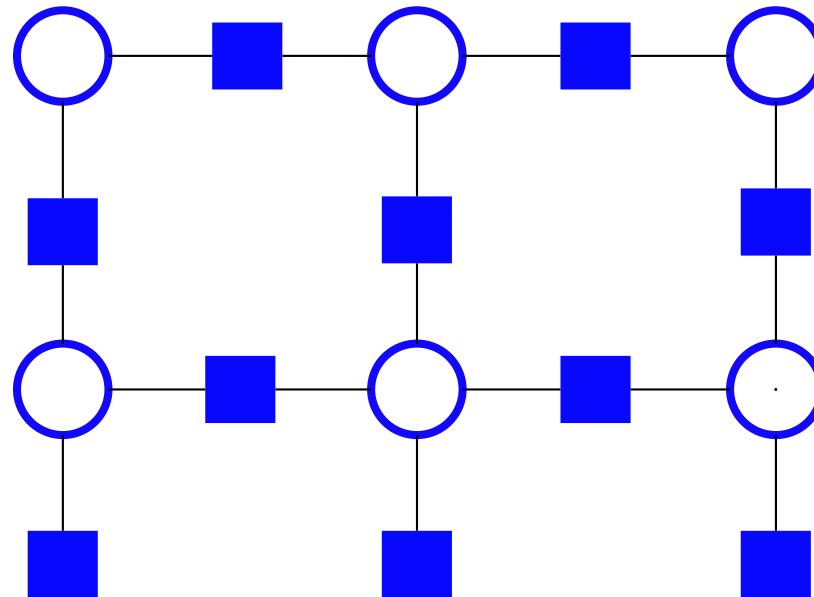
$$\arg \max_{y_1, y_2, \dots, y_n} \sum_I w_i^T \psi(x, y_i) + \sum_{(i,j) \in E} w_{i,j}^T \psi(x, y_i, y_j)$$



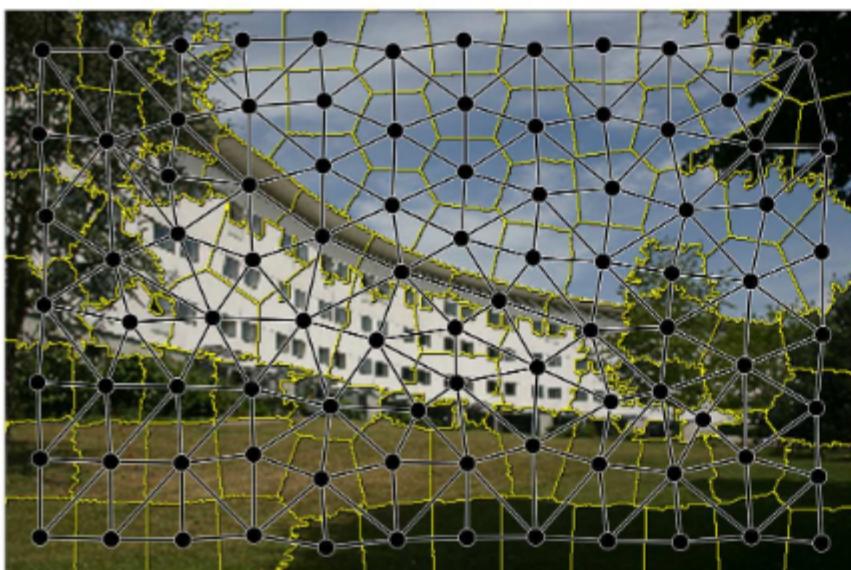
Easy: Dynamic Programming

The Devil is in the Inference

$$\arg \max_{y_1, y_2, \dots, y_n} \sum_I w_i^T \psi(x, y_i) + \sum_{(i,j) \in E} w_{i,j}^T \psi(x, y_i, y_j)$$



HARD!
AD3, QPBO, LP, Loopy BP,



Open Questions in Structured Prediction

- How to learn more efficiently?
- How to best integrate with deep learning?
- How to do inference efficiently in more complex models?

The Open Source Idea

Open exchange

We can learn more from each other when information is open. A free exchange of ideas is critical to creating an environment where people are allowed to learn and use existing information toward creating new ideas.

Participation

When we are free to collaborate, we create. We can solve problems that no one person may be able to solve on their own.

Rapid prototyping

Rapid prototypes can lead to rapid failures, but that leads to better solutions found faster. When you're free to experiment, you can look at problems in new ways and look for answers in new places. You can learn by doing.

Meritocracy

In a meritocracy, the best ideas win. In a meritocracy, everyone has access to the same information. Successful work determines which projects rise and gather effort from the community.

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DAMAGES (INCLUDING, BUT NOT LIMITED TO, PROCUREMENT OF SUBSTITUTE GOODS OR
SERVICES; LOSS OF USE, DATA, OR PROFITS; OR BUSINESS INTERRUPTION) HOWEVER
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LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY
OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH
DAMAGE.

Permissive vs Share-alike

BSD / MIT / Apache

Hadoop

Python (+libraries)

Apache web server

Do whatever you want
= Industry friendly

GPL / LGPL

Linux

Most linux tools (GNU)

Derived software must be licensed
the same way.
Derived web-services must be
open source.

No “free riders”



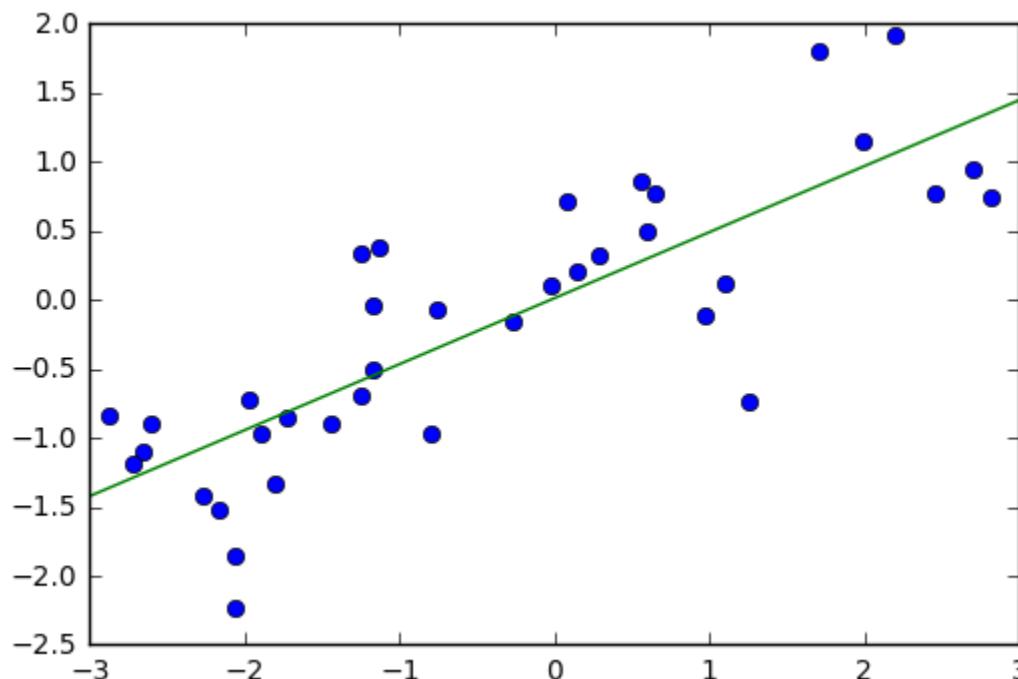
Classification
Regression
Clustering
Semi-Supervised Learning
Feature Selection
Feature Extraction
Manifold Learning
Dimensionality Reduction
Kernel Approximation
Hyperparameter Optimization
Evaluation Metrics
Out-of-core learning

.....



```
: from sklearn.linear_model import LinearRegression  
  
lr = LinearRegression()  
lr.fit(X_train, y_train)  
  
print(lr.predict(X_test))  
print(lr.score(X_test, y_test))
```

```
[-1.07669396 -0.94489099  0.29582604  1.32379186 -1.38209551 -1.42220547  
 0.86691958 -0.63314097  0.79944587  1.28044585  0.64491641  0.23934466  
-0.73008772]  
0.465661173258
```





Alexandre Gramfort
agramfort



bthirion
bthirion



Alexander Fabisch
AlexanderFabisch



Gael Varoquaux
GaelVaroquaux



Joel Nothman
jnothman



Alexandre Passos
alextp



David Cournapeau
cournape



Gilles Louppe
glouppe



Kyle Kastner
kastnerkyle



Andreas Mueller
amueller



Duchesnay
duchesnay



Jake Vanderplas
jakevdp



Lars
larsmans



Arnaud Joly
arjoly



David Warde-Farley
dwf



Jaques Grobler
jaquesgrobler



Shiqiao Du
lucidfrontier45



Brian Holt
bdholt1



Fabian Pedregosa
fabianp



Jan Hendrik Metzen
jmetzen



Mathieu Blondel
mblondel



Manoj Kumar
MechCoder



(Venkat) Raghav (Rajagopalan)
raghavr



Tom Dupré la Tour
TomDLT



Noel Dawe
ndawe



Robert Layton
robertlayton



Vlad Niculae
vene



Nelle Varoquaux
NelleV



Ron Weiss
ronw



Virgile Fritsch
VirgileFritsch



Olivier Grisel
ogrisel



Satrajit Ghosh
satra



Vincent Michel
vmichel



Paolo Losi
paolo-losi



sklearn-cl



Wei Li
weilinear



Peter Prettenhofer
pprett



sklearn-wheels



Yaroslav Halchenko
yarkoptic

[Code](#)[Issues 905](#)[Pull requests 582](#)[Projects 5](#)[Wiki](#)[Settings](#)[Insights](#)[Filters](#) is:pr is:open[Labels](#)[Milestones](#)[New pull request](#) 582 Open ✓ 4,913 Closed[Author](#)[Labels](#)[Projects](#)[Milestones](#)[Reviews](#)[Assignee](#)[Sort](#)

  [classification_report: raise error if labels is None and target_names size is not equal to present classes \(Fixes #9842\)](#) ✓
#9867 opened 10 hours ago by reiinakano

  [retrieve embedded neighbor indexes using KNN search](#) ✓ 6
#9861 opened a day ago by PGryllos • Approved

  [Update performance.rst](#) ✘ 1
#9859 opened 2 days ago by nbmorgan

  [\[MRG\] Add tol parameter and deprecate reorder parameter in auc](#) ✓ 8
#9851 opened 5 days ago by qinhanmin2014

  [FIX Improve check to ensure that ROC curve starts at \(0,0\) point](#) ✘ 7
#9850 opened 5 days ago by alexryndin

  [\[MRG\] speedup confusion_matrix](#) ✓ 14
#9843 opened 6 days ago by Erotemic  5 of 5

  [\[RFC/MRG\] MAINT Use magic to list documentation versions](#) ✓ 5
#9841 opened 6 days ago by jnothman  0.19.1

  [\[MRG\] Remove nose from Cls and documentation](#) ✘ 19
#9840 opened 6 days ago by lesteve  0.20

  [\[MRG\] MAINT pytest test discovery](#) ✓ 3
#9839 opened 6 days ago by rth

```
275      -     y_pred = y_pred[~ind]
277      -     y_true = y_true[~ind]
278      -     # also eliminate weights of eliminated items
279      -     sample_weight = sample_weight[~ind]
269      +     # If labels are not consecutive integers starting from zero, then
270      +     # yt, yp must be converted into index form
271      +     need_index_conversion = not (
```



jnothman 5 days ago Owner

Surely `np.all(labels == np.arange(len(labels))` is just as fast for a reasonable number of classes and much more readable?



Erotemic 3 days ago • edited Contributor

It is both faster and more readable, when I originally wrote this I didn't consider that the ordering of the labels was significant, so the `np.diff` was a quick fix after realizing this. Your solution is simpler and better.

```
In [1]: labels = np.arange(100)

In [2]: %timeit labels.min() == 0 and np.all(np.diff(labels) == 1)
8.3 µs ± 162 ns per loop (mean ± std. dev. of 7 runs, 100000 loops each)

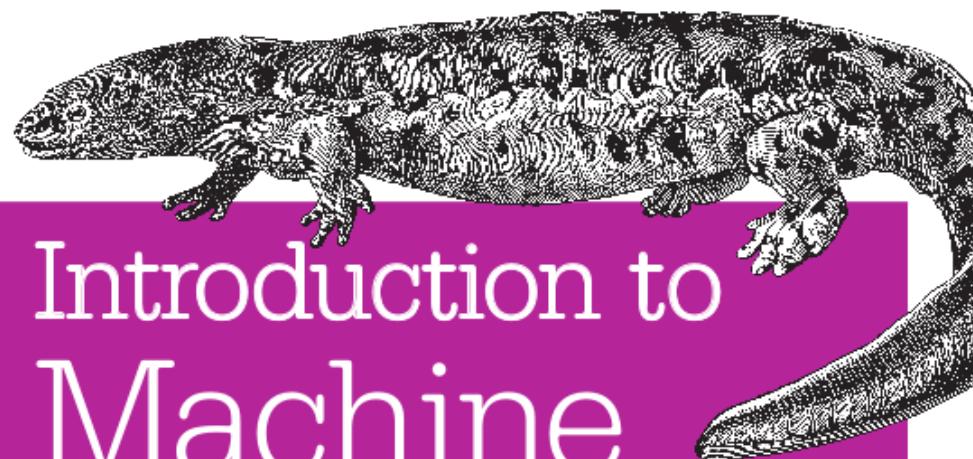
In [3]: %timeit np.all(np.arange(len(labels)) == labels)
3.6 µs ± 47.2 ns per loop (mean ± std. dev. of 7 runs, 100000 loops each)
```



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Start a new conversation

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A GUIDE FOR DATA SCIENTISTS

Andreas C. Müller & Sarah Guido



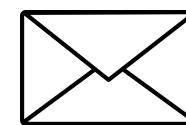
amueller.github.io



@amuellerm!



@amueller



andreas.mueller
@columbia.edu

https://github.com/amueller/talks_odt/